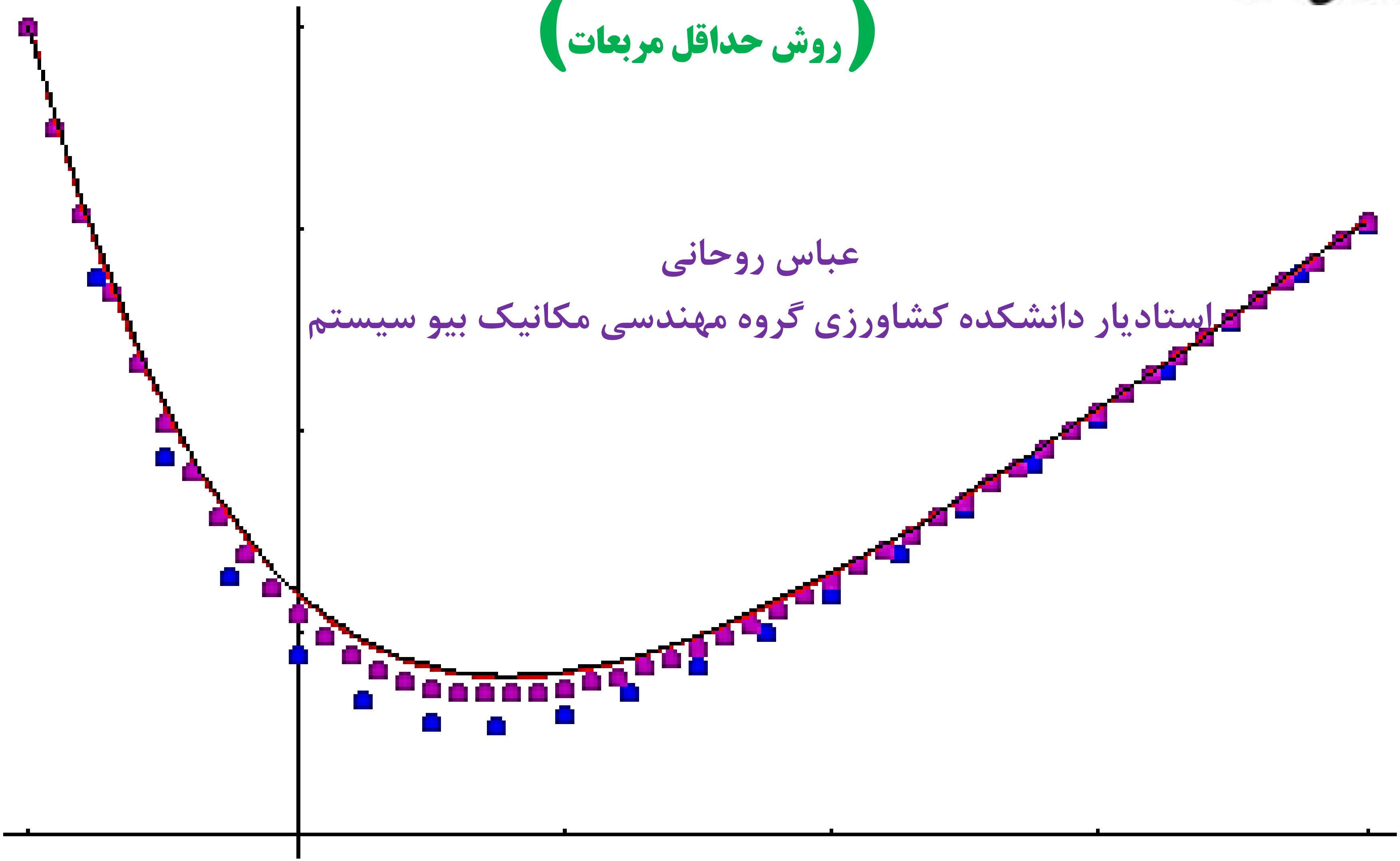
محاسبات عددی

(روش حداقل مربعات)



عباس روحانی

استادیار دانشکده کشاورزی گروه مهندسی مکانیک بیو سیستم

جدول زیر مربوط به تابع $f(x)=\sqrt[3]{x}$ می باشد:

x_i	0	1	8	27	64
f_i	0	1	2	3	4

$$P(x)=L_0(x)f_0+L_1(x)f_1+L_2(x)f_2+L_3(x)f_3+L_4(x)f_4$$

$$P(x)=0+\frac{(x-0)(x-8)(x-27)(x-64)}{1(1-8)(1-27)(1-64)}\times 1+$$

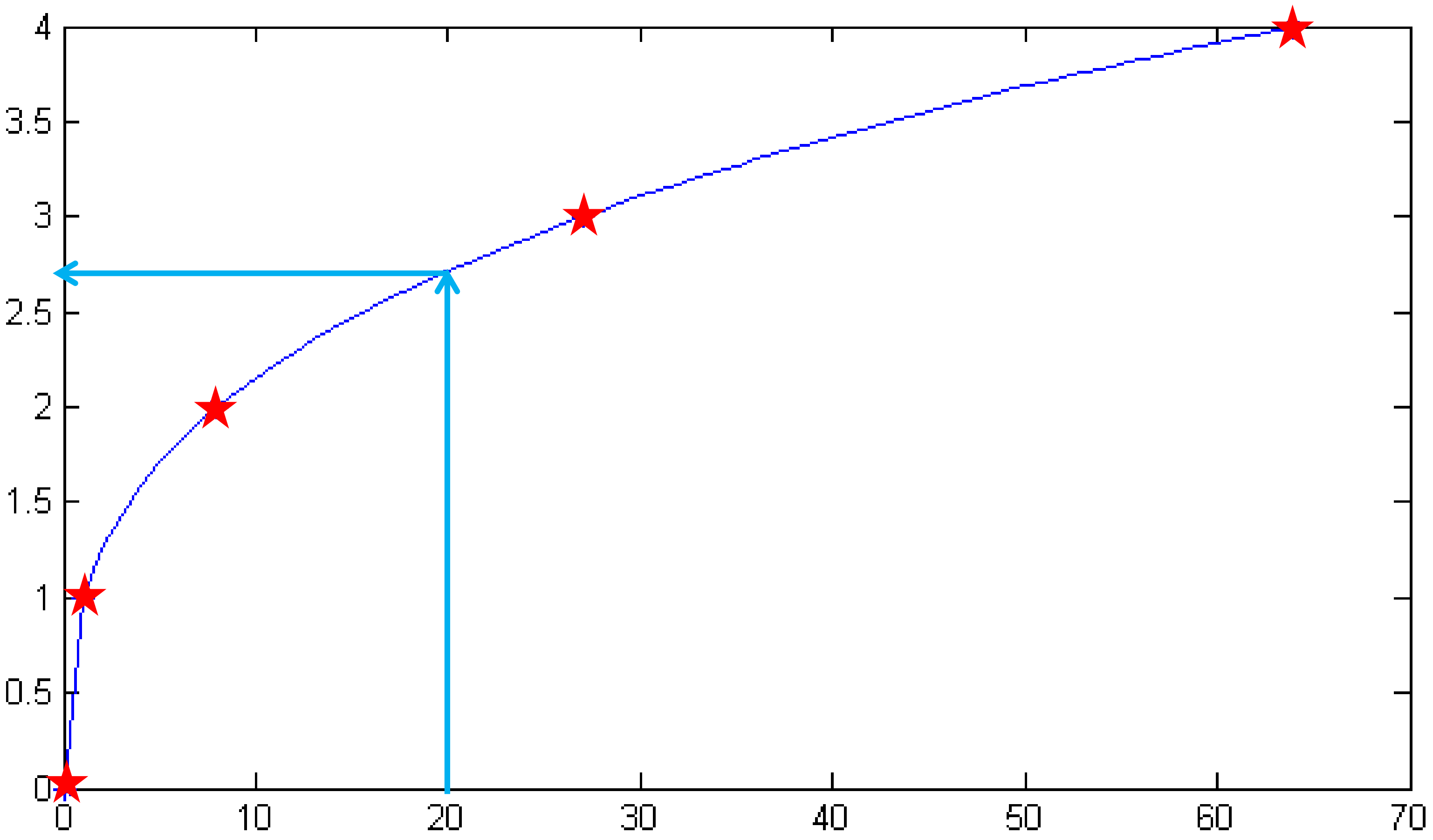
$$\frac{(x-0)(x-1)(x-27)(x-64)}{8(8-1)(8-27)(8-64)}\times 2+$$

$$\frac{(x-0)(x-1)(x-8)(x-64)}{27(27-8)(27-27)(27-64)}\times 3+$$

$$\frac{(x-0)(x-1)(x-8)(x-27)}{64(64-1)(64-8)(64-27)}\times 4$$

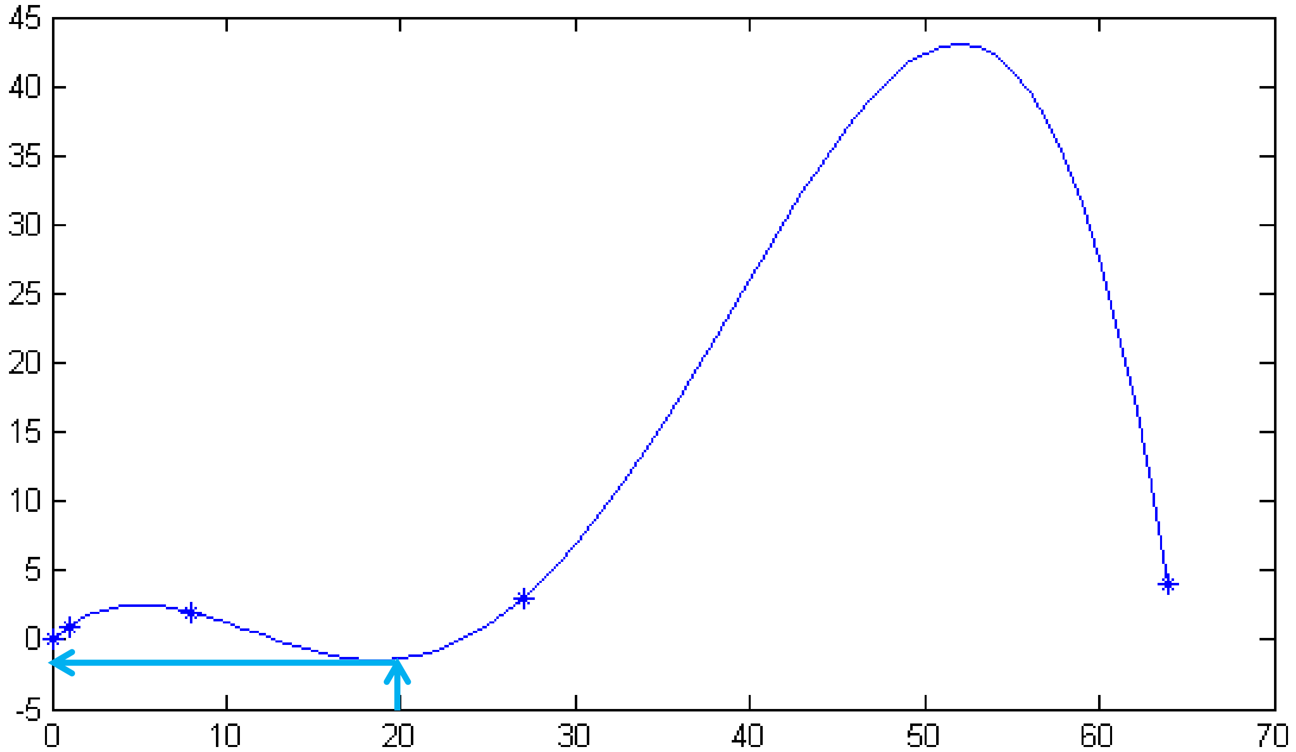
حال به کمک روش لاگرانژ تخمین از $\sqrt[3]{20}$ بدست آوریم:

$$\sqrt[3]{20}\cong P(20)=-1.3139(4D)$$




```
>> xp=0:64;
>> yp=xp.^(1/3);
>> plot(xp,yp)
```

$$\sqrt[3]{20} \cong P(20) = -1.3139(4D)\ ?$$




```
>> x=[0 1 8 27 64];
>> y=[0 1 2 3 4];
>> plot(x,y,'*')
>> p=polyfit(x,y,4)
p =    -0.0001    0.0060   -0.1566    1.1507   -0.0000
>> yp=polyval(p,0:64);
>> hold on
>> plot(0:64,yp)
```

هرگاه در فاصله [۸ ۲۷] چند جمله ای درونیاب درجه اول را به دست آوریم خواهیم داشت:

x_i	0	1	8	27	64
f_i	0	1	2	3	4

$$P(x) = \frac{(x-27)}{(8-27)} \times 2 + \frac{(x-8)}{(27-8)} \times 3$$

$$\sqrt[3]{20} \cong P_1(20) = \frac{50}{19} = 2.6316(4D)$$

این مقدار از مقدار واقعی خیلی دور نیست:

$$\sqrt[3]{20} = 2.7144(4D)$$

بنابراین در برخی موارد با بالاتر بودن درجه چند جمله ای دقت درونیابی نمی تواند بهتر شود

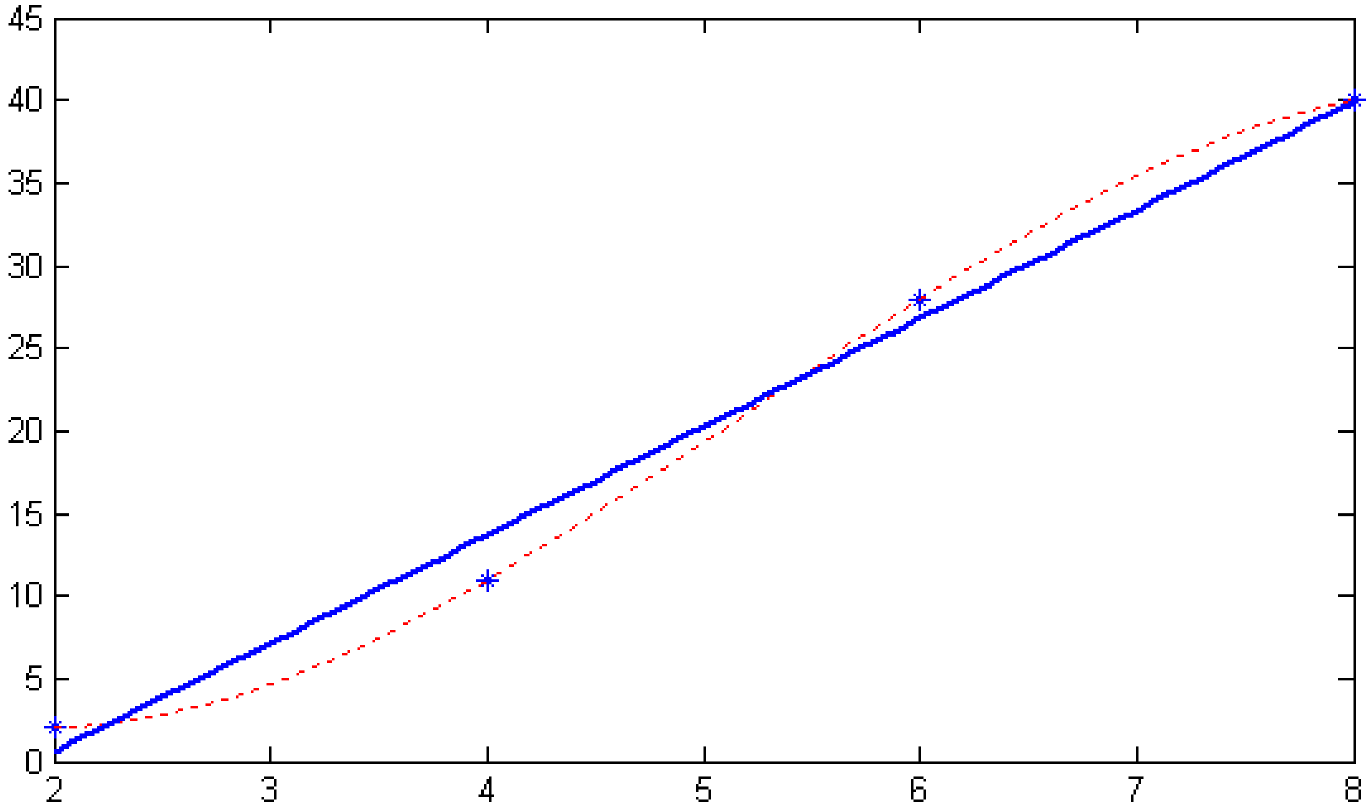
خط حداقل مربعات

مساله تخمین مقادیر یک تابع در نقاط غیر جدولی را برای داده های جدول زیر در نظر بگیرید، که این داده ها از طریق آزمایش به دست آمده اند:

x_i	2	4	6	8
y_i	2	11	28	40

هر گاه از روش لاگرانژ برای ساختن چند جمله ای درونیاب استفاده کنیم، به یک منحنی با حداکثر از درجه ۳ نیاز داریم.

ولی با رسم داده ها می توان به این نتیجه رسید که رابطه بین داده ها خطی می باشد.




```
>> x=[2 4 6 8];
>> y=[2 11 28 40];
>> plot(x,y,'*')
>> p=polyfit(x,y,3)
p =   -0.2708    4.2500  -13.4167   14.0000
>> yp=polyval(p,2:0.1:8);
>> hold on
>> plot(2:0.1:8,yp)
>> p=polyfit(x,y,1)
p =     6.5500  -12.5000
>> yp=polyval(p,2:0.1:8);
>> hold on
>> plot(2:0.1:8,yp)
```

در چنین حالتی بهترین راه، پیدا کردن بهترین خط به عنوان تابع تقریب ساز می باشد ولو اینکه این خط بر داده ها دقیقا منطبق نباشد

هر گاه داشته باشیم

$$P(x) = a_1 x + a_0$$

در اینصورت خواهیم داشت:

$$P(x_i) = a_1 x_i + a_0 = \bar{y}_i$$

در تقریب حداقل مربعات، مساله عبارتست از تعیین ضرایب a_0، a_1 به طوری که مقدار عبارت زیر کمینه شود:

$$S = \sum_{i=1}^{m} (y_i - \bar{y}_i)^2 = \sum_{i=1}^{m} (y_i - (a_1 x_i + a_0))^2$$

که در آن m تعداد کل داده ها و y_iها مقادیر داده شده می باشند.

قضیه (شرط لازم برای وجود اکسترمم در یک نقطه): هر گاه f(x,y) در نقطه (a,b) دارای یک مینیمم(ماکزیمم) باشد، در اینصورت لازم است داشته باشیم:

$$\frac{\partial f}{\partial x}(a,b) = 0 \quad , \qquad \frac{\partial f}{\partial y}(a,b) = 0$$

بنابراین هر گاه S بخواهد در a_0، a_1 کمترین مقدار را داشته باشد، بایستی داشته باشیم:

$$\boxed{\frac{\partial S}{\partial a_0} = 0 \quad , \qquad \frac{\partial S}{\partial a_1} = 0}$$

$$S = \sum_{i=1}^{m} (y_i - a_1 x_i - a_0)^2$$

$$\frac{\partial S}{\partial a_0} = \sum_{i=1}^{m} 2(y_i - a_1 x_i - a_0)(-1) = 0$$

$$\sum_{i=1}^{m} (y_i - a_1 x_i - a_0) = 0$$

$$\sum_{i=1}^{m} y_i - a_1 \sum_{i=1}^{m} x_i - a_0 \sum_{i=1}^{m} 1 = 0$$

$$\sum_{i=1}^{m} y_i - a_1 \sum_{i=1}^{m} x_i - m a_0 = 0$$

$$S = \sum_{i=1}^{m} (y_i - a_1 x_i - a_0)^2$$

$$S = \sum_{i=1}^{m} (y_i - a_1 x_i - a_0)^2$$

$$\frac{\partial S}{\partial a_1} = \sum_{i=1}^{m} 2(y_i - a_1 x_i - a_0)(-x_i) = 0$$

$$\sum_{i=1}^{m} (y_i - a_1 x_i - a_0) x_i = 0$$

$$\sum_{i=1}^{m} x_i y_i - a_1 \sum_{i=1}^{m} {x_i}^2 - a_0 \sum_{i=1}^{m} x_i = 0$$

دستگاه معادلات نرمال

$$\begin{cases} \sum_{i=1}^{m} y_i - a_1 \sum_{i=1}^{m} x_i - m a_0 = 0 \\ \sum_{i=1}^{m} x_i y_i - a_1 \sum_{i=1}^{m} {x_i}^2 - a_0 \sum_{i=1}^{m} x_i = 0 \end{cases}$$

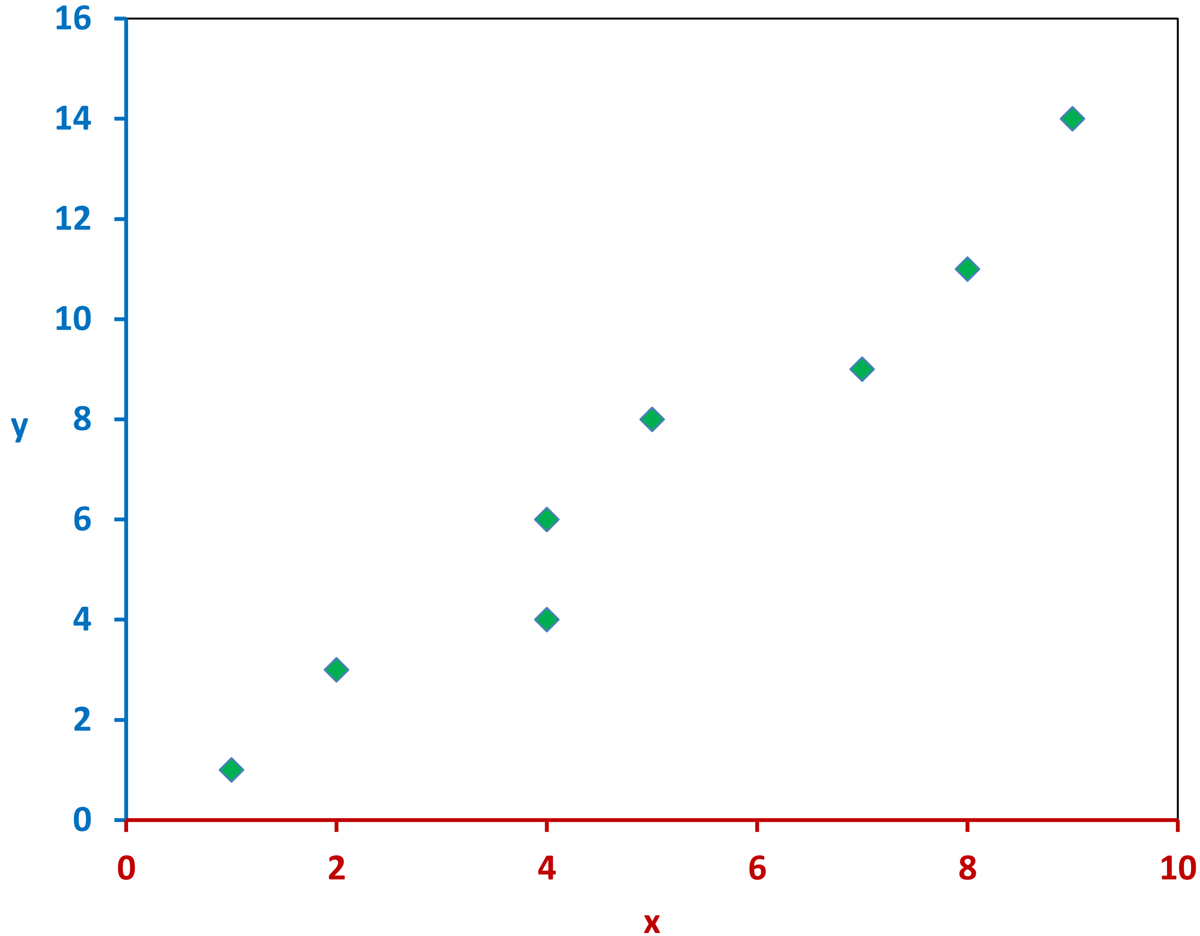
جواب دستگاه به روش کرامر:

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

$$a_0 = \frac{\sum y_i \sum {x_i}^2 - \sum x_i \sum x_i y_i}{m \sum {x_i}^2 - \left(\sum x_i\right)^2}$$

مثال: داده های زیر نتیجه یک آزمایش تجربی می باشد:

x	y
1	1
3	2
4	4
6	4
8	5
9	7
11	8
14	9



x	y	x^2	xy
1	1	1	1
3	2	9	6
4	4	16	16
6	4	36	24
8	5	64	40
9	7	81	63
11	8	121	88
14	9	196	126
56	40	524	364

مجموع

$$a_0 = \frac{\sum y_i \sum x_i^2 - \sum x_i \sum x_i y_i}{m \sum x_i^2 - (\sum x_i)^2}$$

$$a_0 = \frac{40 \times 524 - 56 \times 364}{8 \times 524 - 56^2} = \frac{6}{11}$$

$$a_1 = \frac{m \sum x_i y_i - \sum x_i \sum y_i}{m \sum x_i^2 - (\sum x_i)^2}$$

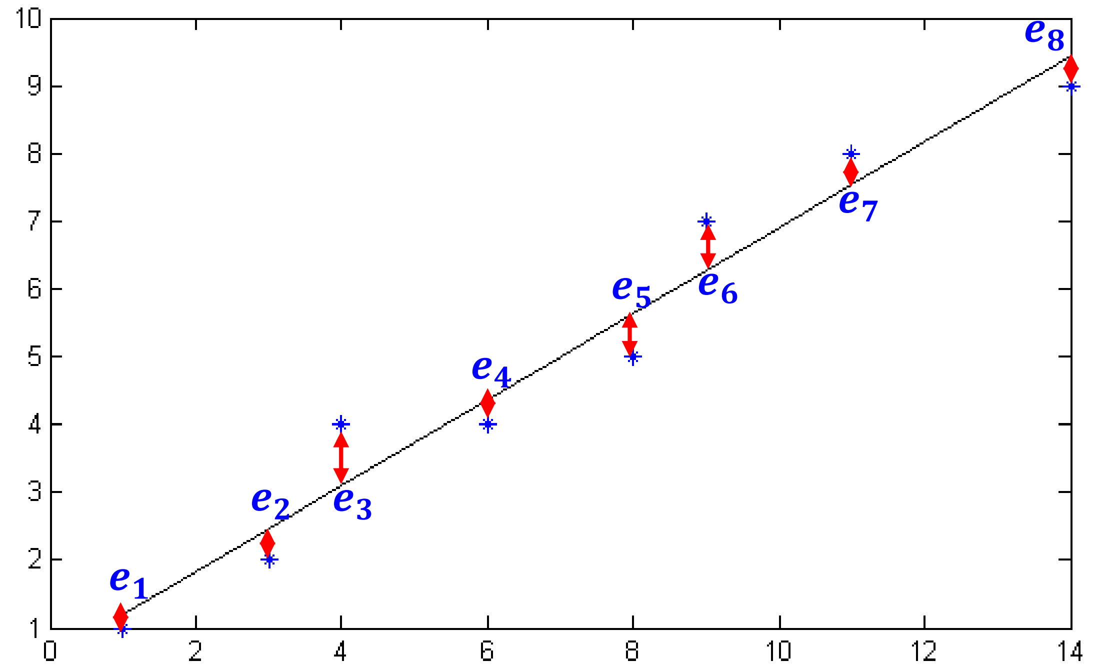
$$a_1 = \frac{8 \times 364 - 56 \times 40}{8 \times 524 - 56^2} = \frac{7}{11}$$

بنابراین معادله خط کمترین مربعات عبارتست از:

$$\bar{y}_i = a_1 x_i + a_0 = \frac{7}{11}x + \frac{6}{11}$$

دستور متلب

```
>> x=[1 3 4 6 8 9 11 14];
>> y=[1 2 4 4 5 7 8 9];
>> p=polyfit(x,y,1)
p =    0.6364    0.5455
>> format rat
>> p
p =       7/11         6/11
```



خطای زیر بهترین خطایی است که می توان با استفاده از یک خط برای برازش داده های جدول به روش حداقل مربعات به دست آورد:

$$E = \sqrt{\sum {e_i}^2} = \left(\sum_{i=1}^{8} (y_i - \overline{y_i})^2\right)^{1/2} = 1.595$$

$$y_1 - \overline{y_1} = 1 - \left(\frac{7}{11} + \frac{6}{11}\right) = -\frac{2}{11}$$

$$y_2 - \overline{y_2} = 2 - \left(\frac{7}{11} \times 3 + \frac{6}{11}\right) = -\frac{5}{11}$$

$$\vdots$$

$$y_8 - \overline{y_8} = 9 - \left(\frac{7}{11} \times 14 + \frac{6}{11}\right) = -\frac{5}{11}$$

متلب

```
>> sqrt(sum((y-yp).^2))
ans =    1.595
```

چند جمله ای حداقل مربعات

مساله تقریب سازی مجموعه ای از داده ها به صورت

$$\{(x_i, y_i): i = 1, \dots, m \}$$

با یک چند جمله ای از درجه n که n<m به شکل زیر خواهد بود:

$$P(x) = \sum_{k=0}^{n} a_k x^k$$

با استفاده از روش حداقل مربعات، مشابه حالت خط کمترین مربعات داریم:

$$P(x) = a_n x^n + \cdots + a_1 \mathbf{x} + a_0$$

و برای $x=x_i$ داریم:

$$\bar{y}_i = P(x_i) = a_n x_i^n + \cdots + a_1 x_i + a_0$$

در اینجا، هدف حداقل ساختن مقدار عبارت زیر است:

$$S = \sum_{i=1}^{m} (y_i - \bar{y}_i)^2$$

$$S = \sum_{i=1}^{m} (y_i - a_n x_i^n - \cdots - a_1 x_i - a_0)^2$$

بنابراین مساله عبارت است از یافتن ثابتهای $a_0, a_1, \ldots, a_n$ به طوری که مقدار S حداقل گردد

مانند حالت خطی، برای آنکه S حداقل شود، لازم است داشته باشیم:

$$\frac{\partial S}{\partial a_j} = 0, \qquad j = 0, 1, \dots, n$$

معادلات نرمال

$$\begin{cases} m a_0 + \left(\sum x_i\right) a_1 + \dots + \left(\sum x_i^k\right) a_k + \dots + \left(\sum x_i^n\right) a_n = \sum y_i \\ \left(\sum x_i\right) a_0 + \left(\sum x_i^2\right) a_1 + \dots + \left(\sum x_i^{k+1}\right) a_k + \dots + \left(\sum x_i^{n+1}\right) a_n = \sum x_i y_i \\ \vdots \\ \left(\sum x_i^n\right) a_0 + \left(\sum x_i^{n+1}\right) a_1 + \dots + \left(\sum x_i^{k+n}\right) a_k + \dots + \left(\sum x_i^{2n}\right) a_n = \sum x_i^n y_i \end{cases}$$

مثال. داده های جدول زیر را با چند جمله ای حداقل مربعات درجه دوم برازش کنید. داده ها و چند جمله ای مربعات درجه دوم را در یک دستگاه مختصات رسم کنید.

i	1	2	3	4	5
x_i	0	0.25	0.5	0.75	1.00
y_i	1.0000	1.2840	1.6487	2.1170	2.7183

$$P(x) = a_2x^2 + a_1x + a_0$$

در این مساله n=2 و m=5 و سه معادله نرمال داریم:

$$\begin{cases} 5a_0 + \left(\sum x_i\right) a_1 + \left(\sum x_i^2\right) a_2 = \sum y_i \\ \left(\sum x_i\right) a_0 + \left(\sum x_i^2\right) a_1 + \left(\sum x_i^{2+1}\right) a_2 = \sum x_i y_i \\ \left(\sum x_i^2\right) a_0 + \left(\sum x_i^{2+1}\right) a_1 + \left(\sum x_i^{2\times 2}\right) a_2 = \sum x_i^2 y_i \end{cases}$$

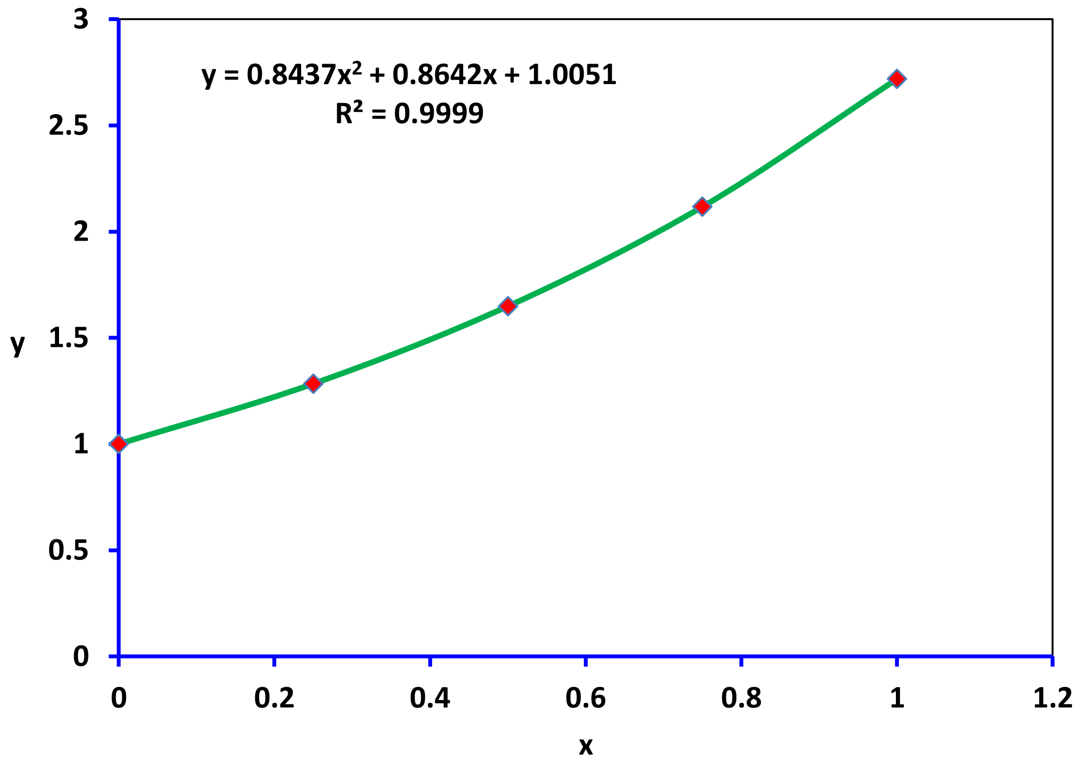
$$\begin{cases} 5a_0 + 2.5a_1 + 1.875a_2 = 8.7680 \\ 2.5a_0 + 1.875a_1 + 1.5625a_2 = 5.4514 \\ 1.875a_0 + 1.5625a_1 + 1.3828a_2 = 4.4015 \end{cases}$$

$a_0 = 1.0052$ $a_1 = 0.8641$ $a_2 = 0.8437$

$$P_2(x) = \mathbf{1.0052} + \mathbf{0.8641}x + \mathbf{0.8437}x^2$$

```
>> x=[0     0.25       0.5          0.75       1];
>> y=[1    1.284       1.6487       2.117      2.7183];
>> plot(x,y,'*')
>> p=polyfit(x,y,2)
p =    0.8437    0.8642    1.0051
>> yp=polyval(p,x);
>> hold on
>> plot(x,yp)
```

$$P(x) = a_2x^2 + a_1\mathrm{x} + a_0$$



i	1	2	3	4	5
x_i	0	0.25	0.5	0.75	1.00
y_i	1.0000	1.2840	1.6487	2.1170	2.7183
$P(x_i)$	1.0052	1.2740	1.6482	2.1279	2.7130
$y_i-P(x_i)$	-0.0052	0.0100	0.0005	-0.0109	0.0053

$$E = \sqrt{\sum {e_i}^2} = \left(\sum_{i=1}^{5} (y_i - P(x_i))^2\right)^{1/2} = 0.0166$$

```
>> sqrt(sum((y-yp).^2))
ans =
   0.0166
```

انواع دیگری از تقریب های حداقل مربعات

برخی موارد تقریب به وسیله چند جمله ای مناسب نیست، زیرا وقتی (x_i , y_i)ها را در یک دستگاه مختصات رسم کنیم، ممکن است مجموعه نقاط رسم شده شبیه یک منحنی نمایی، هذلولی و یا یک منحنی مثلثاتی باشد.

رابطه بین x و y در هر حالت به شکل زیر می تواند باشد:

نمایی

$$y = a_0 e^{a_1 x}$$

هذلولی

$$y = \frac{1}{a_0 + a_1 x}$$

مثلثاتی

wمقدار معلوم است

$$y = a_0 + a_1 \cos wx$$

حالت نمایی

$$y = a_0 e^{a_1 x} \xrightarrow{ln} lny = lna_0 + a_1 x$$

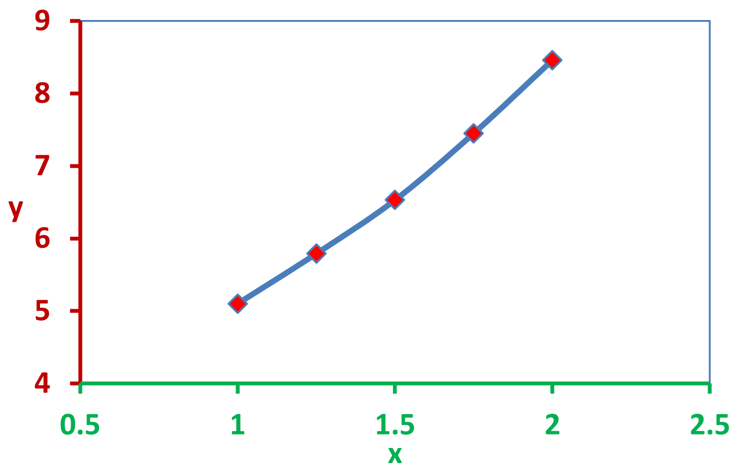
$$\begin{cases} z = lny \\ A = lna_0 \end{cases} \Longrightarrow z = A + a_1 x$$

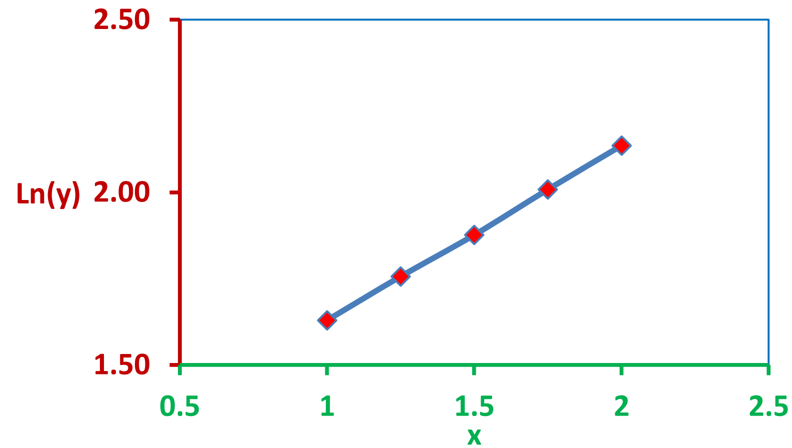
معادلات نرمال

$$\begin{cases} \sum_{i=1}^{m} lny_i - a_1 \sum_{i=1}^{m} x_i - mA = 0 \\ \sum_{i=1}^{m} x_i lny_i - a_1 \sum_{i=1}^{m} {x_i}^2 - A \sum_{i=1}^{m} x_i = 0 \end{cases} \Longrightarrow \begin{cases} a_0 = e^A \\ a_1 \end{cases}$$

مثال. داده های جدول زیر را در نظر بگیرید.

i	1	2	3	4	5
x_i	1.00	1.25	1.50	1.75	2.00
y_i	5.10	5.79	6.53	7.45	8.46





بنابراین بین x و lnx رابطه خطی وجود دارد.

i	x	y	lny	x^2	xlny
1	1.00	5.10	1.629	1.0000	1.629
2	1.25	5.79	1.756	1.5625	2.195
3	1.50	6.53	1.876	2.2500	2.814
4	1.75	7.45	2.008	3.0625	3.514
5	2.00	8.46	2.135	4.0000	4.270
مجموع	7.50		9.404	11.875	14.422

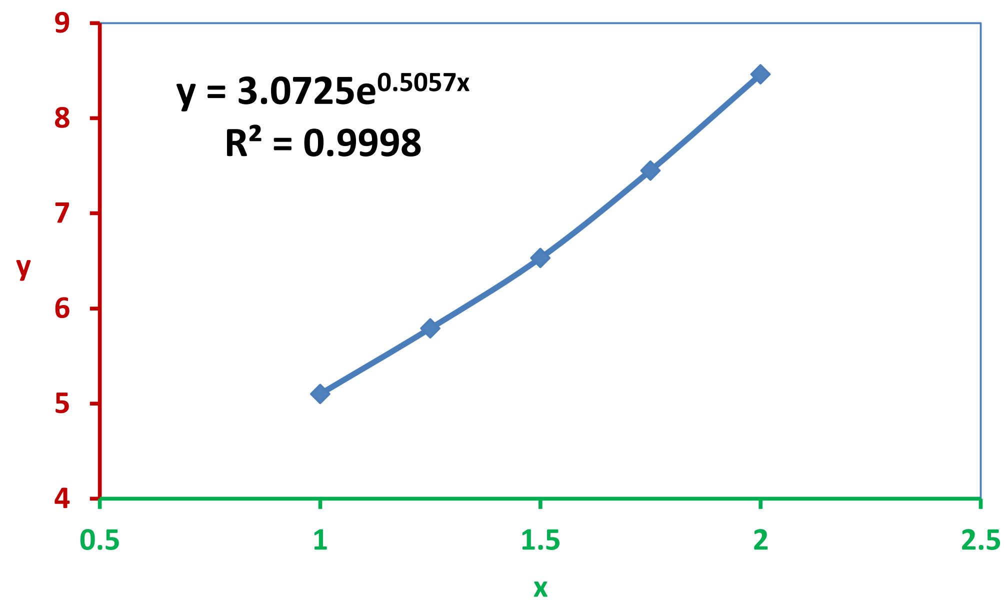
$$\begin{cases} \sum_{i=1}^{m} lny_i - a_1 \sum_{i=1}^{m} x_i - mA = 0 \\ \sum_{i=1}^{m} x_i lny_i - a_1 \sum_{i=1}^{m} {x_i}^2 - A \sum_{i=1}^{m} x_i = 0 \end{cases} \Rightarrow \begin{cases} 9.404 - 7.5a_1 - 5A = 0 \\ 14.422 - 11.875a_1 - 7.5A = 0 \end{cases}$$

$$\begin{cases} 9.404 - 7.5a_1 - 5A = 0 \\ 14.422 - 11.875a_1 - 7.5A = 0 \end{cases} \Rightarrow$$

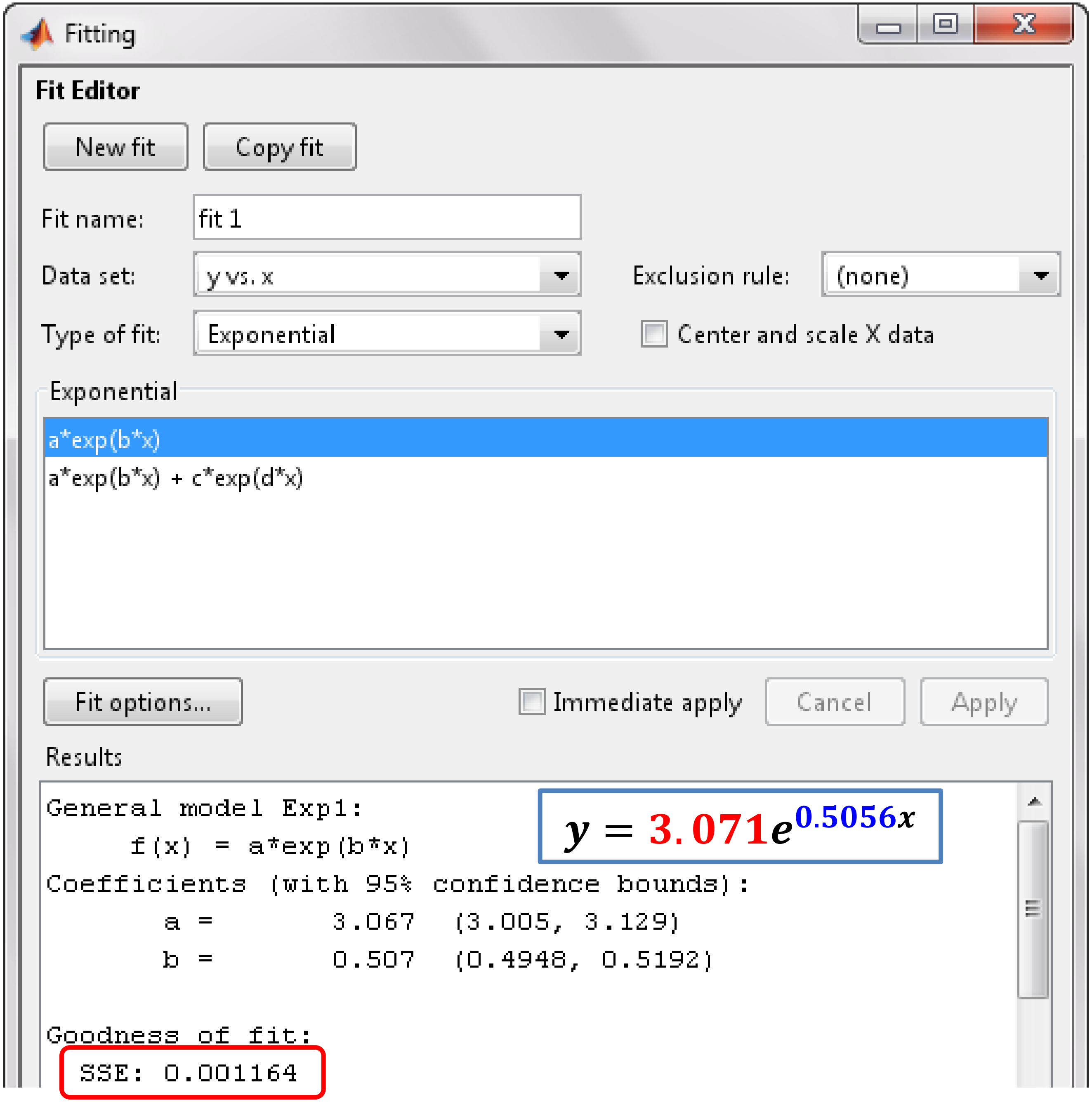
a_1=0.5056

$A = ln a_0$=1.122 $\quad a_0 = e^{1.22} = 3.071$

$$\boxed{y = 3.071e^{0.5056x}}$$



cftool


Fitting
Fit Editor
New fit
Copy fit
Fit name: fit 1
Data set: y vs. x
Exclusion rule: (none)
Type of fit: Exponential
Center and scale X data
Exponential
a*exp(b*x)
a*exp(b*x) + c*exp(d*x)
Fit options...
Immediate apply
Cancel
Apply
Results
General model Exp1:
f(x) = a*exp(b*x)
Coefficients (with 95% confidence bounds):
a = 3.067 (3.005, 3.129)
b = 0.507 (0.4948, 0.5192)
Goodness of fit:
SSE: 0.001164
$y = 3.071e^{0.5056x}$

حالت هذلولی

$$y = \frac{1}{a_0 + a_1 x} \xrightarrow{z = \frac{1}{y}} z = a_0 + a_1 x$$

بنابراین بین x و z رابطه خطی وجود دارد.

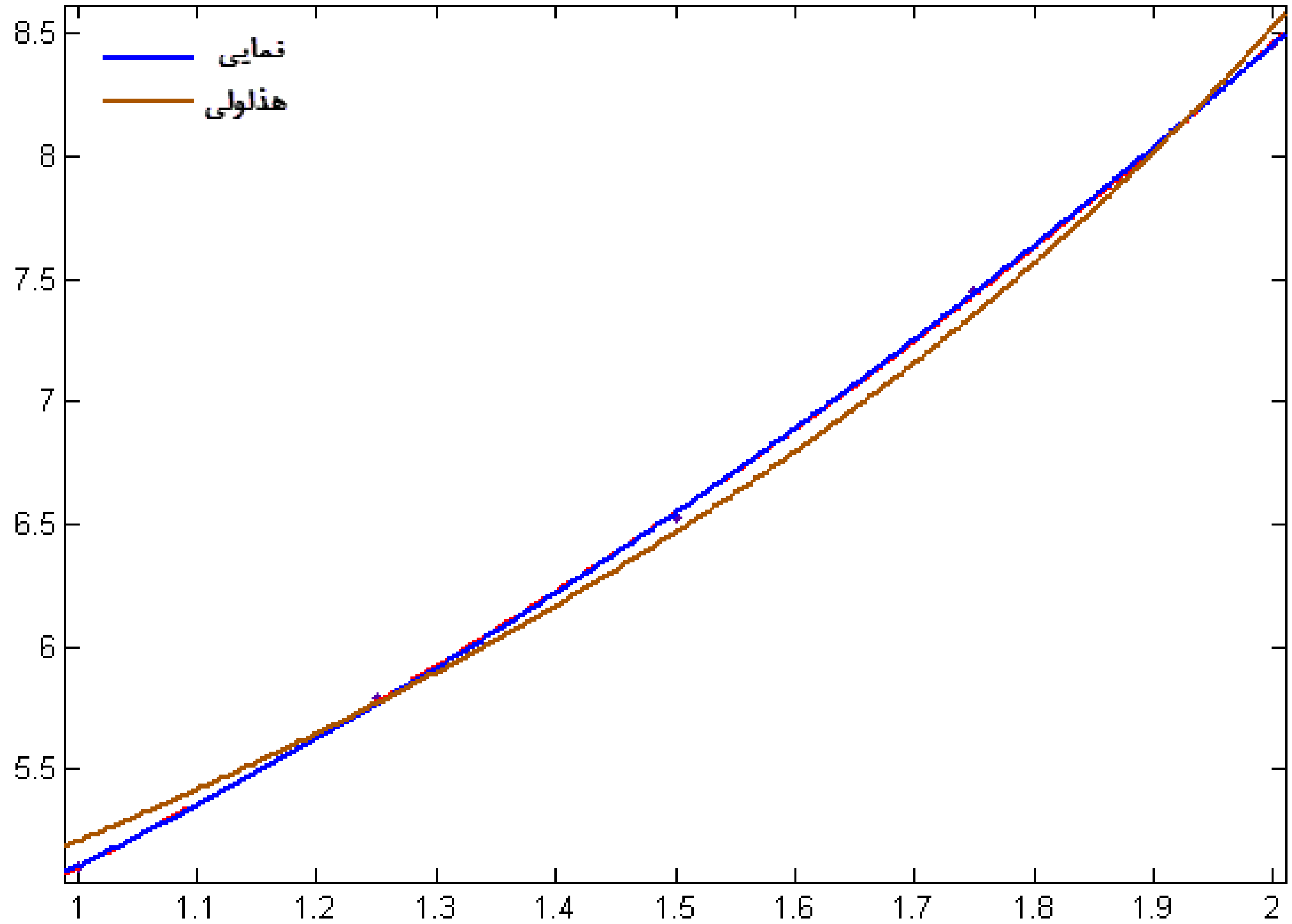
معادلات نرمال

$$\begin{cases} \sum_{i=1}^{m} z_i - a_1 \sum_{i=1}^{m} x_i - m a_0 = 0 \\ \sum_{i=1}^{m} x_i z_i - a_1 \sum_{i=1}^{m} {x_i}^2 - a_0 \sum_{i=1}^{m} x_i = 0 \end{cases}$$

$$S = \sum (z_i - \bar{z}_i)^2$$

```
     f(x) = 1/(a+b*x)
Coefficients (with 95% confidence bounds):
       a =      0.2667  (0.2501, 0.2832)
       b =    -0.07472  (-0.08413, -0.06532)

Goodness of fit:
  SSE: 0.02957
```



حالت مثلثاتی

wمقدار معلوم است

$$y = a_0 + a_1 cos w x \xrightarrow{t = coswx} y = a_0 + a_1 t$$

رابطه خطی بین y و t وجود دارد.

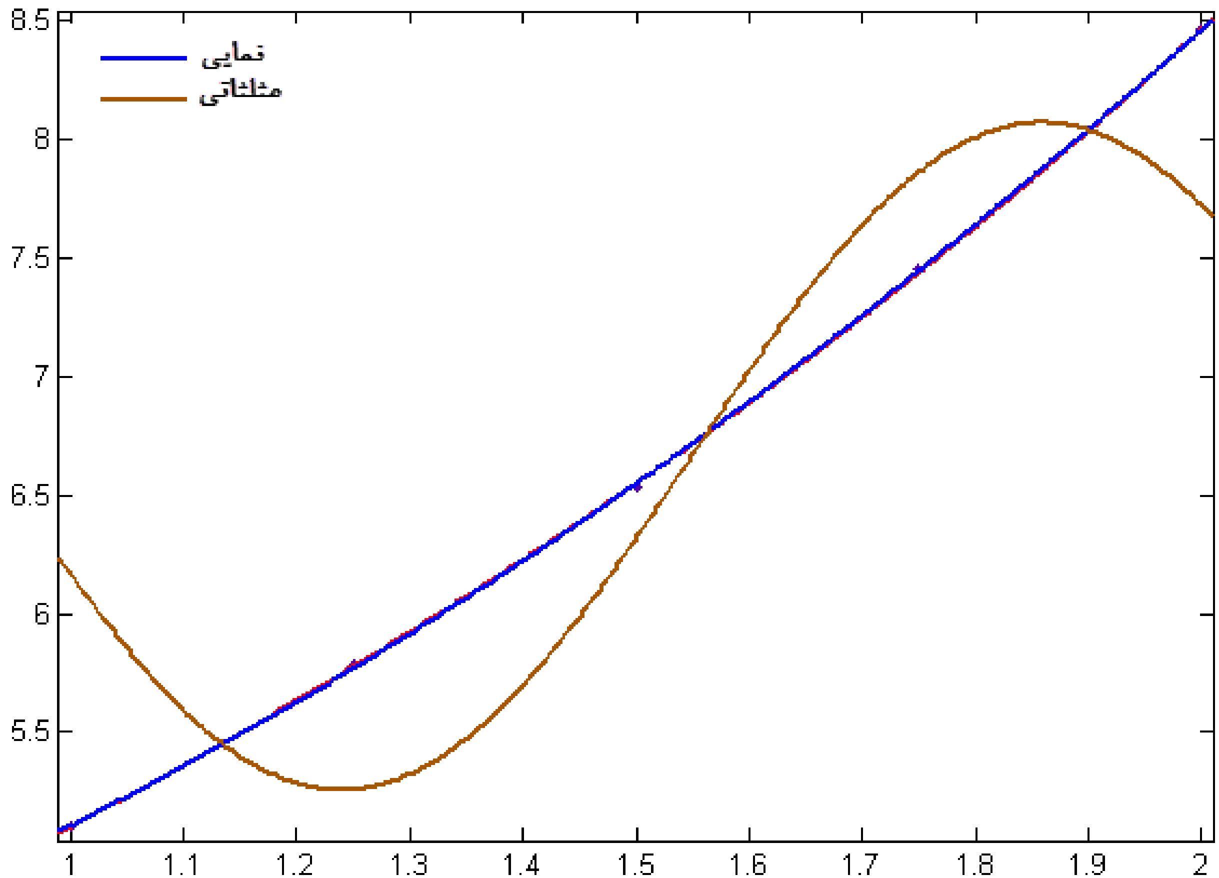
معادلات نرمال

$$\begin{cases} \sum_{i=1}^{m} y_i - a_1 \sum_{i=1}^{m} t_i - m a_0 = 0 \\ \sum_{i=1}^{m} t_i y_i - a_1 \sum_{i=1}^{m} {t_i}^2 - a_0 \sum_{i=1}^{m} t_i = 0 \end{cases}$$

$$S = \sum (y_i - \bar{y}_i)^2$$

```
     f(x) = a0+a1*cos(w*x)
Coefficients (with 95% confidence bounds):
       a0 =       6.663  (4.651, 8.675)
       a1 =      -1.406  (-4.273, 1.462)
       w =      -5.071  (-6.433, -3.709)

Goodness of fit:
  SSE: 2.183
```



منبع مطالب بعدی

http://numericalmethods.eng.usf.edu

What is Regression?

What is regression? Given n data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = f(x)$ to the data. The best fit is generally based on minimizing the sum of the square of the residuals, S_r

Residual at a point is $\varepsilon_i = y_i - f(x_i)$

Sum of the square of the residuals $$S_r = \sum_{i=1}^{n} (y_i - f(x_i))^2$$

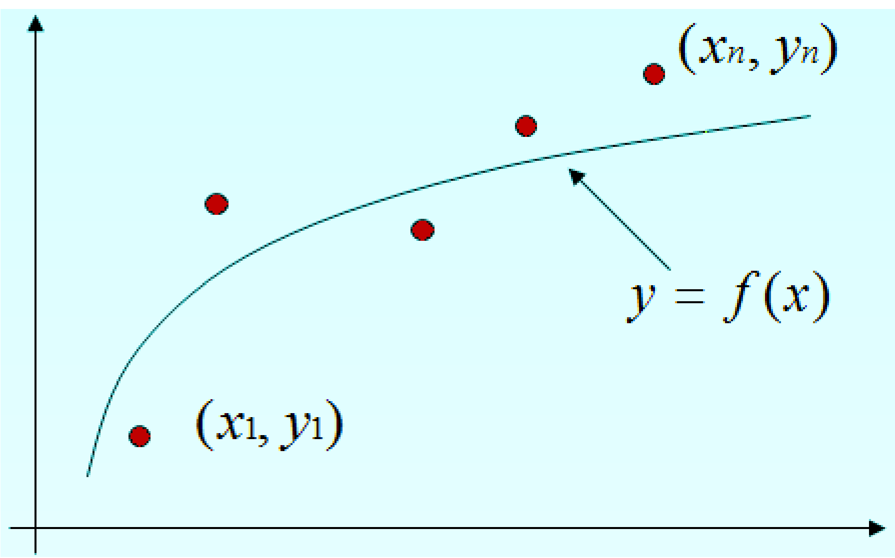


Figure. Basic model for regression

Linear Regression-Criterion#1

Given *n* data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = a_0 + a_1 x$ to the data.

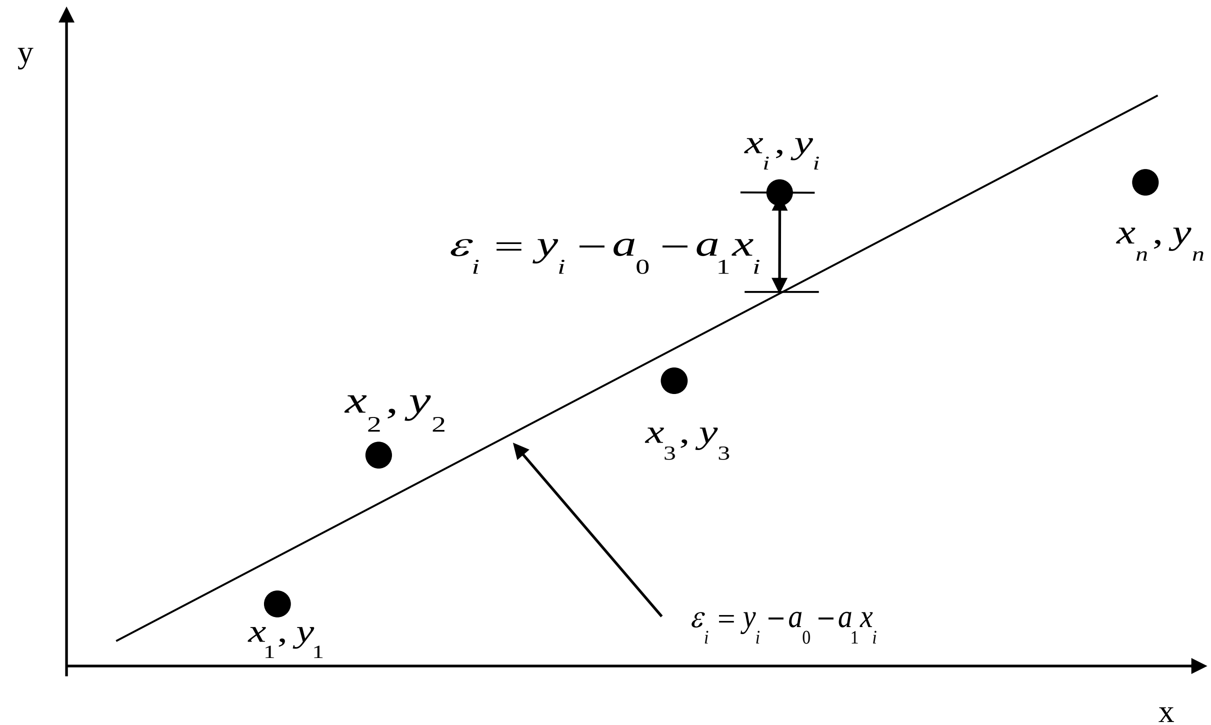


Figure. Linear regression of y vs. x data showing residuals at a typical point, x_i.

Does minimizing $\sum_{i=1}^{n} \varepsilon_i$ work as a criterion, where $\varepsilon_i = y_i - (a_0 + a_1 x_i)$

Least Squares Criterion

The least squares criterion minimizes the sum of the square of the residuals in the model, and also produces a unique line.

$$S_r = \sum_{i=1}^{n} \varepsilon_i^{\,2} = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)^2$$

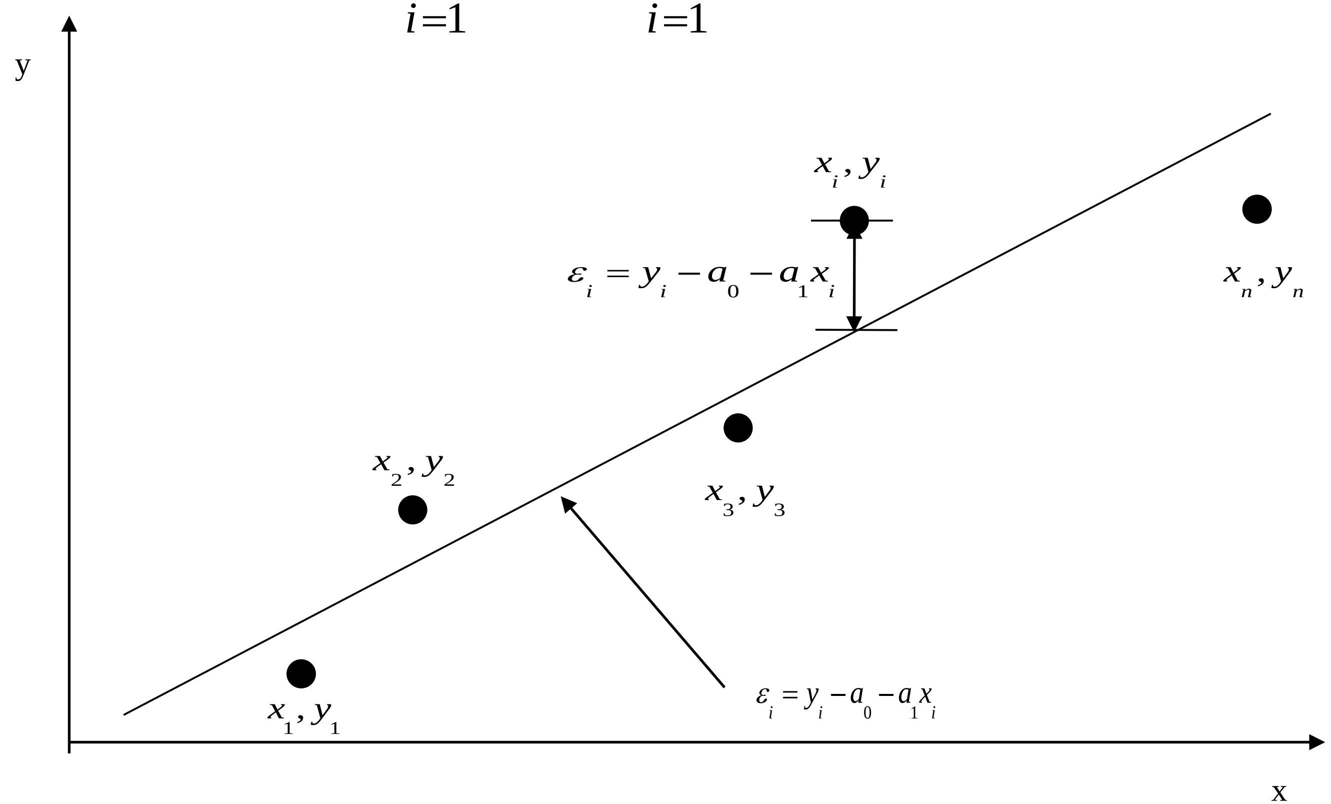


Figure. Linear regression of y vs. x data showing residuals at a typical point, x_i.

Finding Constants of Linear Model

Minimize the sum of the square of the residuals: $S_r = \sum_{i=1}^{n} \varepsilon_i^{\ 2} = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)^2$

To find a_0 and a_1 we minimize S_r with respect to a_1 and a_0.

$$\frac{\partial S_r}{\partial a_0} = -2\sum_{i=1}^{n}\left(y_i - a_0 - a_1 x_i\right)\left(-1\right) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum_{i=1}^{n}\left(y_i - a_0 - a_1 x_i\right)\left(-x_i\right) = 0$$

giving

$$\begin{cases} \sum_{i=1}^{n} a_0 + \sum_{i=1}^{n} a_1 x_i = \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} a_0 x_i + \sum_{i=1}^{n} a_1 x_i^{\ 2} = \sum_{i=1}^{n} y_i x_i \end{cases} \Rightarrow \quad (a_0 = \bar{y} - a_1 \bar{x})$$

Finding Constants of Linear Model

Solving for a_0 and a_1 directly yields,

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

and

$$a_0 = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \qquad (a_0 = \bar{y} - a_1 \bar{x})$$

Example 1

The torque, *T* needed to turn the torsion spring of a mousetrap through an angle, is given below.

Find the constants for the model given by $$T = k_1 + k_2\theta$$

Table: Torque vs Angle for a torsional spring

Angle, θ	**Torque, T**
Radians	***N-m***
0.698132	**0.188224**
0.959931	**0.209138**
1.134464	**0.230052**
1.570796	**0.250965**
1.919862	**0.313707**

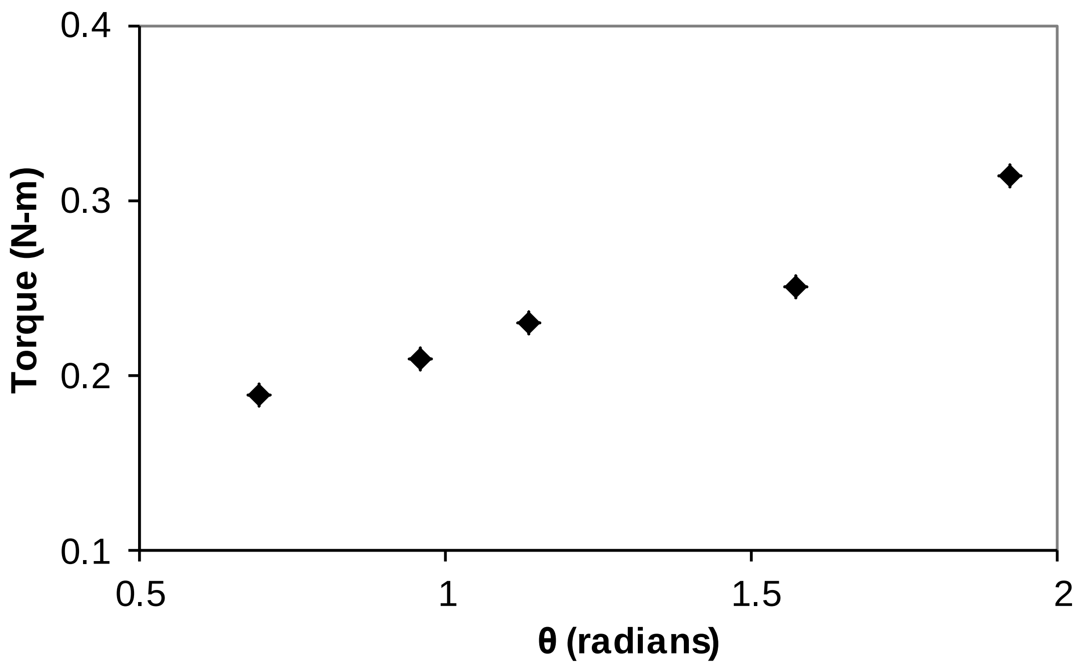


Figure. Data points for Angle vs. Torque data

The following table shows the summations needed for the calculations of the constants in the regression model.

Table. Tabulation of data for calculation of important summations

	θ	T	θ^2	$T\theta$
	Radians	*N-m*	*Radians*^{2}	*N-m-Radians*
	0.698132	**0.188224**	**0.487388**	**0.131405**
	0.959931	**0.209138**	**0.921468**	**0.200758**
	1.134464	**0.230052**	**1.2870**	**0.260986**
	1.570796	**0.250965**	**2.4674**	**0.394215**
	1.919862	**0.313707**	**3.6859**	**0.602274**
$\sum_{i=1}^{5} =$	**6.2831**	**1.1921**	**8.8491**	**1.5896**

Using equations described for a_0 and a_1 with $n = 5$

$$k_2 = \frac{n\sum_{i=1}^{5}\theta_i T_i - \sum_{i=1}^{5}\theta_i \sum_{i=1}^{5} T_i}{n\sum_{i=1}^{5}\theta_i^2 - \left(\sum_{i=1}^{5}\theta_i\right)^2}$$

$$= \frac{5(1.5896)-(6.2831)(1.1921)}{5(8.8491)-(6.2831)^2}$$

$$= 9.6091\times10^{-2} \text{ N-m/rad}$$

Use the average torque and average angle to calculate k_1

$$\bar{T} = \frac{\sum_{i=1}^{5} T_i}{n} = \frac{1.1921}{5} = 2.3842 \times 10^{-1}$$

$$\bar{\theta} = \frac{\sum_{i=1}^{5} \theta_i}{n} = \frac{6.2831}{5} = 1.2566$$

Using,

$$k_1 = \bar{T} - k_2\,\bar{\theta} = 2.3842 \times 10^{-1} - (9.6091 \times 10^{-2})(1.2566)$$

$$= 1.1767 \times 10^{-1} \quad \textit{N-m}$$

Example 1 Results

Using linear regression, a trend line is found from the data

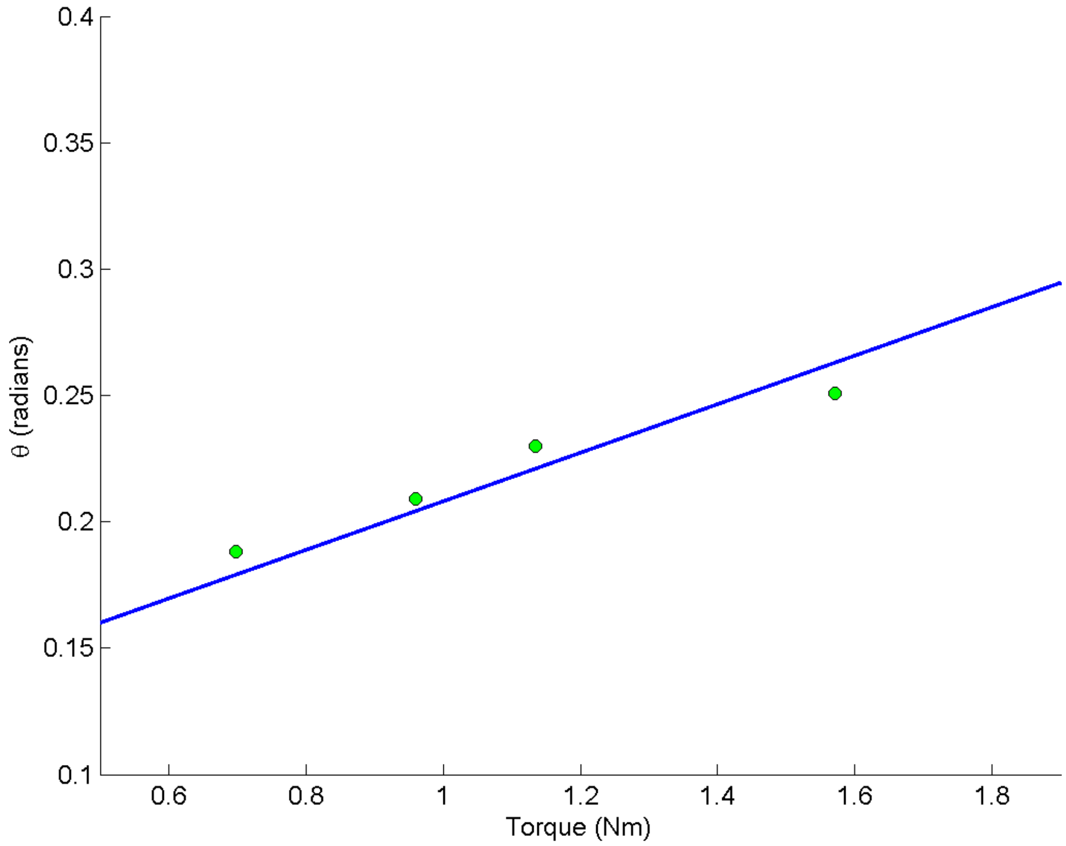


Figure. Linear regression of Torque versus Angle data

Can you find the energy in the spring if it is twisted from 0 to 180 degrees?

Example 2

To find the longitudinal modulus of composite, the following data is collected. Find the longitudinal modulus, E using the regression model

$$\sigma = E\varepsilon$$

and the sum of the square of the residuals.

Table. Stress vs. Strain data

Strain	Stress
(%)	*(MPa)*
0	0
0.183	306
0.36	612
0.5324	917
0.702	1223
0.867	1529
1.0244	1835
1.1774	2140
1.329	2446
1.479	2752
1.5	2767
1.56	2896

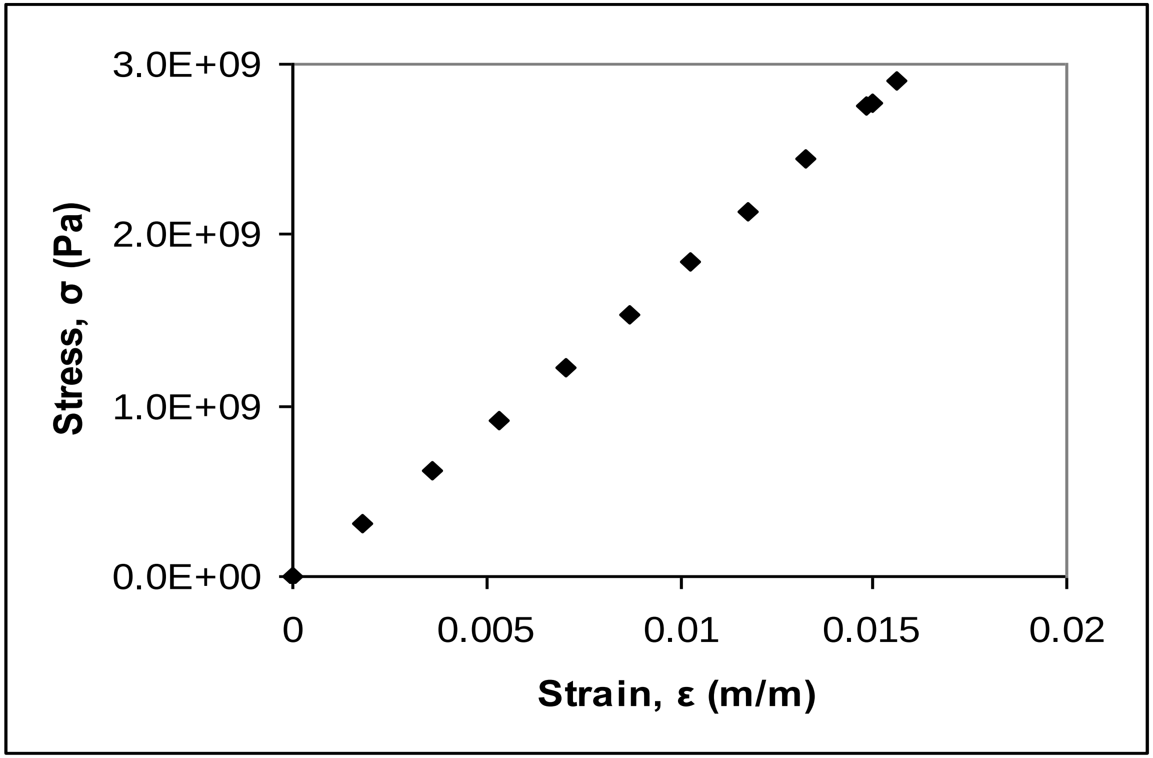


Figure. Data points for Stress vs. Strain data

Residual at each point is given by $\gamma_i = \sigma_i - E\varepsilon_i$

The sum of the square of the residuals then is

$$S_r = \sum_{i=1}^{n} \gamma_i^2 = \sum_{i=1}^{n} \left(\sigma_i - E\varepsilon_i\right)^2$$

Differentiate with respect to E $\quad \dfrac{\partial S_r}{\partial E} = \sum_{i=1}^{n} 2\left(\sigma_i - E\varepsilon_i\right)\left(-\varepsilon_i\right) = 0$

Therefore

$$E = \frac{\sum_{i=1}^{n} \sigma_i \varepsilon_i}{\sum_{i=1}^{n} \varepsilon_i^{\,2}}$$

Table. Summation data for regression model

i	ε	σ	ε²	εσ
1	0.0000	0.0000	0.0000	0.0000
2	1.8300×10^{-3}	3.0600×10^{8}	3.3489×10^{-6}	5.5998×10^{5}
3	3.6000×10^{-3}	6.1200×10^{8}	1.2960×10^{-5}	2.2032×10^{6}
4	5.3240×10^{-3}	9.1700×10^{8}	2.8345×10^{-5}	4.8821×10^{6}
5	7.0200×10^{-3}	1.2230×10^{9}	4.9280×10^{-5}	8.5855×10^{6}
6	8.6700×10^{-3}	1.5290×10^{9}	7.5169×10^{-5}	1.3256×10^{7}
7	1.0244×10^{-2}	1.8350×10^{9}	1.0494×10^{-4}	1.8798×10^{7}
8	1.1774×10^{-2}	2.1400×10^{9}	1.3863×10^{-4}	2.5196×10^{7}
9	1.3290×10^{-2}	2.4460×10^{9}	1.7662×10^{-4}	3.2507×10^{7}
10	1.4790×10^{-2}	2.7520×10^{9}	2.1874×10^{-4}	4.0702×10^{7}
11	1.5000×10^{-2}	2.7670×10^{9}	2.2500×10^{-4}	4.1505×10^{7}
12	1.5600×10^{-2}	2.8960×10^{9}	2.4336×10^{-4}	4.5178×10^{7}
$\sum_{i=1}^{12}$			1.2764×10^{-3}	2.3337×10^{8}

With

$$\sum_{i=1}^{12}\varepsilon_i^2 = 1.2764\times10^{-3}$$

and

$$\sum_{i=1}^{12}\sigma_i\varepsilon_i = 2.3337\times10^{8}$$

Using

$$E = \frac{\sum_{i=1}^{12}\sigma_i\varepsilon_i}{\sum_{i=1}^{12}\varepsilon_i^2} = \frac{2.3337\times10^{8}}{1.2764\times10^{-3}} = 182.84\ GPa$$

The equation $\sigma = 182.84\varepsilon$ describes the data.

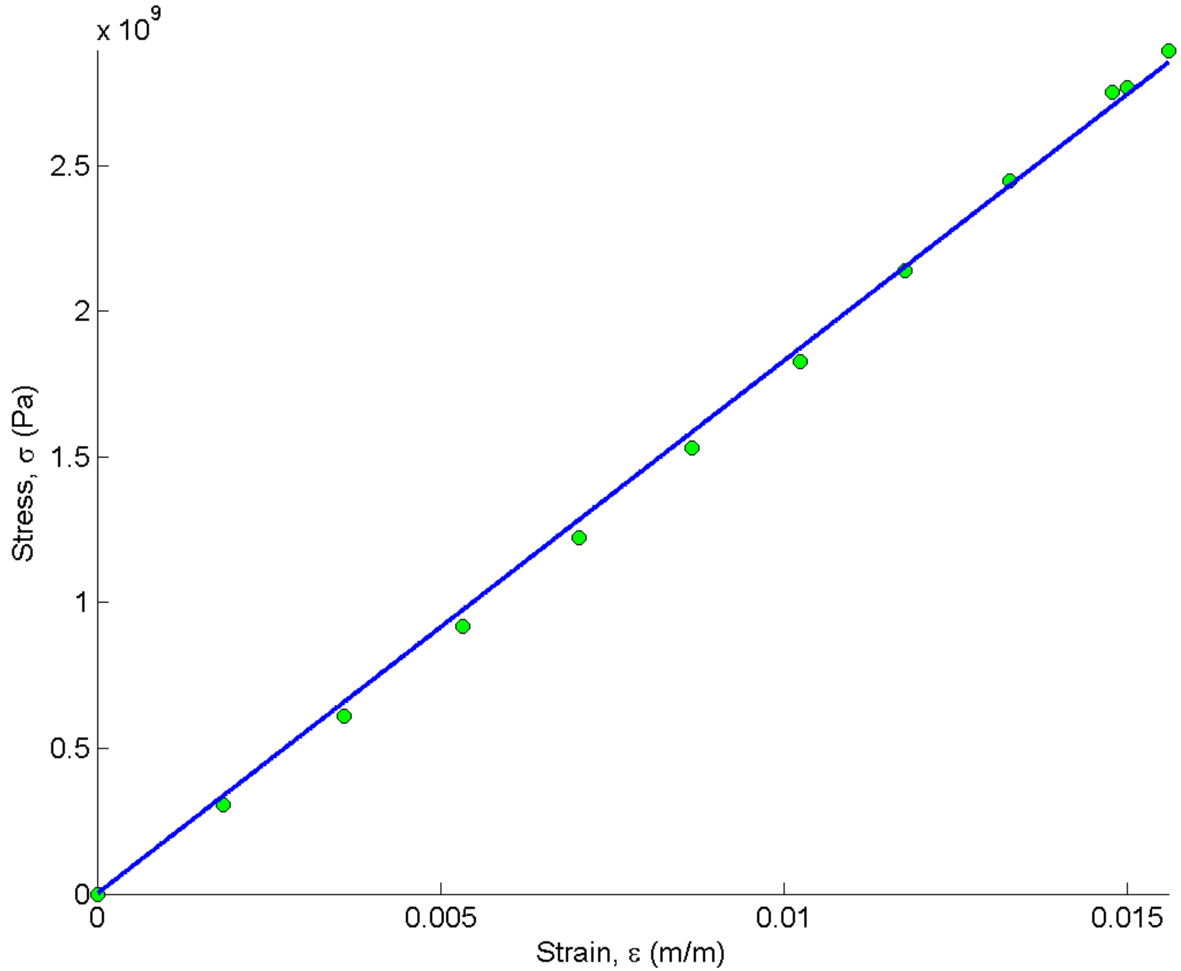


Figure. Linear regression for Stress vs. Strain data

Nonlinear Regression

Some popular nonlinear regression models:

1. Exponential model: $(y = ae^{bx})$

2. Power model: $(y = ax^{b})$

3. Saturation growth model: $\left(y = \dfrac{ax}{b+x}\right)$

4. Polynomial model: $(y = a_0 + a_1x + \ldots + a_mx^{m})$

Exponential Model

Given $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ best fit $y = ae^{bx}$ to the data.

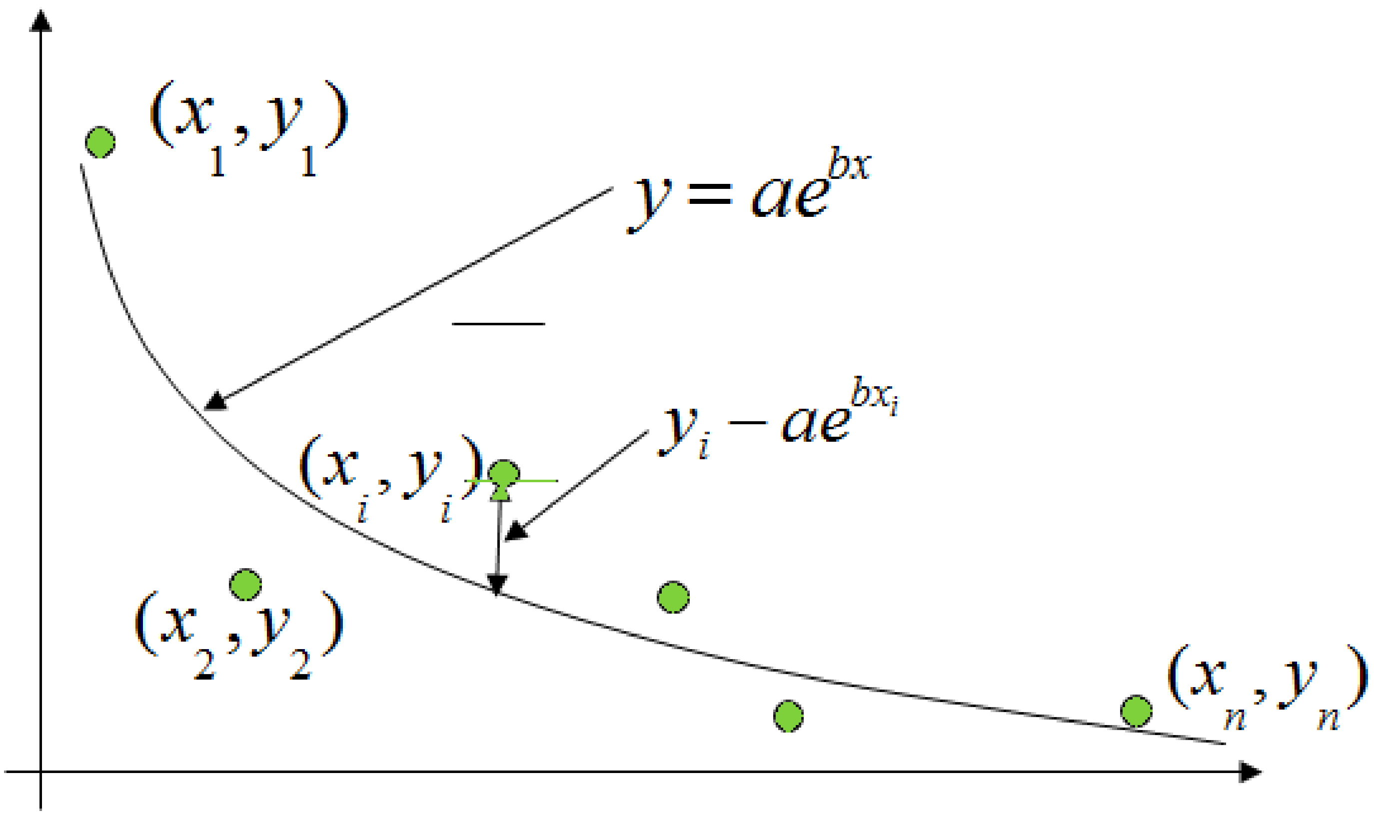


Figure. Exponential model of nonlinear regression for y vs. x data

Finding Constants of Exponential Model

The sum of the square of the residuals is defined as

$$S_r = \sum_{i=1}^{n} \left(y_i - ae^{bx_i} \right)^2$$

Differentiate with respect to *a* and *b*

$$\frac{\partial S_r}{\partial a} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i} \right)\left(-e^{bx_i} \right) = 0$$

$$\frac{\partial S_r}{\partial b} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i} \right)\left(-ax_i e^{bx_i} \right) = 0$$

Finding Constants of Exponential Model

Rewriting the equations, we obtain

$$-\sum_{i=1}^{n} y_i e^{bx_i} + a\sum_{i=1}^{n} e^{2bx_i} = 0$$

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - a\sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

Finding constants of Exponential Model

Solving the first equation for a yields

$$a = \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}}$$

Substituting a back into the previous equation

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

The constant b can be found through numerical methods such as bisection method.

Example 1-Exponential Model

Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the techritium-99m would be gone in about 6 hours. It, however, takes about 24 hours for the radiation levels to reach what we are exposed to in day-to-day activities. Below is given the relative intensity of radiation as a function of time.

Table. Relative intensity of radiation as a function of time.

t(hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

The relative intensity is related to time by the equation

$$\gamma = Ae^{\lambda t}$$

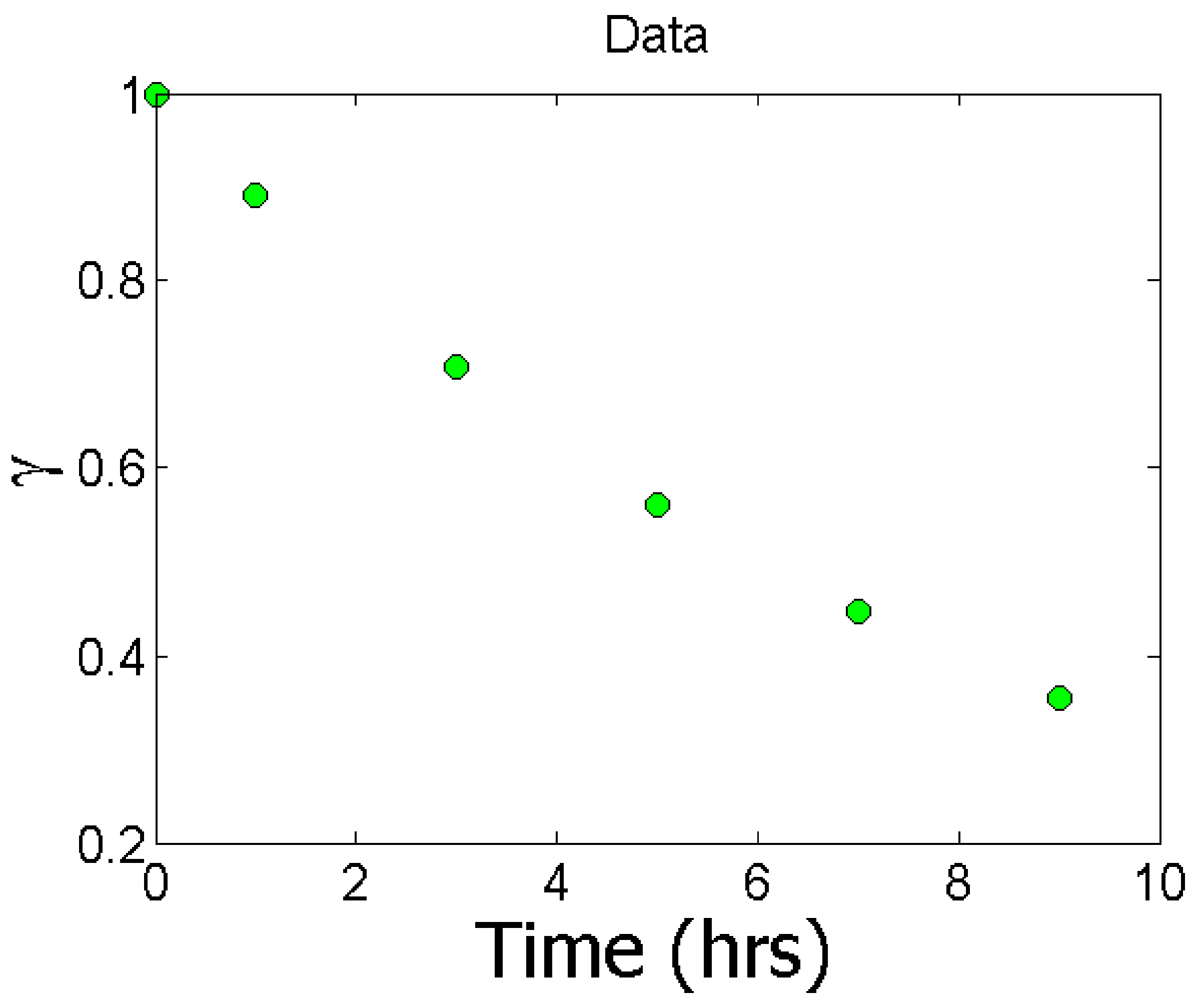
Find:

a) The value of the regression constants A and λ

b) The half-life of Technium-99m

c) Radiation intensity after 24 hours

Plot of data



Constants of the Model

$$\gamma = Ae^{\lambda t}$$

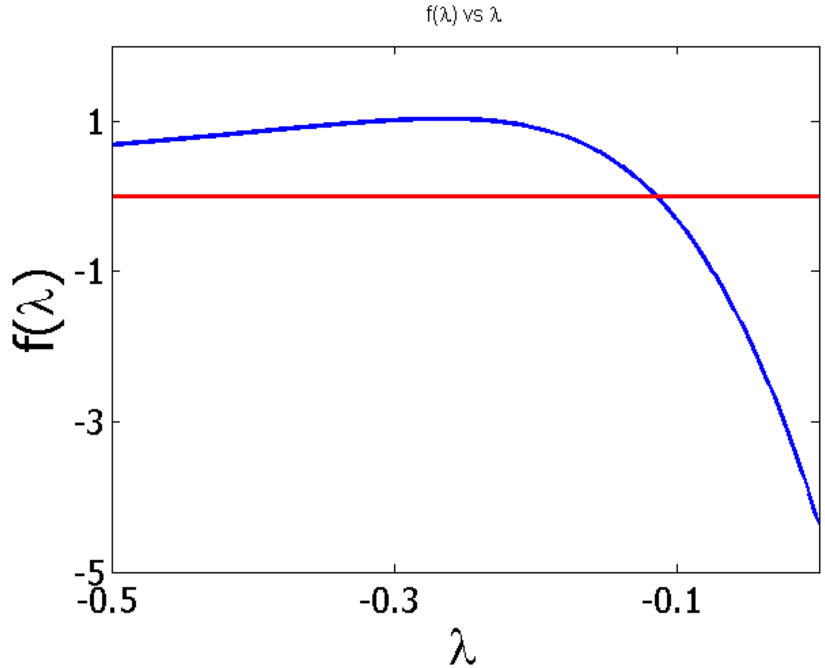
The value of λ is found by solving the nonlinear equation

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$

$$A = \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}}$$

Setting up the Equation in MATLAB

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$



t (hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

Setting up the Equation in MATLAB

$$f(\lambda)=\sum_{i=1}^{n}\gamma_i t_i e^{\lambda t_i}-\frac{\sum_{i=1}^{n}\gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}}\sum_{i=1}^{n} t_i e^{2\lambda t_i}=0$$

$$\lambda=-0.1151$$

```
t=[0 1  3  5  7  9]
gamma=[1  0.891  0.708  0.562  0.447  0.355]
syms lamda
sum1=sum(gamma.*t.*exp(lamda*t));
sum2=sum(gamma.*exp(lamda*t));
sum3=sum(exp(2*lamda*t));
sum4=sum(t.*exp(2*lamda*t));
f=sum1-sum2/sum3*sum4;
```

Calculating the Other Constant

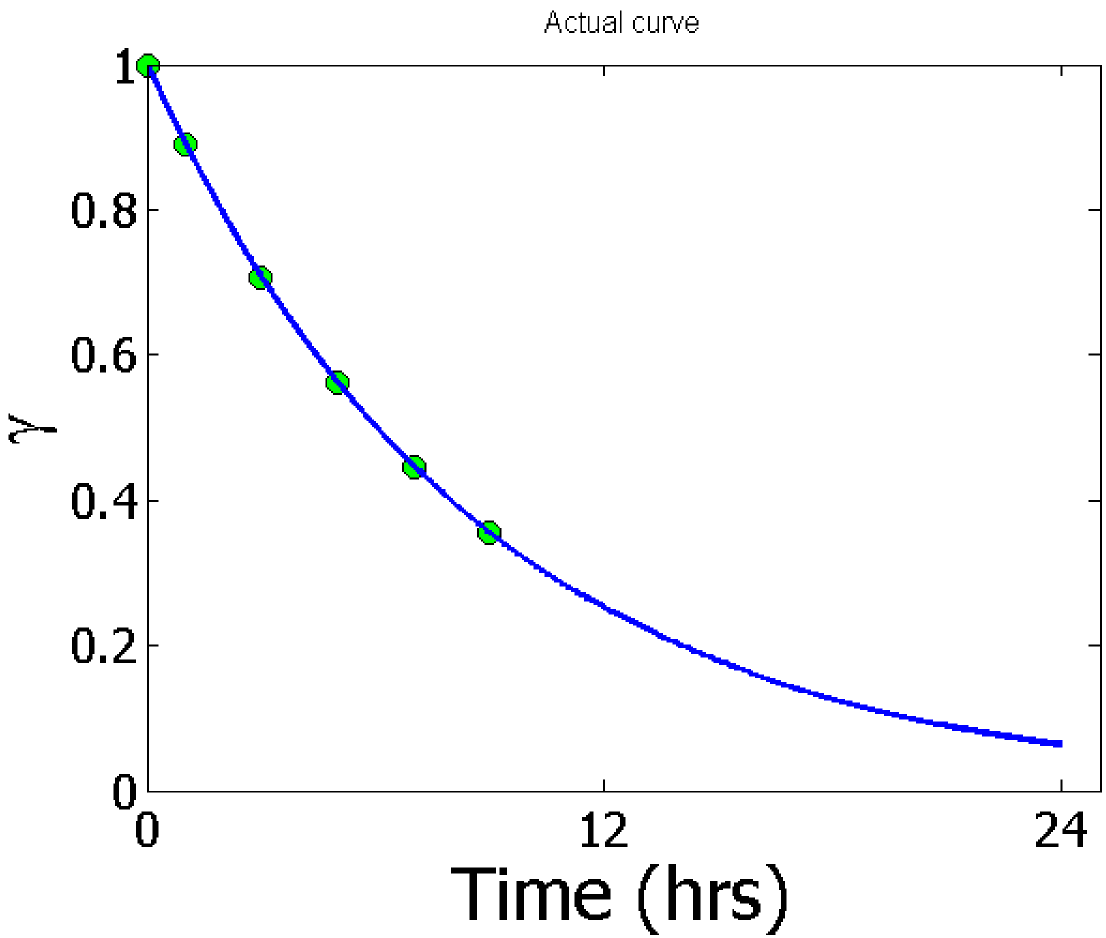
The value of *A* can now be calculated

$$A = \frac{\sum_{i=1}^{6} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{6} e^{2\lambda t_i}} = 0.9998$$

The exponential regression model then is

$$\gamma = 0.9998\, e^{-0.1151t}$$

Plot of data and regression curve



Relative Intensity After 24 hrs

The relative intensity of radiation after 24 hours

$$\gamma = 0.9998 \times e^{-0.1151(24)}$$

$$= 6.3160 \times 10^{-2}$$

This result implies that only

$$\frac{6.316 \times 10^{-2}}{0.9998} \times 100 = 6.317\%$$

radioactive intensity is left after 24 hours.

Polynomial Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = a_0 + a_1 x + \ldots + a_m x^m$ $(m \le n-2)$ to a given data set.

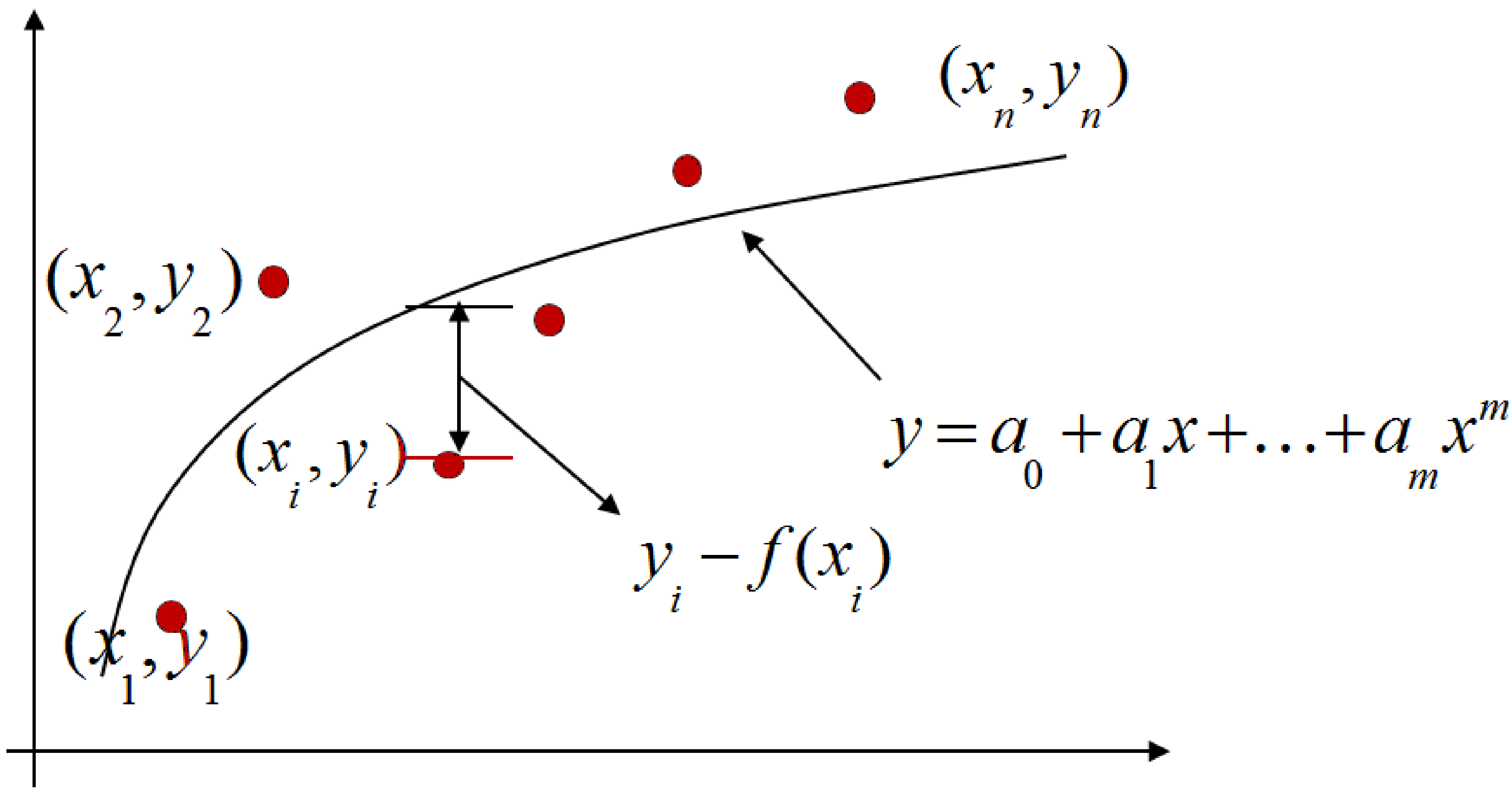


Figure. Polynomial model for nonlinear regression of y vs. x data

Polynomial Model cont.

The residual at each data point is given by

$$E_i = y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m$$

The sum of the square of the residuals then is

$$S_r = \sum_{i=1}^{n} E_i^2$$

$$= \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m \right)^2$$

Polynomial Model cont.

To find the constants of the polynomial model, we set the derivatives with respect to a_i where $i = 1, \ldots m,$ equal to zero.

$$\frac{\partial S_r}{\partial a_0} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - . \ . \ . - a_m x_i^m\right)(-1) = 0$$

$$\frac{\partial S_r}{\partial a_1} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - . \ . \ . - a_m x_i^m\right)(-x_i) = 0$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$\frac{\partial S_r}{\partial a_m} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - . \ . \ . - a_m x_i^m\right)(-x_i^m) = 0$$

Polynomial Model cont.

These equations in matrix form are given by

$$
\begin{bmatrix}
n & \left(\sum_{i=1}^{n} x_i\right) & \cdots & \left(\sum_{i=1}^{n} x_i^{m}\right) \\
\left(\sum_{i=1}^{n} x_i\right) & \left(\sum_{i=1}^{n} x_i^{2}\right) & \cdots & \left(\sum_{i=1}^{n} x_i^{m+1}\right) \\
\cdots & \cdots & \cdots & \cdots \\
\left(\sum_{i=1}^{n} x_i^{m}\right) & \left(\sum_{i=1}^{n} x_i^{m+1}\right) & \cdots & \left(\sum_{i=1}^{n} x_i^{2m}\right)
\end{bmatrix}
\begin{bmatrix} a_0 \\ a_1 \\ \cdots \\ a_m \end{bmatrix}
=
\begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \\ \cdots \\ \sum_{i=1}^{n} x_i^{m} y_i \end{bmatrix}
$$

The above equations are then solved for $a_0, a_1, \ldots, a_m$

Example 2-Polynomial Model

Regress the thermal expansion coefficient vs. temperature data to a second order polynomial.

Table. Data points for temperature vs α

Temperature, T(°F)	Coefficient of thermal expansion, α (in/in/°F)
80	6.47×10^{-6}
40	6.24×10^{-6}
−40	5.72×10^{-6}
−120	5.09×10^{-6}
−200	4.30×10^{-6}
−280	3.33×10^{-6}
−340	2.45×10^{-6}

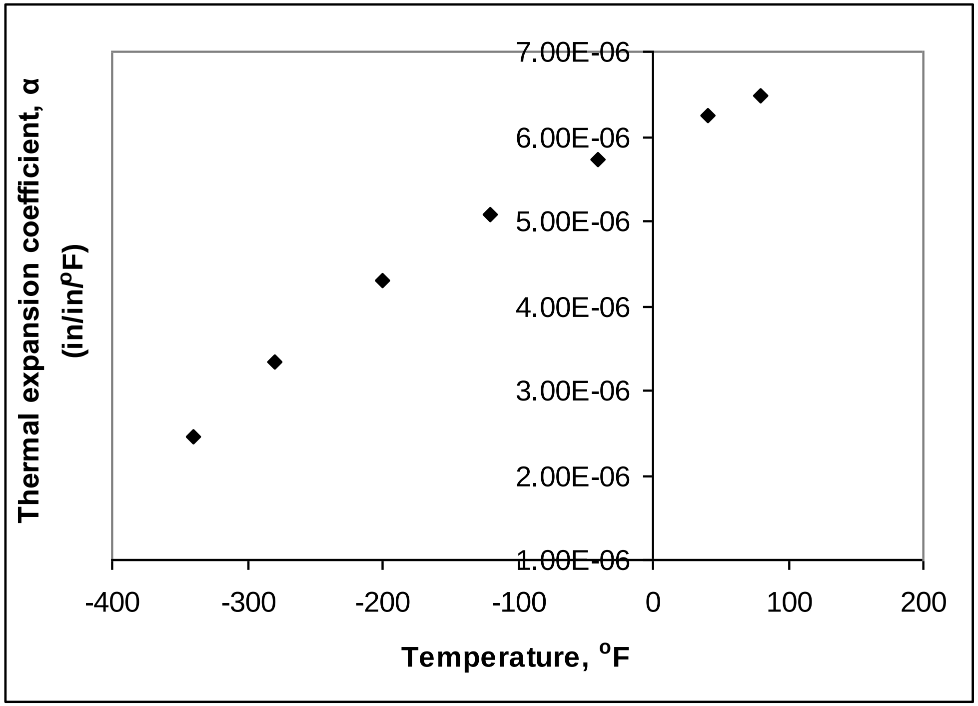


Figure. Data points for thermal expansion coefficient vs temperature.

Example 2-Polynomial Model cont.

We are to fit the data to the polynomial regression model

$$\alpha = a_0 + a_1 T + a_2 T^2$$

The coefficients a_0, a_1, a_2 are found by differentiating the sum of the square of the residuals with respect to each variable and setting the values equal to zero to obtain

$$\begin{bmatrix} n & \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) \\ \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) \\ \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) & \left(\sum_{i=1}^{n} T_i^4\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} \alpha_i \\ \sum_{i=1}^{n} T_i \, \alpha_i \\ \sum_{i=1}^{n} T_i^2 \alpha_i \end{bmatrix}$$

Example 2-Polynomial Model cont.

The necessary summations are as follows

Table. Data points for temperature vs.

Temperature, T (°F)	Coefficient of thermal expansion, α (in/in/°F)
80	6.47×10^{-6}
40	6.24×10^{-6}
−40	5.72×10^{-6}
−120	5.09×10^{-6}
−200	4.30×10^{-6}
−280	3.33×10^{-6}
−340	2.45×10^{-6}

$$\sum_{i=1}^{7} T_i^2 = 2.5580\times10^{5}$$

$$\sum_{i=1}^{7} T_i^3 = -7.0472\times10^{7}$$

$$\sum_{i=1}^{7} T_i^4 = 2.1363\times10^{10}$$

$$\sum_{i=1}^{7} \alpha_i = 3.3600\times10^{-5}$$

$$\sum_{i=1}^{7} T_i\alpha_i = -2.6978\times10^{-3}$$

$$\sum_{i=1}^{7} T_i^2\alpha_i = 8.5013\times10^{-1}$$

Example 2-Polynomial Model cont.

Using these summations, we can now calculate a_0, a_1, a_2

$$\begin{bmatrix} 7.0000 & -8.6000\times10^{2} & 2.5800\times10^{5} \\ -8.600\times10^{2} & 2.5800\times10^{5} & -7.0472\times10^{7} \\ 2.5800\times10^{5} & -7.0472\times10^{7} & 2.1363\times10^{10} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 3.3600\times10^{-5} \\ -2.6978\times10^{-3} \\ 8.5013\times10^{-1} \end{bmatrix}$$

Solving the above system of simultaneous linear equations we have

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 6.0217\times10^{-6} \\ 6.2782\times10^{-9} \\ -1.2218\times10^{-11} \end{bmatrix}$$

The polynomial regression model is then

$$\alpha = a_0 + a_1 T + a_2 T^2$$

$$= 6.0217\times10^{-6} + 6.2782\times10^{-9}\,\mathrm{T} - 1.2218\times10^{-11}\,\mathrm{T}^2$$

Transformation of Data

To find the constants of many nonlinear models, it results in solving simultaneous nonlinear equations. For mathematical convenience, some of the data for such models can be transformed. For example, the data for an exponential model can be transformed.

As shown in the previous example, many chemical and physical processes are governed by the equation,

$$y = ae^{bx}$$

Taking the natural log of both sides yields, $\ln y = \ln a + bx$

Let $z = \ln y$ and $a_0 = \ln a$

We now have a linear regression model where $z = a_0 + a_1 x$

(implying) $a = e^{a_o}$ with $a_1 = b$

Linearization of data cont.

Using linear model regression methods,

$$a_1 = \frac{n\sum_{i=1}^{n} x_i z_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$a_0 = \bar{z} - a_1 \bar{x}$$

Once a_o, a_1 are found, the original constants of the model are found as

$$b = a_1$$

$$a = e^{a_0}$$

Example 3-Linearization of data

Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the technetium-99m would be gone in about *6* hours. It, however, takes about *24* hours for the radiation levels to reach what we are exposed to in day-to-day activities. Below is given the relative intensity of radiation as a function of time.

Table. Relative intensity of radiation as a function of time

t(hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

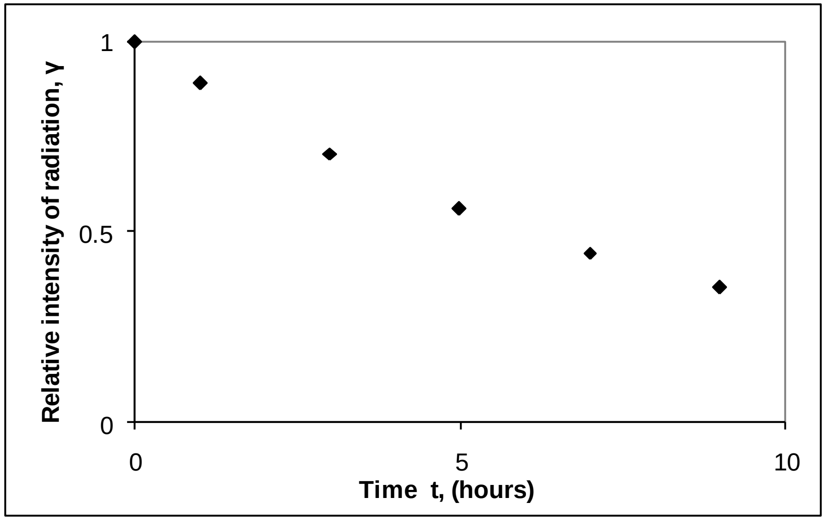


Figure. Data points of relative radiation intensity vs. time

Find:

a) The value of the regression constants A and λ

b) The half-life of Technium-99m

c) Radiation intensity after 24 hours

The relative intensity is related to time by the equation

$$\gamma = Ae^{\lambda t}$$

Example 3-Linearization of data cont.

Exponential model given as, $\gamma = Ae^{\lambda t}$ $\ln(\gamma) = \ln(A) + \lambda t$

Assuming $z = \ln\gamma$, $a_o = \ln(A)$ and $a_1 = \lambda$ we obtain

$$z = a_0 + a_1 t$$

This is a linear relationship between z and t

Example 3-Linearization of data cont.

Using this linear relationship, we can calculate a_0, a_1 where

$$a_1 = \frac{n\sum_{i=1}^{n} t_i z_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} t_1^2 - \left(\sum_{i=1}^{n} t_i\right)^2}$$

and

$$a_0 = \bar{z} - a_1 \bar{t}$$

$$\lambda = a_1$$

$$A = e^{a_0}$$

Example 3-Linearization of Data cont.

Summations for data linearization are as follows

Table. Summation data for linearization of data model

i	t_i	γ_i	$z_i = \ln \gamma_i$	$t_i z_i$	t_i^2
1	0	1	0.00000	0.0000	0.0000
2	1	0.891	−0.11541	−0.11541	1.0000
3	3	0.708	−0.34531	−1.0359	9.0000
4	5	0.562	−0.57625	−2.8813	25.000
5	7	0.447	−0.80520	−5.6364	49.000
6	9	0.355	−1.0356	−9.3207	81.000
$\sum$	25.000		−2.8778	−18.990	165.00

With $n = 6$

$$\sum_{i=1}^{6} t_i = 25.000$$

$$\sum_{i=1}^{6} z_i = -2.8778$$

$$\sum_{i=1}^{6} t_i z_i = -18.990$$

$$\sum_{i=1}^{6} t_i^2 = 165.00$$

Example 3-Linearization of Data cont.

Calculating a_0, a_1

$$a_1 = \frac{6(-18.990)-(25)(-2.8778)}{6(165.00)-(25)^2} = -0.11505$$

$$a_0 = \frac{-2.8778}{6} - (-0.11505)\frac{25}{6} = -2.6150\times 10^{-4}$$

Since

$$a_0 = \ln(A)$$

$$A = e^{a_0}$$

$$= e^{-2.6150\times 10^{-4}} = 0.99974$$

also

$$\lambda = a_1 = -0.11505$$

Example 3-Linearization of Data cont.

Resulting model is $\gamma = 0.99974 \times e^{-0.11505t}$

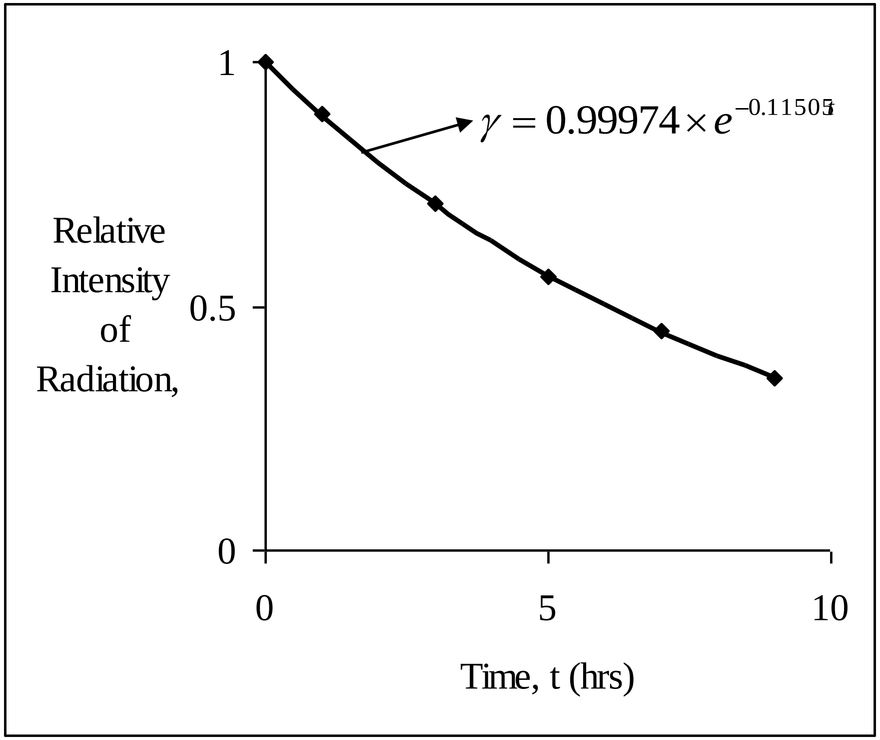


Figure. Relative intensity of radiation as a function of temperature using linearization of data model.

Example 3-Linearization of Data cont.

The regression formula is then $\gamma = 0.99974 \times e^{-0.11505t}$

b) Half life of Technetium 99 is when $\gamma = \frac{1}{2}\gamma\Big|_{t=0}$

$$0.99974 \times e^{-0.11505t} = \frac{1}{2}(0.99974)e^{-0.11505(0)}$$

$$e^{-0.11508t} = 0.5$$

$$-0.11505t = \ln(0.5)$$

$$t = 6.0248 \ hours$$

Example 3-Linearization of Data cont.

c) The relative intensity of radiation after 24 hours is then

$$\gamma = 0.99974e^{-0.11505(24)} = 0.063200$$

This implies that only $\frac{6.3200 \times 10^{-2}}{0.99983} \times 100 = 6.3216\%$ of the radioactive material is left after 24 hours.

Comparison

Comparison of exponential model with and without data linearization:

Table. Comparison for exponential model with and without data linearization.

	With data linearization (Example 3)	Without data linearization (Example 1)
A	0.99974	0.99983
λ	-0.11505	-0.11508
Half-Life (hrs)	6.0248	6.0232
Relative intensity after 24 hrs.	6.3200×10^{-2}	6.3160×10^{-2}

The values are very similar so data linearization was suitable to find the constants of the nonlinear exponential model in this case.