Nonlinear Regression

Chemical Engineering Majors

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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: $(y = a_0 + a_1 x + ... + a_m x^m)$

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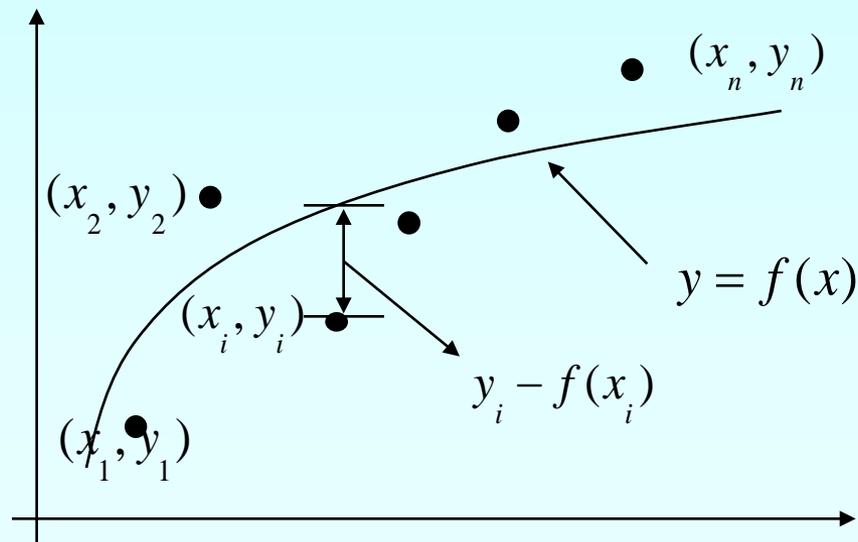
Figure. Nonlinear regression model for discrete y vs. x data

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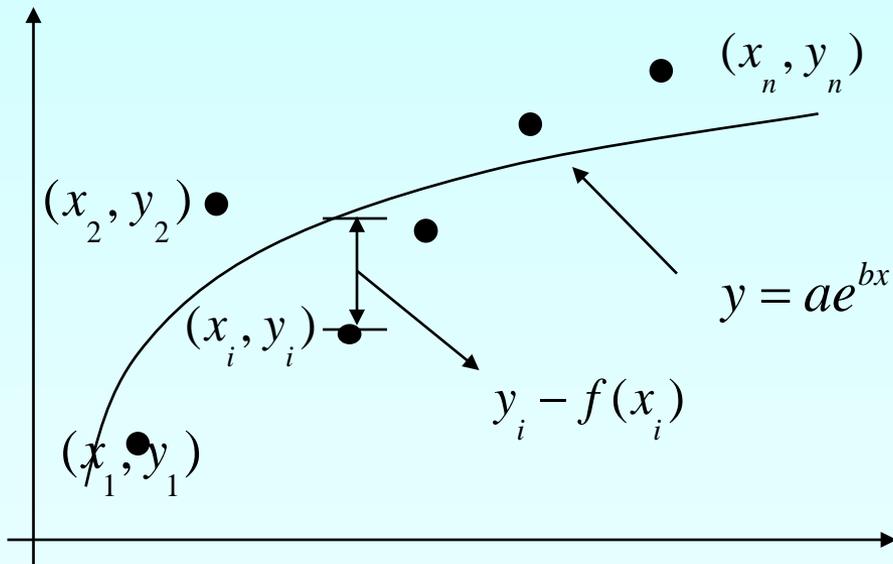
Figure. Exponential model of nonlinear regression for y vs. x data

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*

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

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

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

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

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
	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
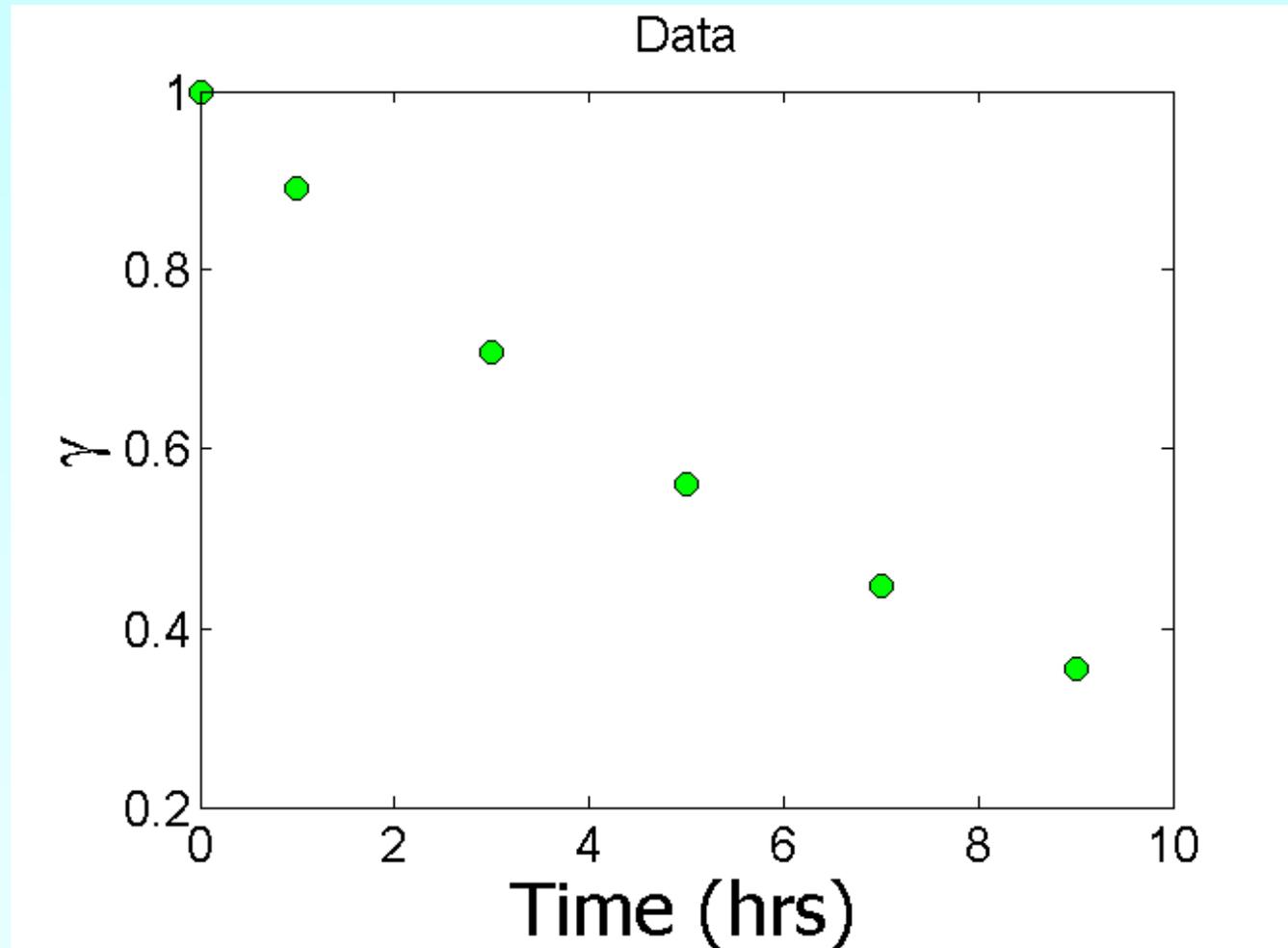
Constants of the Model

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

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

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$
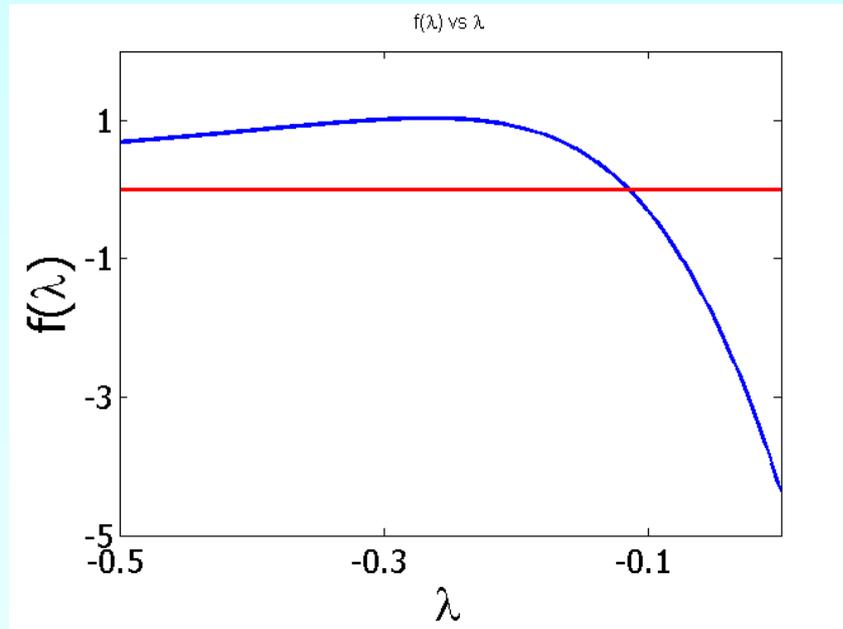
t (hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

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

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

The exponential regression model then is

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

Plot of data and regression curve
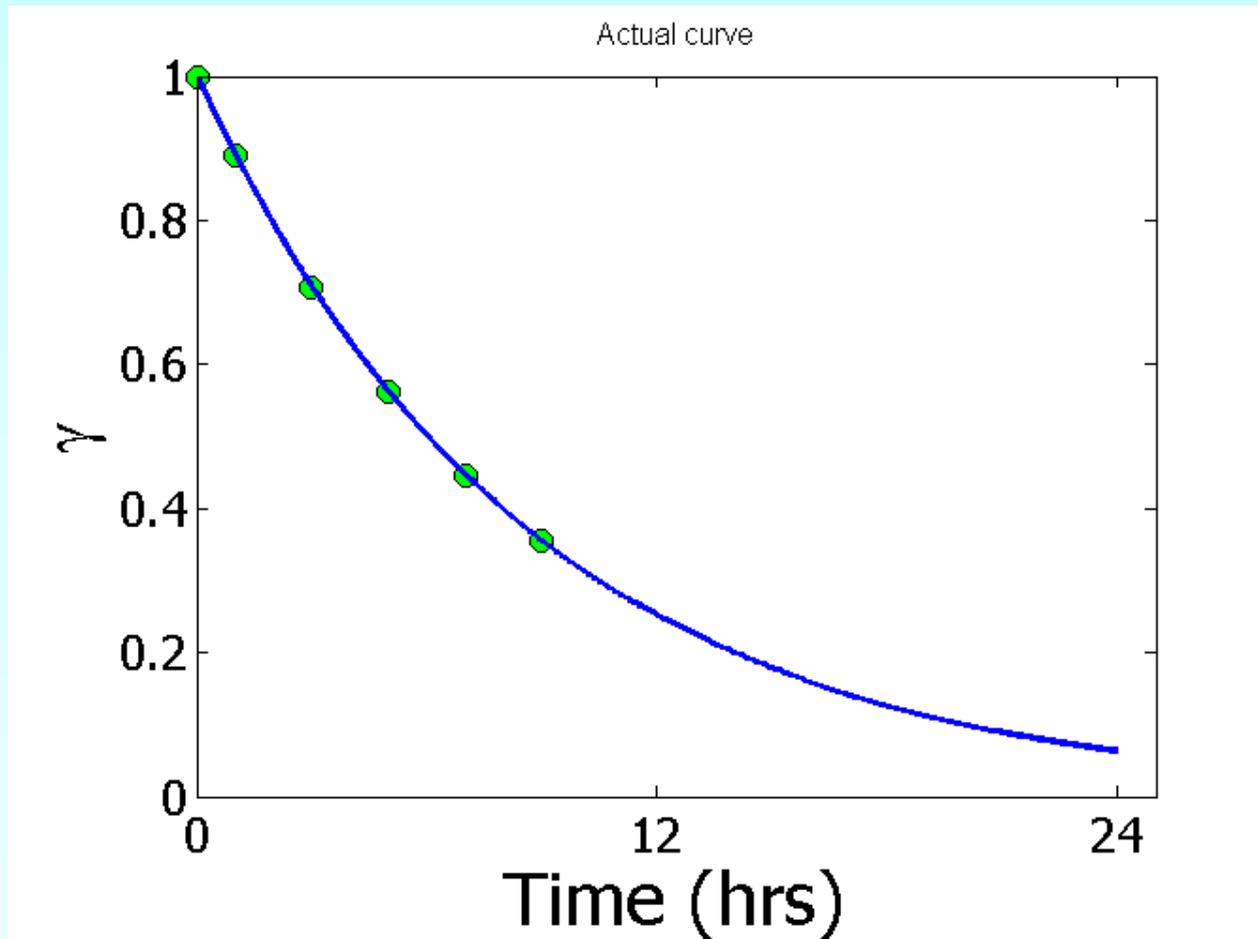
Relative Intensity After 24 hrs

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

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

$(m \leq n - 2)$ to a given data set.

$$y = a_0 + a_1 x + \ldots + a_m x^m$$
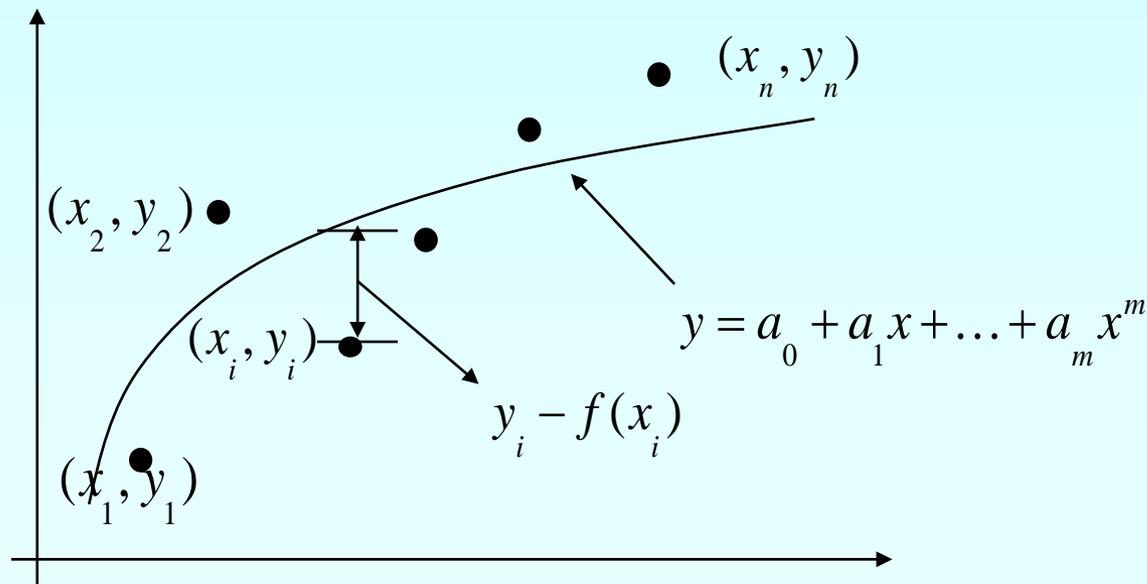
Figure. Polynomial model for nonlinear regression of y vs. x data

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.

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

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

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

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

Polynomial Model cont.

These equations in matrix form are given by

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

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

Example 2-Polynomial Model

Below is given the FT-IR (Fourier Transform Infra Red) data of a 1:1 (by weight) mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC). Absorbance P is given as a function of wavenumber m.

Table. Absorbance vs Wavenumber data

Wavenumber, m (cm^{-1})	Absorbance, P (arbitrary unit)
804.184	0.1591
827.326	0.0439
846.611	0.0050
869.753	0.0073
889.038	0.0448
892.895	0.0649
900.609	0.1204
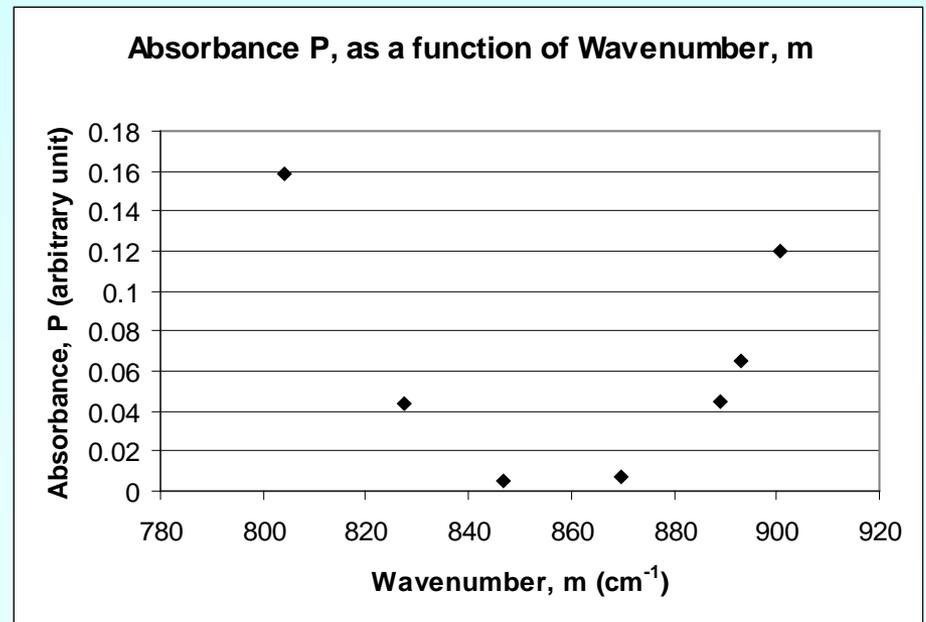
Figure. Absorbance vs. Wavenumber data

Example 2-Polynomial Model cont.

Regress the data to a second order polynomial where $P = a_0 + a_1 m + a_2 m^2$

and find the absorbance at $m = 1000 \text{cm}^{-1}$

The coefficients a_0, a_1, a_2 are found as follows

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

Example 2-Polynomial Model cont.

The necessary summations are as follows

Table. Necessary summations for calculation of polynomial model constants

i	Wavenumber, m (cm^{-1})	Absorbance, P (arbitrary unit)	m^2	m^3
1	804.18	0.1591	6.4671 10^5	5.2008 10^8
2	827.33	0.0439	6.8447 10^5	5.6628 10^8
3	846.61	0.0050	7.1675 10^5	6.0681 10^8
4	869.75	0.0073	7.5647 10^5	6.5794 10^8
5	889.04	0.0448	7.9039 10^5	7.0269 10^8
6	892.90	0.0649	7.9726 10^5	7.1187 10^8
7	900.61	0.1204	8.1110 10^5	7.3048 10^8
$\sum_{i=1}^{7}$	6030.4	0.4454	5.2031 10^6	4.4961 10^9

Example 2-Polynomial Model cont.

Necessary summations continued:

Table. Necessary summations for calculation of polynomial model constants.

i	m^4	$m \quad P$	$m^2 \quad P$
1	$4.1824 \quad 10^{11}$	127.95	$1.0289 \quad 10^5$
2	$4.6849 \quad 10^{11}$	36.319	$3.0048 \quad 10^4$
3	$5.1373 \quad 10^{11}$	4.233	$3.583 \quad 10^3$
4	$5.7225 \quad 10^{11}$	6.349	$5.522 \quad 10^3$
5	$6.2471 \quad 10^{11}$	39.828	$3.5409 \quad 10^4$
6	$6.3563 \quad 10^{11}$	57.948	$5.1742 \quad 10^4$
7	$6.5787 \quad 10^{11}$	108.43	$9.7655 \quad 10^4$
$\sum_{i=1}^{7}$	$3.8909 \quad 10^{12}$	381.06	$3.2685 \quad 10^5$

Example 2-Polynomial Model cont.

Using these summations we have

$$\begin{bmatrix} 7.0000 & 6.0304 \times 10^3 & 5.2031 \times 10^6 \\ 6.0304 \times 10^3 & 5.2031 \times 10^6 & 4.4961 \times 10^9 \\ 5.2031 \times 10^6 & 4.4961 \times 10^9 & 3.8909 \times 10^{12} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0.4454 \\ 381.06 \\ 3.2685 \times 10^5 \end{bmatrix}$$

Solving this system of equations we find

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} -8.6623 \\ 2.0798 \times 10^{-2} \\ -1.2365 \times 10^{-5} \end{bmatrix}$$

The regression model is then

$$P = a_0 + a_1 m + a_2 m^2$$
$$= -8.6623 + 2.0798 \times 10^{-2} m - 1.2365 \times 10^{-5} m^2$$

Example 2-Polynomial Model cont.

With the model is given by

$$P = -8.6623 + 2.0798 \times 10^{-2} m - 1.2365 \times 10^{-5} m^2$$
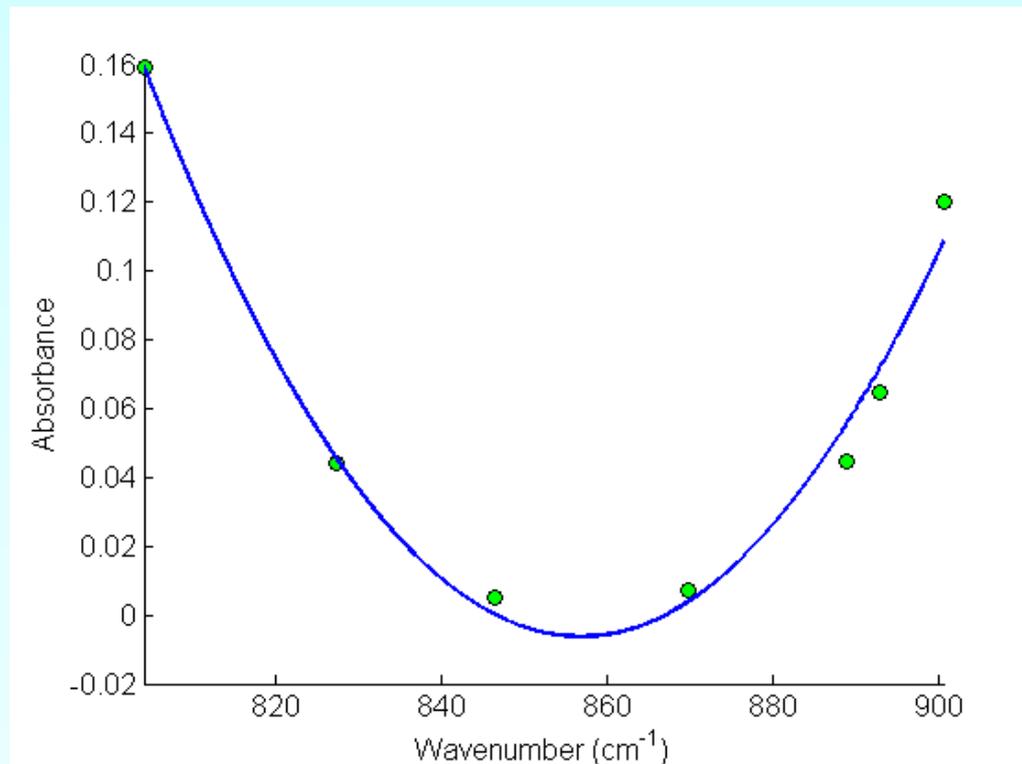
Figure. Polynomial model of Absorbance vs. Wavenumber.

Example 2-Polynomial Model cont.

To find P where $\mathrm{m} = 1000\mathrm{cm}^{-1}$ we have

$$P = a_0 + a_1 m + a_2 m^2$$
$$= -8.6623 + 2.0798 \times 10^{-2} m - 1.2365 \times 10^{-5} m^2$$
$$= -8.6623 + 2.0798 \times 10^{-2} (1000) - 1.2365 \times 10^{-5} (1000)^2$$
$$= -0.22970$$

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
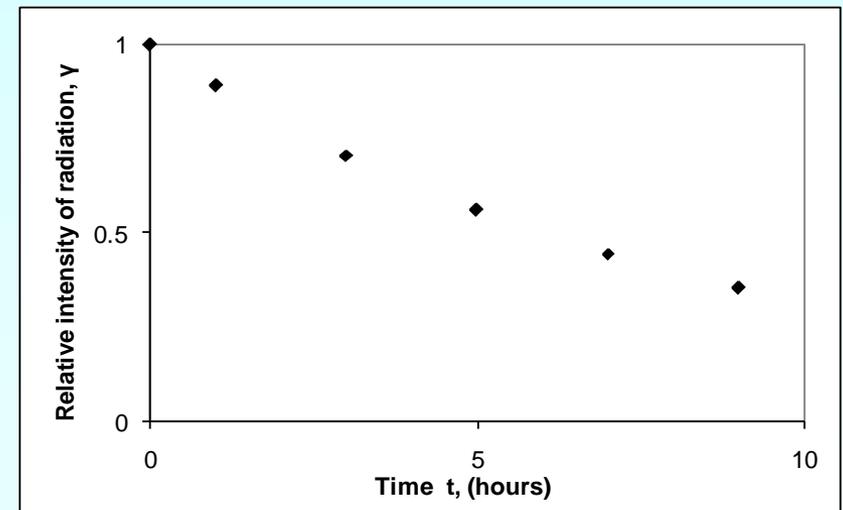
Figure. Data points of relative radiation intensity vs. time

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

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

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 $\gamma = 0.99974 \times e^{-0.11505t}$
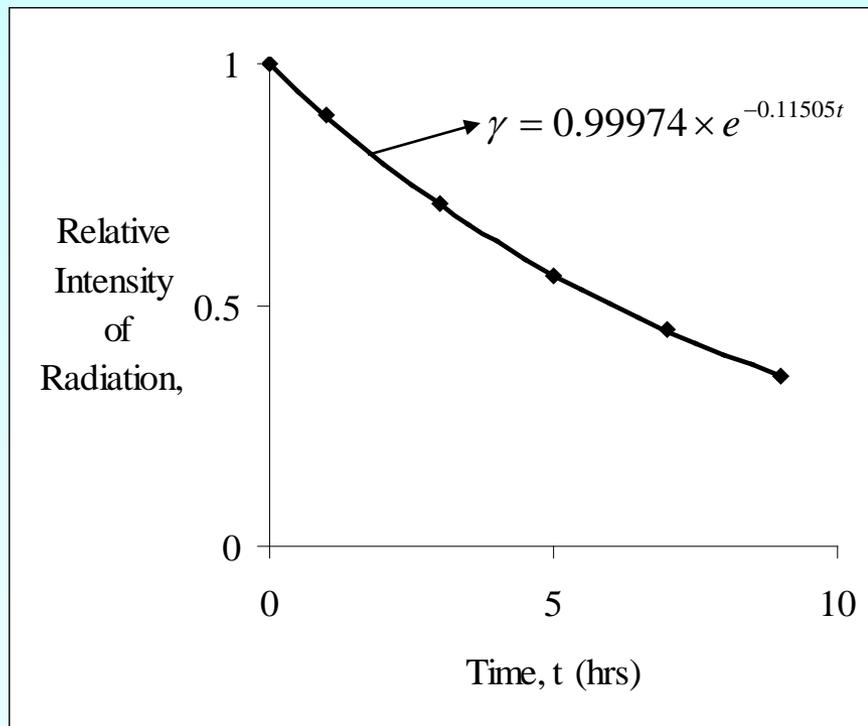
Figure. Relative intensity of radiation as a function of temperature using linearization of data model.

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

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

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

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

$$t = 6.0248 \ hours$$

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