Nonlinear Regression

Industrial Engineering Major

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Transforming Numerical Methods Education for STEM Undergraduates

Nonlinear Regression

Nonlinear Regression

Some popular nonlinear regression models:
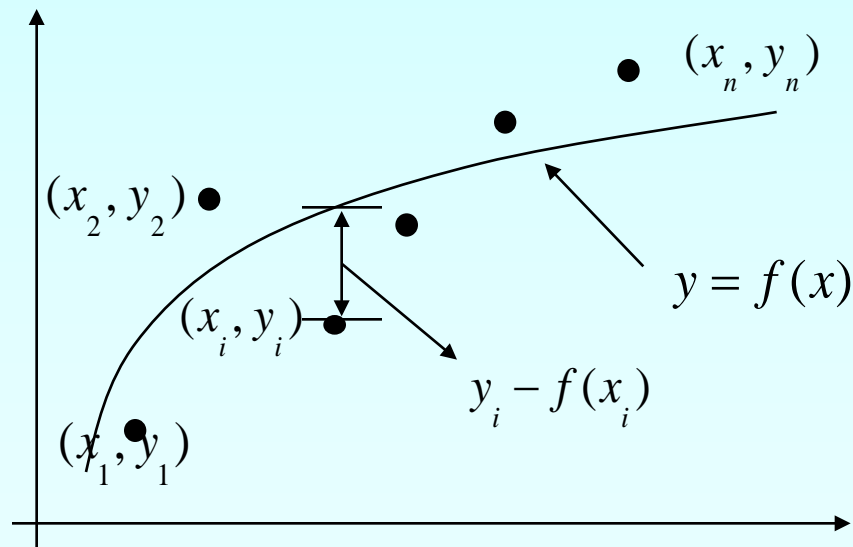
1. Exponential model: $(y = ae^{bx})$

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

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

4. Polynomial model: $(y = a_0 + a_1 x + \ldots + a_m x^m)$

Nonlinear 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, where $f(x)$ is a nonlinear function of x.
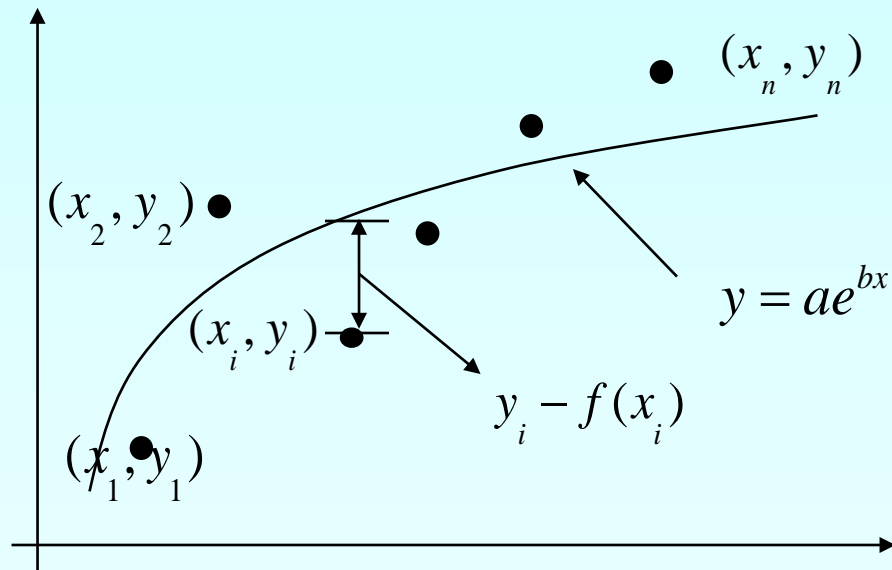

Figure. Nonlinear regression model for discrete y vs. x data

Regression
Exponential Model

Exponential Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ 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*

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

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

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

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

Substituting a back into the previous equation

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

Nonlinear equation in terms of b

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

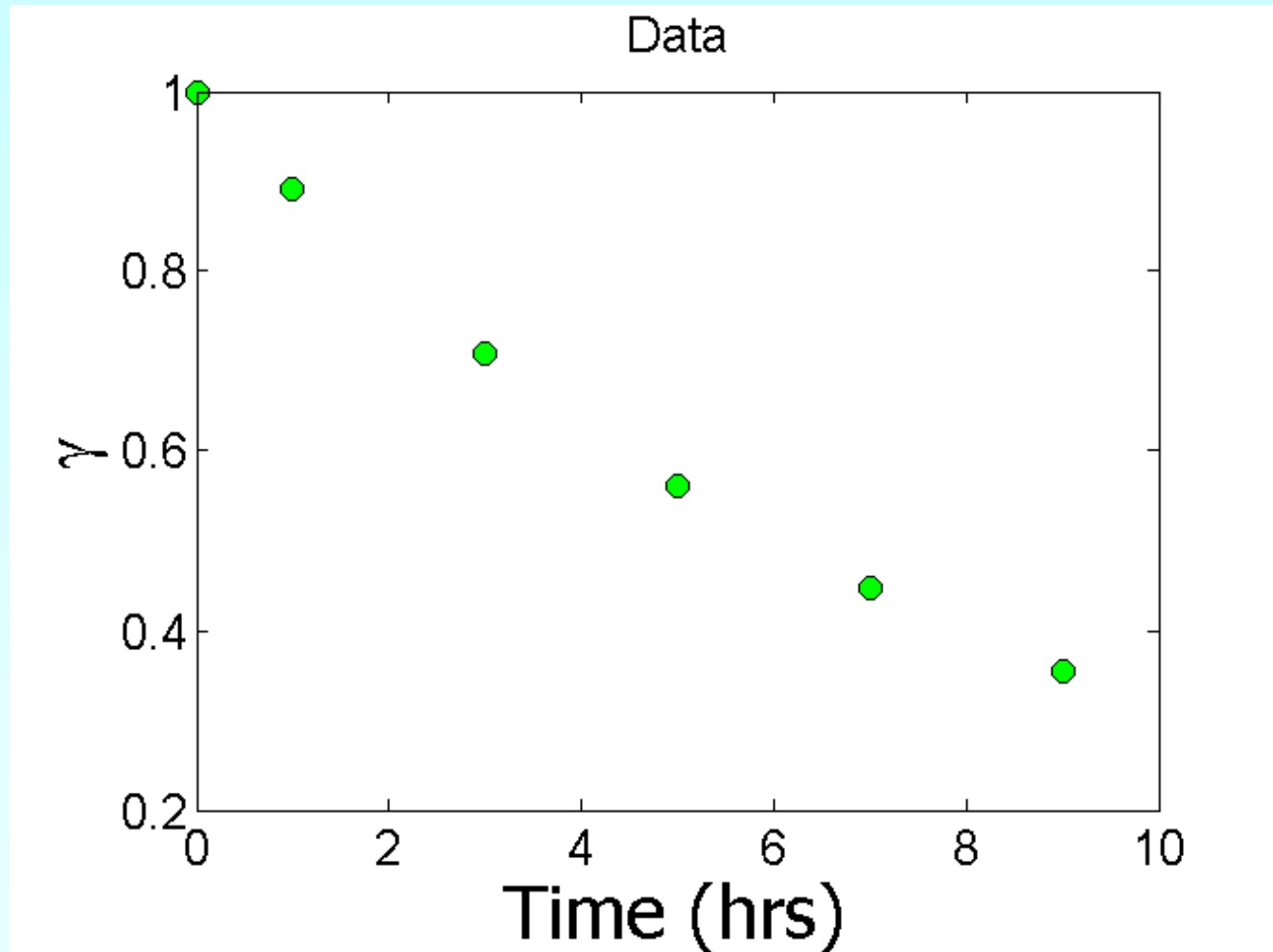| t(hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

Example 1-Exponential Model cont.

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
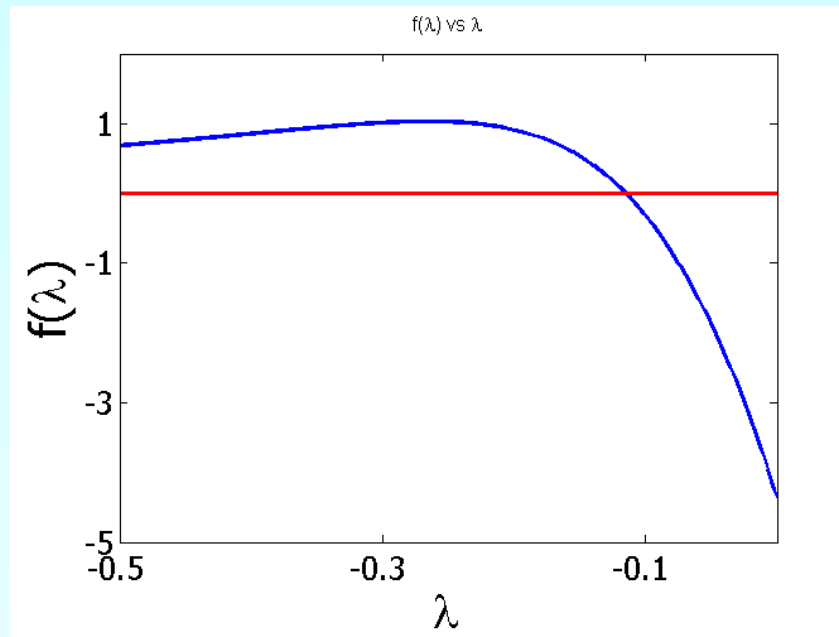
Constants of the Model

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

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

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

f(λ) vs λ

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

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0 \qquad \lambda = -0.1151$$

```
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;
```

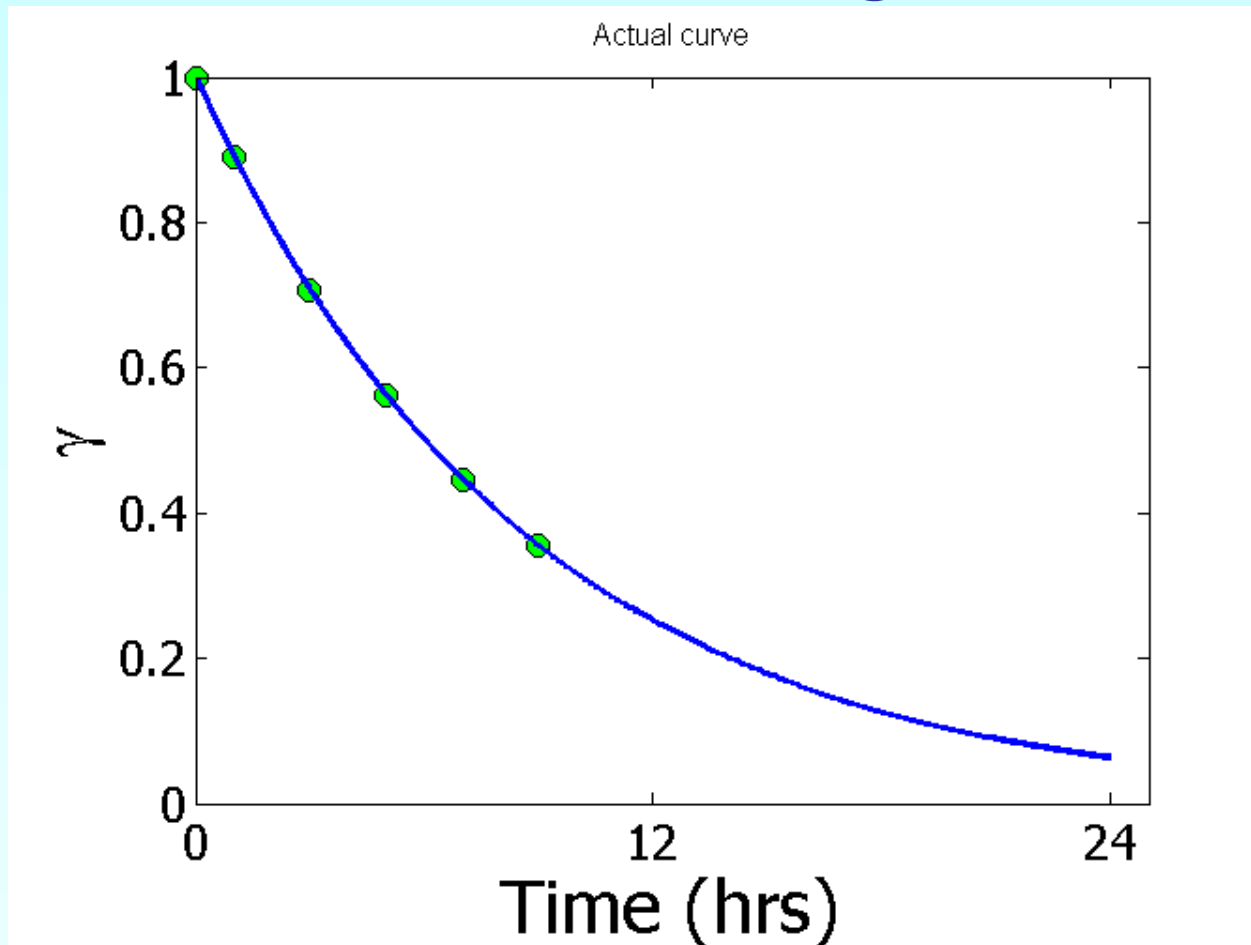# Calculating the Other Constant

The value of A can now be calculated

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

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

radioactive intensity is left after 24 hours.

Homework

1. What is the half-life of technetium 99m isotope?

2. Compare the constants of this regression model with the one where the data is transformed.

3. Write a program in the language of your choice to find the constants of the model.

THE END

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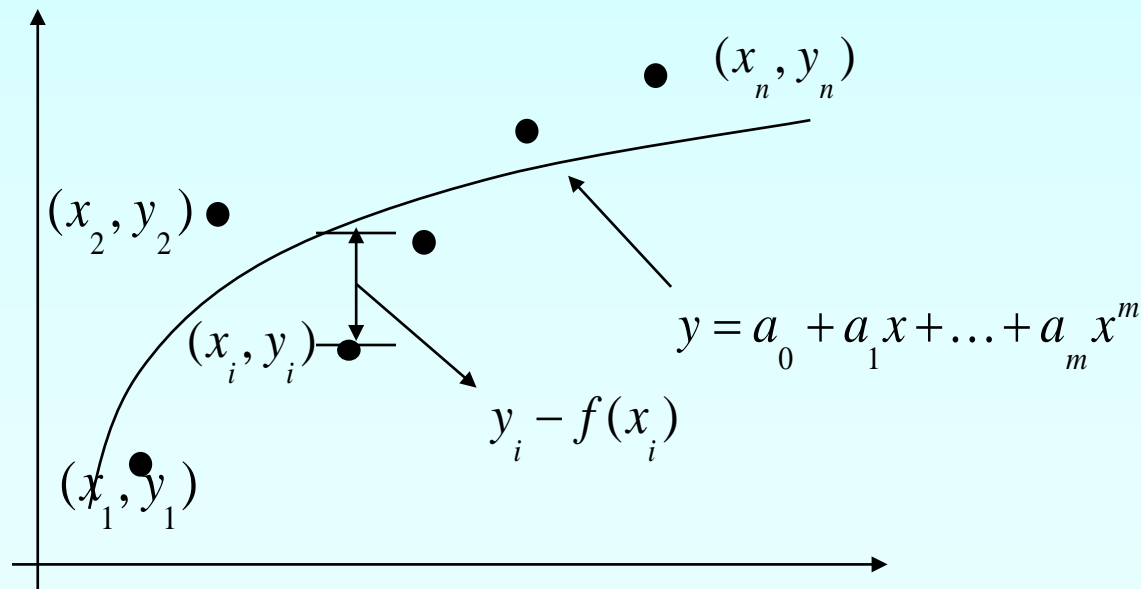
Figure. Polynomial model for nonlinear regression of y vs. x data

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.

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

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

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

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

Polynomial Model cont.

These equations in matrix form are given by

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

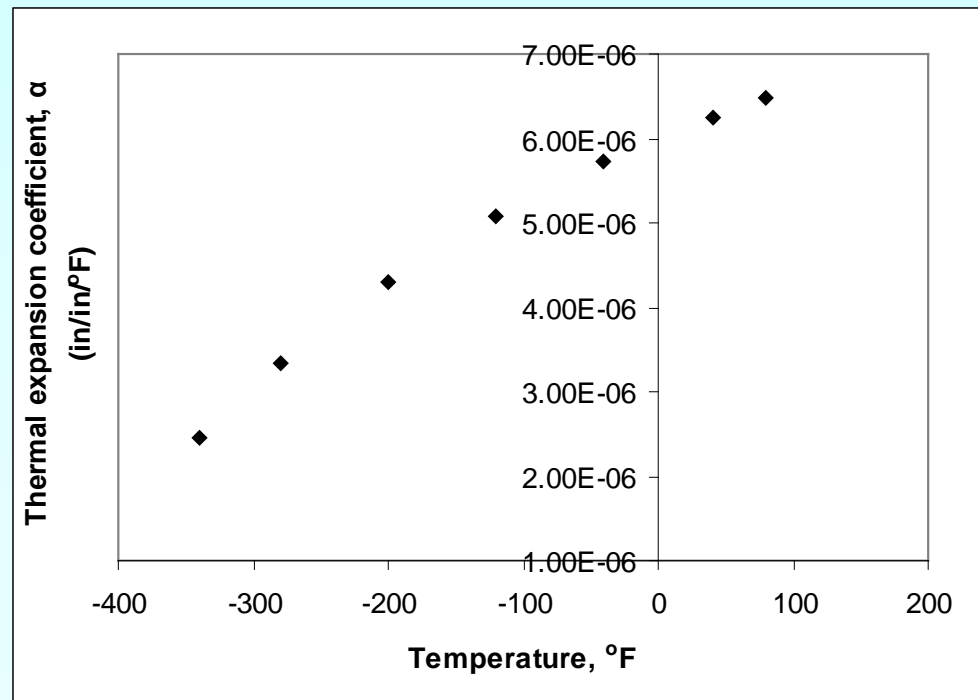The above equations are then solved for $a_0, a_1, \ldots, a_m$

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. α

Temperature, T (ºF)	Coefficient of thermal expansion, α (in/in/ºF)
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}

$$\sum_{i=1}^{7} T_i^2 = 2.5580 \times 10^5$$

$$\sum_{i=1}^{7} T_i^3 = -7.0472 \times 10^7$$

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

$$\sum_{i=1}^{7} \alpha_i = 3.3600 \times 10^{-5}$$

$$\sum_{i=1}^{7} T_i \alpha_i = -2.6978 \times 10^{-3}$$

$$\sum_{i=1}^{7} T_i^2 \alpha_i = 8.5013 \times 10^{-1}$$

Example 2-Polynomial Model cont.

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

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

Solving the above system of simultaneous linear equations we have

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 6.0217 \times 10^{-6} \\ 6.2782 \times 10^{-9} \\ -1.2218 \times 10^{-11} \end{bmatrix}$$

The polynomial regression model is then

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

$$= 6.0217 \times 10^{-6} + 6.2782 \times 10^{-9}\, \text{T} - 1.2218 \times 10^{-11}\, \text{T}^2$$

Linearization 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 linearized. For example, the data for an exponential model can be linearized.

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,

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

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

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
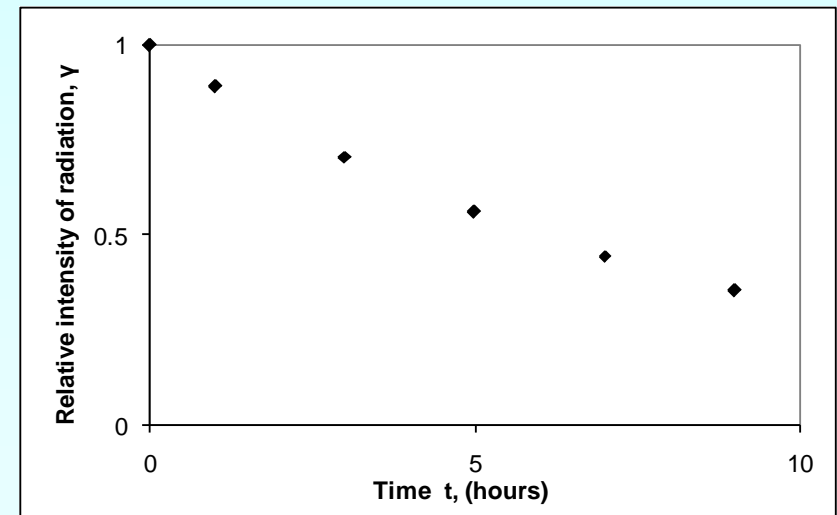
Figure. Data points of relative radiation intensity vs. time

Example 3-Linearization of data cont.

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

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

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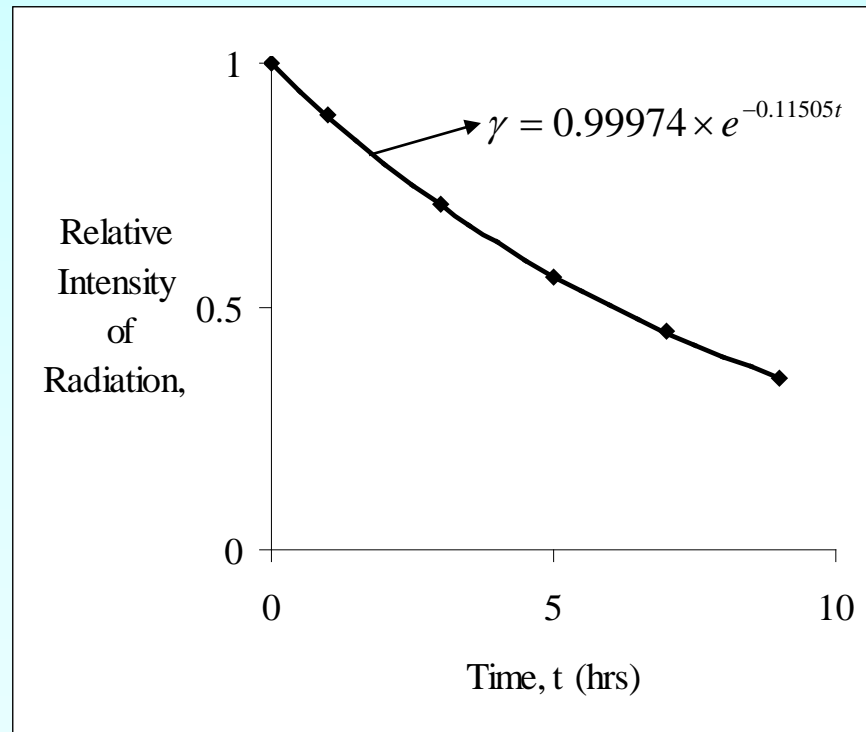
Since

$$a_0 = \ln(A)$$

$$A = e^{a_0}$$

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

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 $\gamma = \dfrac{1}{2}\gamma \Big|_{t=0}$

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

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

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

$$t = 6.0248 \; hours$$

Example 3-Linearization of Data cont.

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

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

This implies that only $\dfrac{6.3200 \times 10^{-2}}{0.99983} \times 100 = 6.3216\%$ 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.

Additional Resources

For all resources on this topic such as digital audiovisual lectures, primers, textbook chapters, multiple-choice tests, worksheets in MATLAB, MATHEMATICA, MathCad and MAPLE, blogs, related physical problems, please visit

http://numericalmethods.eng.usf.edu/topics/nonlinear_regression.html

THE END