

## 6.04: Nonlinear Regression

### Lesson 1: Introduction to Nonlinear Regression

#### Learning Objectives

After successful completion of this lesson, you should be able to:

- 1) identify different nonlinear regression models,
- 2) recall the formula for the sum of the squares of the residuals for a general regression model.

#### Introduction

Many physical phenomena have a nonlinear relationship between variables. For example, unlike the linear spring you see in a weighing machine at your local grocery store in the produce section, a spring in the car's suspension system follows a nonlinear relationship between force and its displacement. However, the fundamentals of finding the constants of nonlinear regression models are similar to what we use for linear regression models.

The problem statement for a nonlinear regression model is still the same, that is, given  $n$  data pairs  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = f(x)$  to the data.

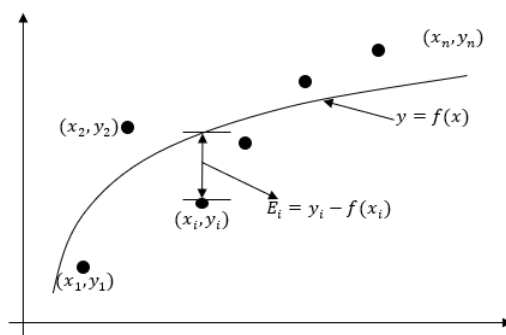


Figure 6.4.1.1. Nonlinear regression model for discrete  $y$  vs.  $x$  data.

The residual at each data point  $x_i$  is found

$$E_i = y_i - f(x_i) \quad (6.4.1.1)$$

to get the sum of the square of the residuals as

$$\begin{aligned} S_r &= \sum_{i=1}^n E_i^2 \\ &= \sum_{i=1}^n (y_i - f(x_i))^2 \end{aligned} \quad (6.4.1.2)$$

Now, one minimizes the square of the residuals  $S_r$  with respect to the constants of the regression model  $y = f(x)$ .

Common nonlinear models in science and engineering include the following.

#### Exponential model

Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = ae^{bx}$  to the data. In this model, the constants of the regression model are  $a$  and  $b$ . An example of the model is the case of a radioactive dye such as Technetium-99 given to patients who are going through a CT scan of their body to diagnose an illness such as excess fat on a liver. The radiation intensity of the radioactive dye decreases with time and is governed by an exponentially decaying model (Figure 6.4.1.2). The interest in such a model would be to find out how long substantial radiation stays in the body.

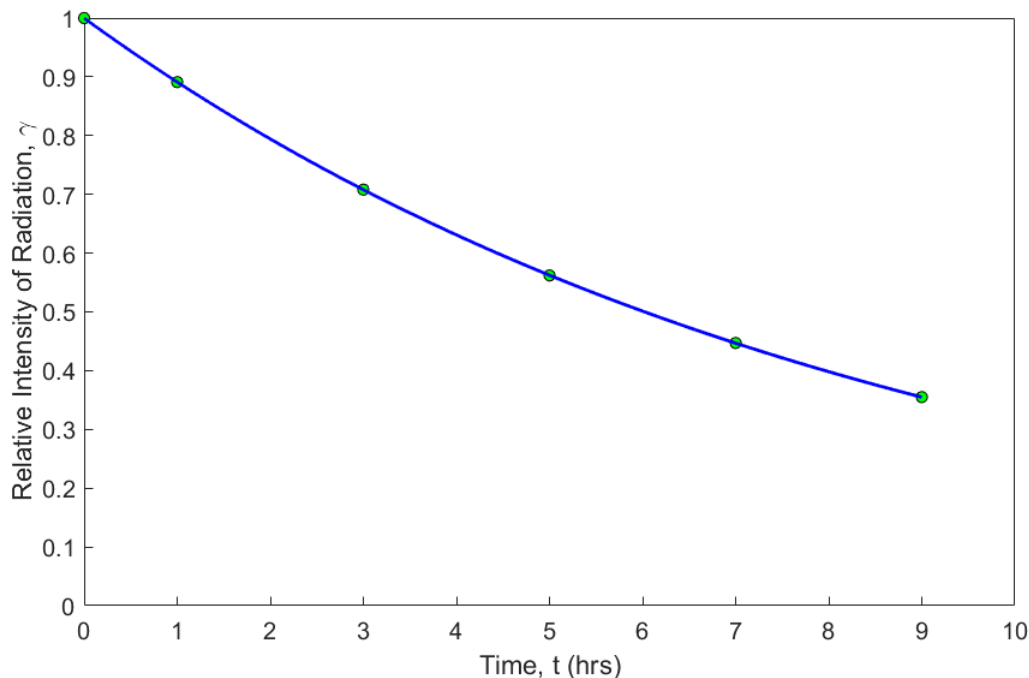


Figure 6.4.1.2. Relative intensity of radiation as a function of time using an exponential regression model.

#### Power model

Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = ax^b$  to the data. In this model, the constants of the regression model are  $a$  and  $b$ . An example of the model is a falling parachutist, where the drag force on the parachute is related through the power of the velocity with which they are falling. An interest in such a model would arise from designing the parachute such that the drag is low enough to maintain control of fall but high enough for the fall to be safe.

#### Saturation growth model

Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = \frac{ax}{b+x}$  to the data. In this model, the constants of the regression model are  $a$  and  $b$ . An example of the model is the case of how good animation looks. How good an animation looks is measured by a variable called performance and is a function of the frame rate. Frame rate is the frequency at which consecutive frames (images) appear on display. The higher the frame rate, the more natural animation looks to the human eye, but the human eye cannot distinguish the increased performance after a certain frame rate. This model is an example of a saturation growth model where at zero frame rate, the performance is zero as one is looking at a static image, and at high frame rates, the performance level saturates.

#### Harmonic decline model

Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = \frac{b}{1+ax}$  to the data. In this model, the constants of the regression model are  $a$  and  $b$ . An example of the model is how much oil would be produced from a well as a function of time. An interest in such a model would arise to estimate the life of the oil well to find out when it should be abandoned.

In all the above examples, one would find the sum of the square of the residuals and minimize it with respect to the constants of the model.

For example, take the case of the exponential model. Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = ae^{bx}$  to the data. The variables  $a$  and  $b$  are the constants of the exponential model. The residual at each data point  $x_i$  is

$$E_i = y_i - ae^{bx_i} \quad (6.4.1.3)$$

The sum of the square of the residuals is

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

$$= \sum_{i=1}^n (y_i - ae^{bx_i})^2 \quad (6.4.1.4)$$

All one must do is to minimize the sum of the square of the residuals with respect to  $a$  and  $b$ . The challenge lies as the resulting equations, unlike in linear regression, turn out to be simultaneous nonlinear equations. We cover this issue in the upcoming lessons.

### Audiovisual Lecture

**Title:** Nonlinear Regression - Introduction

**Summary:** This video will get you introduced to nonlinear regression and show you that its fundamentals are not any different than linear regression.



## Lesson 2: Exponential Regression Model with Transformation

### Learning Objectives

After successful completion of this lesson, you should be able to:

- 1) derive constants of nonlinear regression models using transformation of data,
- 2) use the derived formula to find the constants of the nonlinear regression model from given data.

### Derivation of nonlinear regression models

In a previous lesson, we have discussed linear regression models. But when data is following a nonlinear trend, we need to develop nonlinear regression models. A simple example of such models is the drag force on a parachute, which is related to the square of the velocity of the parachutist. Other examples are the decay of radioactivity intensity of nuclear material, which is related exponentially to passage of time, or the height of a human that saturates as the person ages.

The derivation of the nonlinear models follows the same concept of finding the sum of the squares of the residuals and minimizing with respect to the constants of the regression model. For brevity, we limit our discussion to the exponential model in this lesson.

### 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 6.4.2.1).

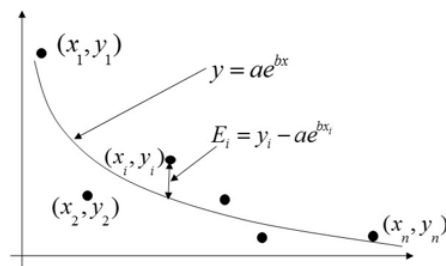


Figure 6.4.2.1. Exponential regression model for  $y$  vs.  $x$  data.

The variables  $a$  and  $b$  are the constants of the exponential model. The residual  $E_i$  at each data point  $x_i$  is

$$E_i = y_i - ae^{bx_i} \quad (6.4.2.1)$$

The sum of the square of the residuals is

$$\begin{aligned} S_r &= \sum_{i=1}^n E_i^2 \\ &= \sum_{i=1}^n (y_i - ae^{bx_i})^2 \end{aligned} \quad (6.4.2.2)$$

To find the constants  $a$  and  $b$  of the exponential model, we minimize  $S_r$  by differentiating with respect to  $a$  and  $b$  and equating the resulting equations to zero

$$\begin{aligned} \frac{\partial S_r}{\partial a} &= \sum_{i=1}^n 2 (y_i - ae^{bx_i}) (-e^{bx_i}) = 0 \\ \frac{\partial S_r}{\partial b} &= \sum_{i=1}^n 2 (y_i - ae^{bx_i}) (-ax_i e^{bx_i}) = 0 \end{aligned} \quad (6.4.2.3a, b)$$

Expanding Equations (6.4.2.3a, b) gives

$$\begin{aligned} -2 \sum_{i=1}^n y_i e^{bx_i} + 2a \sum_{i=1}^n e^{2bx_i} &= 0 \\ -2a \sum_{i=1}^n y_i x_i e^{bx_i} + 2a^2 \sum_{i=1}^n x_i e^{2bx_i} &= 0 \end{aligned} \quad (6.4.2.4a, b)$$

Examining Equations (6.4.4a, b) above shows that we need to solve simultaneous nonlinear equations for the regression constants  $a$  and  $b$  and need numerical methods. Is there an alternative?

It is sometimes possible to use simple linear regression formulas to estimate the parameters of a nonlinear model. This procedure involves first transforming the given data, followed by using formulas derived for linear regression. Data for several nonlinear models such as exponential, power, and growth can be transformed, but not so for all nonlinear models.

### Exponential Model through Transformation of Data

Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = ae^{bx}$  to the data by using the transformation of data. The variables  $a$  and  $b$  are the constants of the exponential model

$$y = ae^{bx} \quad (6.4.2.5)$$

Taking the natural log of both sides of Equation (6.4.2.5) gives

$$\ln y = \ln a + bx \quad (6.4.2.6)$$

Let

$$z = \ln y$$

$$a_0 = \ln a \text{ implying } a = e^{a_0}$$

$$a_1 = b \quad (6.4.2.7)$$

then

$$z = a_0 + a_1 x \quad (6.4.2.8)$$

For the transformed data of  $z$  versus  $x$ , we can use the linear regression formulas. Hence, the constants  $a_0$  and  $a_1$  can be found as

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

$$a_0 = \bar{z} - a_1 \bar{x} \quad (6.4.2.9a, b)$$

When the constants  $a_0$  and  $a_1$  are found, the original constants of the exponential model are found as given in Equation (6.4.2.7)

$$b = a_1$$

$$a = e^{a_0}$$

#### ✓ Example 6.4.2.1

Many patients get concerned when a medical test involves an injection of radioactive material. For example, to scan a gallbladder, a few drops of Technetium-99m isotope are used. Half of the Technetium-99m would be gone in about 6 hours. However, it 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 6.4.2.1. Relative intensity of radiation as a function of time.

$t(\text{hrs})$	0	1	3	5	7	9
$\gamma$	1.000	0.891	0.708	0.562	0.447	0.355

If the level of the relative intensity of radiation is related to time via an exponential formula  $\gamma = Ae^{\lambda t}$ , using the transformation of data, find

- the value of the regression constants  $A$  and  $\lambda$ ,
- the half-life of Technium-99m, and
- the radiation intensity after 24 hours.

#### Solution

a)

$$\gamma = Ae^{\lambda t} \quad (6.4.2.E1.1)$$

Taking the natural logarithm on both sides,

$$\ln(\gamma) = \ln(A) + \lambda t \quad (6.4.2.E1.2)$$

Assuming

$$y = \ln \gamma$$

$$a_0 = \ln(A) \quad (6.4.2.E1.3)$$

$$a_1 = \lambda \quad (6.4.2.E1.4)$$

we get

$$y = a_0 + a_1 t$$

This is a linear relationship between  $y$  and  $t$ . Then

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

$$a_0 = \bar{y} - a_1 \bar{t} \quad (6.4.2.E1.5a, b)$$

Table 6.4.2.2 shows the summations one would need for calculating  $a_0$  and  $a_1$ .

Table 6.4.2.2. Summations of data to calculate constants of the model.

$i$	$t_i$	$y_i$	$y_i = \ln y_i$	$t_i y_i$	$t_i^2$
1	0	1	0.00000	0.0000	0.0000
2	1	0.891	-0.11541	<b>-0.11541</b>	1.0000
3	3	0.708	-0.34531	-1.0359	9.0000
4	5	0.562	-0.57625	-2.8813	25.0000
5	7	0.447	-0.80520	-5.6364	49.0000
6	9	0.355	-1.0356	-9.3207	81.0000
$\sum_{i=1}^6$	25.0000		-2.8778	-18.990	165.00

$$n = 6$$

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

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

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

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

From Equation (6.4.2.E1.5a, b) we have

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

$$= -0.11505$$

$$a_0 = \frac{-2.8778}{6} - (-0.11505) \frac{25}{6}$$

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

Since

$$a_0 = \ln(A)$$

$$A = e^{a_0}$$

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

$$= 0.99974$$

$$\lambda = a_1 = -0.11505$$

The regression formula then is

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

b) Half-life is when

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

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

$$e^{-0.11505t} = 0.5$$

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

$$t = 6.0248 \text{ hours}$$

c) The relative intensity of radiation after 24 hours is

$$\begin{aligned} \gamma &= 0.99974 e^{-0.11505(24)} \\ &= 0.063200 \end{aligned}$$

This value of relative intensity implies that only

$$\frac{6.3200 \times 10^{-2}}{0.99974} \times 100 = 6.3216\%$$

of the initial radioactivity is left after 24 hours.

### Audiovisual Lecture

**Title:** Nonlinear Regression - Exponential Model

**Summary:** This video will teach you how to find the constants of an exponential regression model by transforming the data.



## Lesson 3: Nonlinear Regression Model Without Transformation

### Learning Objectives

After successful completion of this lesson, you should be able to:

- 1) derive constants of a nonlinear exponential regression model,
- 2) use the derived formula to find the constants of the exponential regression model from given data.

## Nonlinear models using least squares

The development of the least-squares estimation for nonlinear models does not generally yield linear equations and hence is not easy to solve. Solving for the constants of the nonlinear models mostly results in simultaneous nonlinear equations. We illustrate this challenge through an exponential model.

### Exponential model

Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , best fit  $y = ae^{bx}$  to the data. The variables  $a$  and  $b$  are the constants of the exponential model. The residual at each data point  $x_i$ , is

$$E_i = y_i - ae^{bx_i} \quad (6.4.3.1)$$

The sum of the square of the residuals is

$$\begin{aligned} S_r &= \sum_{i=1}^n E_i^2 \\ &= \sum_{i=1}^n (y_i - ae^{bx_i})^2 \end{aligned} \quad (6.4.3.2)$$

To find the constants  $a$  and  $b$  of the exponential model, we minimize  $S_r$  by differentiating  $S_r$  with respect to  $a$  and  $b$  and equating the resulting equations to zero

$$\begin{aligned} \frac{\partial S_r}{\partial a} &= \sum_{i=1}^n 2 (y_i - ae^{bx_i}) (-e^{bx_i}) = 0 \\ \frac{\partial S_r}{\partial b} &= \sum_{i=1}^n 2 (y_i - ae^{bx_i}) (-ax_i e^{bx_i}) = 0 \end{aligned} \quad (6.4.3.3a, b)$$

Expanding Equation (6.4.3.3a, b) gives

$$\begin{aligned} -2 \sum_{i=1}^n y_i e^{bx_i} + 2a \sum_{i=1}^n e^{2bx_i} &= 0 \\ -2a \sum_{i=1}^n y_i x_i e^{bx_i} + 2a^2 \sum_{i=1}^n x_i e^{2bx_i} &= 0 \end{aligned} \quad (6.4.3.4a, b)$$

Simplifying Equation (6.4.3.4a, b) gives

$$\begin{aligned} - \sum_{i=1}^n y_i e^{bx_i} + a \sum_{i=1}^n e^{2bx_i} &= 0 \\ - \sum_{i=1}^n y_i x_i e^{bx_i} + a \sum_{i=1}^n x_i e^{2bx_i} &= 0 \end{aligned} \quad (6.4.3.5a, b)$$

Equations (6.4.3.5a) and (6.4.3.5b) are nonlinear in  $a$  and  $b$  and thus not in a closed-form to be solved as was the case for linear regression. In general, iterative methods (such as Gauss-Newton iteration method, method of steepest descent, Marquardt's method, direct search, etc) must be used to find values of  $a$  and  $b$ .

However, in this case, from Equation (6.4.3.5a)  $a$  can be written explicitly in terms of  $b$  as

$$a = \frac{\sum_{i=1}^n y_i e^{bx_i}}{\sum_{i=1}^n e^{2bx_i}} \quad (6.4.3.6)$$

Substituting Equation (6.4.3.6) in (6.4.3.5b) gives



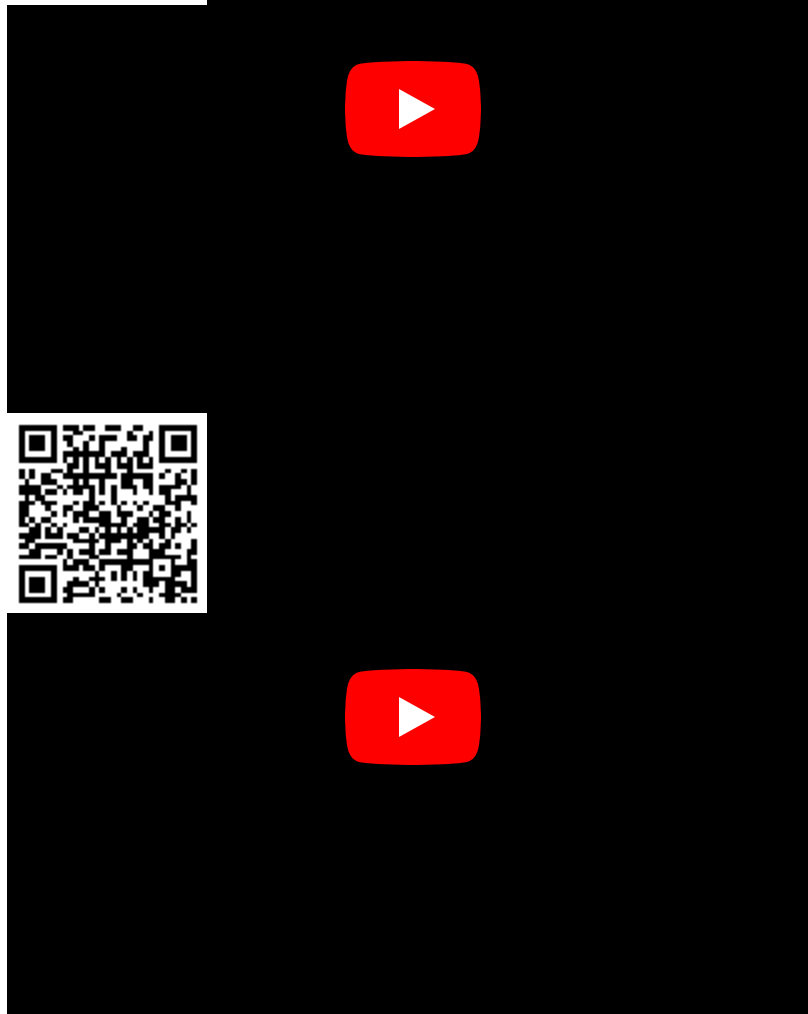
$$\sum_{i=1}^n y_i x_i e^{bx_i} - \frac{\sum_{i=1}^n y_i e^{bx_i}}{\sum_{i=1}^n e^{2bx_i}} \sum_{i=1}^n x_i e^{2bx_i} = 0 \quad (6.4.3.7)$$

This equation is still nonlinear in  $b$  and can be solved best by numerical methods such as the bisection method or the secant method.

#### Audiovisual Lecture

**Title:** Exponential Model Regression - Derivation

**Summary:** This video discusses how to derive the formula for the constants of an exponential regression model.



### ✓ Example 6.4.3.1

Many patients get concerned when a test involves an injection of radioactive material. For example, to scan a gallbladder, a few drops of Technetium-99m isotope are 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 6.4.3.1. Relative intensity of radiation as a function of time.

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

If the level of the relative intensity of radiation is related to time via an exponential formula  $\gamma = Ae^{\lambda t}$ , find

- the value of the regression constants  $A$  and  $\lambda$ ,
- the half-life of Technetium-99m, and
- the radiation intensity after 24 hours.

### Solution

a) The value of  $\lambda$  is given by solving the nonlinear Equation (6.4.3.7),

$$f(\lambda) = \sum_{i=1}^n \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^n \gamma_i e^{\lambda t_i}}{\sum_{i=1}^n e^{2\lambda t_i}} \sum_{i=1}^n t_i e^{2\lambda t_i} = 0 \quad (6.4.3.E1.1)$$

Then the value of  $A$  from Equation (6.4.3.6) takes the form,

$$A = \frac{\sum_{i=1}^n \gamma_i e^{\lambda t_i}}{\sum_{i=1}^n e^{2\lambda t_i}} \quad (6.4.3.E1.2)$$

Equation (6.4.3.E1.1) can be solved for  $\lambda$  using the bisection method. To estimate the initial guesses, we assume  $\lambda = -0.120$  and  $\lambda = -0.110$ . We need to check whether these values first bracket the root of  $f(\lambda) = 0$ . At  $\lambda = -0.120$ , the table below shows the evaluation of  $f(-0.120)$ .

Table 6.4.3.2. Summation value for calculation of constants of the model.

$i$	$t_i$	$\gamma_i$	$\gamma_i t_i e^{\lambda t_i}$	$\gamma_i e^{\lambda t_i}$	$e^{2\lambda t_i}$	$t_i e^{2\lambda t_i}$
1	0	1	0.00000	1.00000	1.00000	0.00000
2	1	0.891	0.79205	0.79205	0.78663	0.78663
3	3	0.708	1.4819	0.49395	0.48675	1.4603
4	5	0.562	1.5422	0.30843	0.30119	1.5060
5	7	0.447	1.3508	0.19297	0.18637	1.3046
6	9	0.355	1.0850	0.12056	0.11533	1.0379
$\sum_{i=1}^6$			6.2501	2.9062	2.8763	6.0954

From Table 6.4.3.2

$$n = 6$$

$$\sum_{i=1}^6 \gamma_i t_i e^{-0.120 t_i} = 6.2501$$

$$\sum_{i=1}^6 \gamma_i e^{-0.120 t_i} = 2.9062$$

$$\sum_{i=1}^6 e^{2(-0.120) t_i} = 2.8763$$

$$\sum_{i=1}^6 t_i e^{2(-0.120) t_i} = 6.0954$$

$$f(-0.120) = (6.2501) - \frac{2.9062}{2.8763}(6.0954) \\ = 0.091357$$

Similarly

$$f(-0.110) = -0.10099$$

Since

$$f(-0.120) \times f(-0.110) < 0,$$

the value of  $\lambda$  falls in the bracket of  $[-0.120, -0.110]$  The next guess of the root then is

$$\lambda = \frac{-0.120 + (-0.110)}{2} \\ = -0.115$$

Continuing with the bisection method, the root of  $f(\lambda) = 0$  is found as  $\lambda = -0.11508$ . This value of the root was obtained after 20 iterations with an absolute relative approximate error of less than 0.000008%

From Equation (6.4.3.E1.2)  $A$  can be calculated as

$$A = \frac{\sum_{i=1}^6 \gamma_i e^{\lambda t_i}}{\sum_{i=1}^6 e^{2\lambda t_i}} \\ = \frac{1 \times e^{-0.11508(0)} + 0.891 \times e^{-0.11508(1)} + 0.708 \times e^{-0.11508(3)} + 0.562 \times e^{-0.11508(5)} + 0.447 \times e^{-0.11508(7)} + 0.355 \times e^{-0.11508(9)}}{e^{2(-0.11508)(0)} + e^{2(-0.11508)(1)} + e^{2(-0.11508)(3)} + e^{2(-0.11508)(5)} + e^{2(-0.11508)(7)} + e^{2(-0.11508)(9)}} \\ = \frac{2.9373}{2.9378} \\ = 0.99983$$

The regression formula is hence given by

$$\gamma = 0.99983 e^{-0.11508 t}$$

b) Half-life of Technetium-99m is when

$$\gamma = \frac{1}{2} \gamma \Big|_{t=0} \\ 0.99983 \times e^{-0.11508 t} = \frac{1}{2} (0.99983) e^{-0.11508(0)} \\ e^{-0.11508 t} = 0.5$$

$$-0.11508t = \ln(0.5)$$

$$t = 6.0232 \text{ hours}$$

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

$$\begin{aligned}\gamma &= 0.99983 \times e^{-0.11508(24)} \\ &= 6.3160 \times 10^{-2}\end{aligned}$$

This value of relative intensity implies that only

$$\frac{6.3160 \times 10^{-2}}{0.99983} \times 100 = 6.3171\%$$

of the initial radioactivity is left after 24 hours.

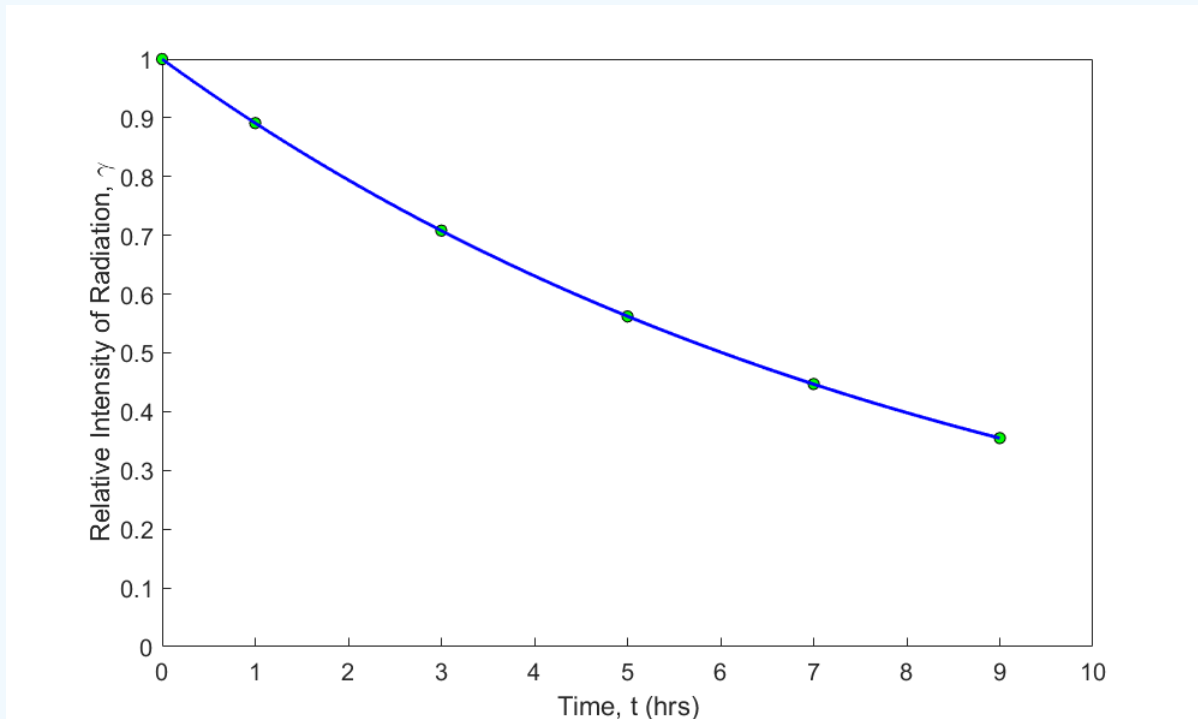


Figure 6.4.1. Relative intensity of radiation as a function of time using an exponential regression model.

How different are the constants of the model when compared to when the data is transformed?

The regression formula obtained without transforming the data is

$$\gamma = 0.99983 e^{-0.11508t}$$

and the regression formula obtained with transforming the data is

$$\gamma = 0.99974 e^{-0.11505t}$$

Such proximity of the constants of the model for this example may lead us to believe that it does not matter much whether we transform the data or not. Far from it, as we will see in the next example.

### Audiovisual Lecture

**Title:** Exponential Model Regression - Example

**Summary:** This video shows an example of how you can regress data to an exponential model.



### ✓ Example 6.4.3.2

Given the data below, regress the data to  $y = e^{bx}$  with and without data transformation.

$x$	$y$
0	1.0000
5	0.8326
10	0.6738
15	0.5837
20	0.5150
25	0.4163
40	0.3219
60	0.2466

$x$	$y$
90	0.1803

## Solution

Regress  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  data to

$$y = e^{bx} \quad (6.4.3.E2.1)$$

regression model.

### Transforming the data

The value of  $b$  can be found by transforming the data by taking the natural log of both sides of the model equation as

$$\ln(y) = \ln(e^{bx}) \quad (6.4.3.E2.2)$$

$$\ln(y) = bx \quad (6.4.3.E2.3)$$

Assuming

$$z = \ln y \quad (6.4.3.E2.4),$$

we get a special linear model (intercept is zero) relating the  $z$  data to  $x$ ,

$$z = bx \quad (6.4.3.E2.5)$$

and this linear model on minimizing the sum of the squares of the residuals gives

$$b = \frac{\sum_{i=1}^n x_i \ln(y_i)}{\sum_{i=1}^n x_i^2} \quad (6.4.3.E2.6)$$

Substituting the values of the data points gives

$$\sum_{i=1}^9 x_i \ln(y_i) = -331.64$$

$$\sum_{i=1}^n x_i^2 = 14675$$

$$b = \frac{-331.64}{14675} = -0.02260$$

The regression model obtained with transforming the data is hence given by

$$y = e^{-0.02260x}$$

### Without transforming the data

Here we need to start from the sum of the square of the residuals of the original model (Equation 6.4.3.E2.1), and minimize the sum with respect to  $b$ . The residual is given by

$$E_i = y_i - ae^{bx_i} \quad (6.4.3.E2.7)$$

The sum of the square of the residuals is

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

$$= \sum_{i=1}^n (y_i - e^{bx_i})^2 \quad (6.4.3.E2.8)$$

To find the constant  $b$  of the exponential model, we minimize  $S_r$  by differentiating with respect to  $b$  and equating the resulting expression to zero

$$\frac{dS_r}{db} = \sum_{i=1}^n 2 (y_i - e^{bx_i}) (-x_i e^{bx_i}) = 0 \quad (6.4.3.E2.9)$$

Expanding and simplifying Equation (6.4.3.E2.9) gives

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

This is a nonlinear equation in terms of  $b$ , and can be solved by numerical methods such as bisection method. The value of  $b$  obtained is

$$b = -0.03071$$

From the above solution, the regression formula obtained without transforming the data is

$$y = e^{-0.03071x}$$

The regression formula obtained with transforming the data is

$$y = e^{-0.02260x}$$

Clearly, the two models are not close, and you can see this in Figure 6.4.3.2 as well.

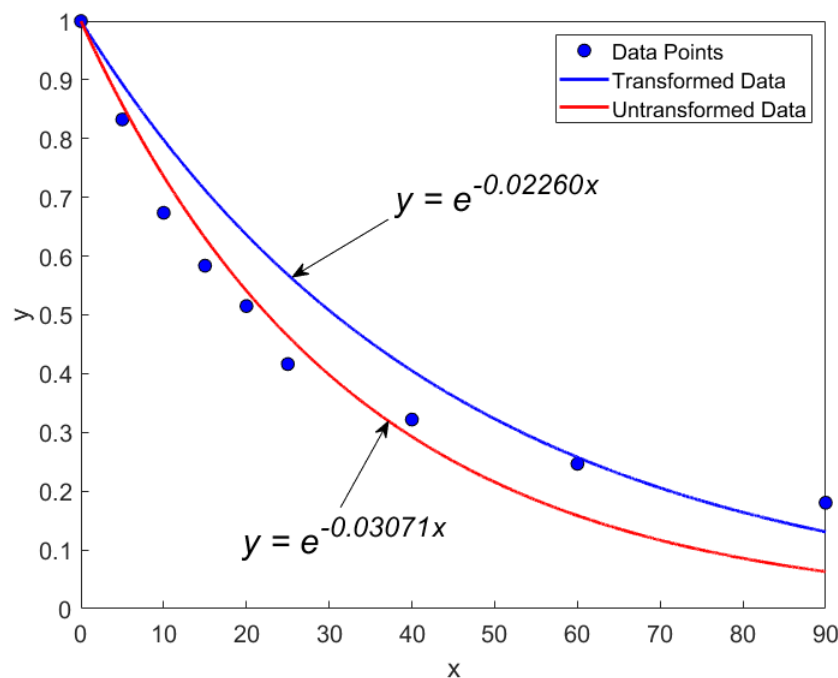


Figure 6.4.3.2. Comparing an exponential regression model with and without data transformation.

## Lesson 4: Polynomial Regression Model

### Learning Objectives

After successful completion of this lesson, you should be able to:

- 1) derive formulas for the regression constants of a polynomial regression model
- 2) apply the polynomial regression model to given data.

### Polynomial Models

Given  $n$  data points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , use the least-squares method to regress the data to an  $m^{th}$  order polynomial.

$$y = a_0 + a_1x + a_2x^2 + \dots + a_mx^m, \quad m < n \quad (6.4.4.1)$$

The residual at each data point is given by

$$E_i = y_i - a_0 - a_1x_i - \dots - a_mx_i^m \quad (6.4.4.2)$$

The sum of the square of the residuals is given by

$$\begin{aligned} S_r &= \sum_{i=1}^n E_i^2 \\ &= \sum_{i=1}^n (y_i - a_0 - a_1x_i - \dots - a_mx_i^m)^2 \end{aligned} \quad (6.4.4.3)$$

To find the constants of the polynomial regression model, we put the derivatives with respect to  $a_i$ ,  $i = 1, 2, \dots, m$  to zero, that is,

$$\begin{aligned} \frac{\partial S_r}{\partial a_0} &= \sum_{i=1}^n 2(y_i - a_0 - a_1x_i - \dots - a_mx_i^m)(-1) = 0 \\ \frac{\partial S_r}{\partial a_1} &= \sum_{i=1}^n 2(y_i - a_0 - a_1x_i - \dots - a_mx_i^m)(-x_i) = 0 \\ &\vdots \\ \frac{\partial S_r}{\partial a_m} &= \sum_{i=1}^n 2(y_i - a_0 - a_1x_i - \dots - a_mx_i^m)(-x_i^m) = 0 \end{aligned}$$

Setting these equations in matrix form gives

$$\begin{bmatrix} n & \left(\sum_{i=1}^n x_i\right) & \dots & \left(\sum_{i=1}^n x_i^m\right) \\ \left(\sum_{i=1}^n x_i\right) & \left(\sum_{i=1}^n x_i^2\right) & \dots & \left(\sum_{i=1}^n x_i^{m+1}\right) \\ \dots & \dots & \dots & \dots \\ \left(\sum_{i=1}^n x_i^m\right) & \left(\sum_{i=1}^n x_i^{m+1}\right) & \dots & \left(\sum_{i=1}^n x_i^{2m}\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \dots \\ a_m \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \\ \dots \\ \sum_{i=1}^n x_i^m y_i \end{bmatrix} \quad (6.4.4.4)$$

The above equations are solved for  $a_0, a_1, \dots, a_m$ .

### Audiovisual Lecture

**Title:** Polynomial Regression Model: Derivation

**Summary:** This video discusses how to derive polynomial regression formula.





#### ✓ Example 6.4.4.1

To find the contraction of a steel cylinder, one wishes to regress the coefficient of linear thermal expansion data to temperature.

Table 6.4.4.1. Coefficient of linear thermal expansion at given different temperatures

Temperature, $T$ ( $^{\circ}\text{F}$ )	Coefficient of thermal expansion, $\alpha$ (in/in/ $^{\circ}\text{F}$ )
80	$6.47 \times 10^{-6}$
40	$6.24 \times 10^{-6}$
-40	$5.72 \times 10^{-6}$
-120	$5.09 \times 10^{-6}$
-200	$4.30 \times 10^{-6}$
-280	$3.33 \times 10^{-6}$
-340	$2.45 \times 10^{-6}$

Regress the above data to  $\alpha = a_0 + a_1T + a_2T^2$  .

### Solution

Since  $\alpha = a_0 + a_1T + a_2T^2$  is the quadratic relationship between the coefficient of linear thermal expansion and the temperature, the coefficients  $a_0$ ,  $a_1$ ,  $a_2$  are found as follows

$$\begin{bmatrix} n & \left(\sum_{i=1}^n T_i\right) & \left(\sum_{i=1}^n T_i^2\right) \\ \left(\sum_{i=1}^n T_i\right) & \left(\sum_{i=1}^n T_i^2\right) & \left(\sum_{i=1}^n T_i^3\right) \\ \left(\sum_{i=1}^n T_i^2\right) & \left(\sum_{i=1}^n T_i^3\right) & \left(\sum_{i=1}^n T_i^4\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n \alpha_i \\ \sum_{i=1}^n T_i \alpha_i \\ \sum_{i=1}^n T_i^2 \alpha_i \end{bmatrix} \quad (6.4.4.E1.1)$$

Table 6.4.4.2. Summations for calculating constants of the model .

$i$	$T(^{\circ}\text{F})$	$\alpha(\text{in/in}/^{\circ}\text{F})$	$T^2$	$T^3$	$T^4$	$T \times \alpha$	$T^2 \times \alpha$
1	80	$6.4700 \times 10^{-6}$	$6.4000 \times 10^3$	$5.1200 \times 10^5$	$4.0960 \times 10^7$	$5.1760 \times 10^{-4}$	$4.1408 \times 10^{-2}$
2	40	$6.2400 \times 10^{-6}$	$1.6000 \times 10^3$	$6.4000 \times 10^4$	$2.5600 \times 10^6$	$2.4960 \times 10^{-4}$	$9.9840 \times 10^{-3}$
3	-40	$5.7200 \times 10^{-6}$	$1.6000 \times 10^3$	$-6.4000 \times 10^4$	$2.5600 \times 10^6$	$-2.2880 \times 10^{-4}$	$9.1520 \times 10^{-3}$
4	-120	$5.0900 \times 10^{-6}$	$1.4400 \times 10^4$	$-1.7280 \times 10^6$	$2.0736 \times 10^8$	$-6.1080 \times 10^{-4}$	$7.3296 \times 10^{-2}$
5	-200	$4.3000 \times 10^{-6}$	$4.0000 \times 10^4$	$-8.0000 \times 10^6$	$1.6000 \times 10^9$	$-8.6000 \times 10^{-4}$	$1.7200 \times 10^{-1}$
6	-280	$3.3300 \times 10^{-6}$	$7.8400 \times 10^4$	$-2.1952 \times 10^7$	$6.1466 \times 10^9$	$-9.3240 \times 10^{-4}$	$2.6107 \times 10^{-1}$
7	-340	$2.4500 \times 10^{-6}$	$1.1560 \times 10^5$	$-3.9304 \times 10^7$	$1.3363 \times 10^{10}$	$-8.3300 \times 10^{-4}$	$2.8322 \times 10^{-1}$
$\sum_{i=1}^7$	$-8.6000 \times 10^2$	$3.3600 \times 10^{-5}$	$2.5800 \times 10^5$	$-7.0472 \times 10^7$	$2.1363 \times 10^{10}$	$-2.6978 \times 10^{-3}$	$8.5013 \times 10^{-1}$

$$n = 7$$

$$\sum_{i=1}^7 T_i = -8.6000 \times 10^2$$

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

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

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

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

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

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

From Equation (6.4.4.E1.1) we have

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

Solving the above system of simultaneous linear equations, we get

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

The polynomial regression model hence is

$$\begin{aligned} \alpha &= a_0 + a_1 T + a_2 T^2 \\ &= 6.0217 \times 10^{-6} + 6.2782 \times 10^{-9} T - 1.2218 \times 10^{-11} T^2 \end{aligned}$$

### Audiovisual Lecture

**Title:** Polynomial Regression Model: Example

**Summary:** This video shows an example how to conduct polynomial regression.





## Lesson 5: Optimum Order of a Polynomial Regression Model

### Learning Objectives

After successful completion of this lesson, you should be able to:

- 1) Choose an optimum order of polynomial for polynomial regression models.

### Introduction

Often, you may not have the privilege or enough knowledge of the problem to choose the type of regression model. Some may suggest fitting the data to a polynomial model. But the question that you would begin to ask then is – What order of polynomial should I use?

Say, if you are given  $n$  data points,  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , you could use the least-squares method to regress the data to an  $m^{\text{th}}$  order polynomial, where the order,  $m$  can be as low as 0 and as high as  $n - 1$ .

$$y = a_0 + a_1x + a_2x^2 + \dots + a_mx^m, \quad 0 \leq m \leq n - 1 \quad (6.4.5.1)$$

Look at Figures 6.4.5.1 and 6.4.5.2 where the data from Table 6.4.5.1, which has 22 data points, has been regressed to a first-order and second-order polynomial.

Table 6.4.5.1. Instantaneous thermal expansion coefficient as a function of temperature for steel.

Temperature	Instantaneous Thermal Expansion
°F	$\mu\text{in/in}/^\circ\text{F}$
80	6.47
60	6.36
40	6.24
20	6.12
0	6.00
–20	5.86
–40	5.72
–60	5.58
–80	5.43
–100	5.28

Temperature	Instantaneous Thermal Expansion
-120	5.09
-140	4.91
-160	4.72
-180	4.52
-200	4.30
-220	4.08
-240	3.83
-260	3.58
-280	3.33
-300	3.07
-320	2.76
-340	2.45

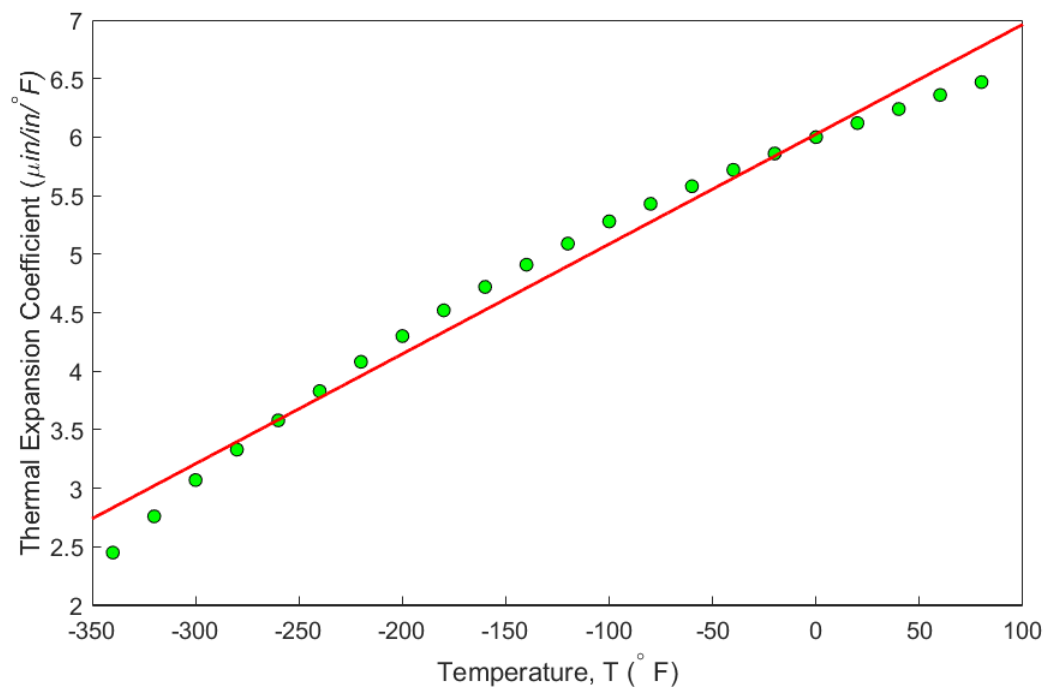


Figure 6.4.5.1(a). Polynomial regression model  $\alpha = 0.009387T + 6.025$  for the linear coefficient of thermal expansion vs. temperature data for steel.

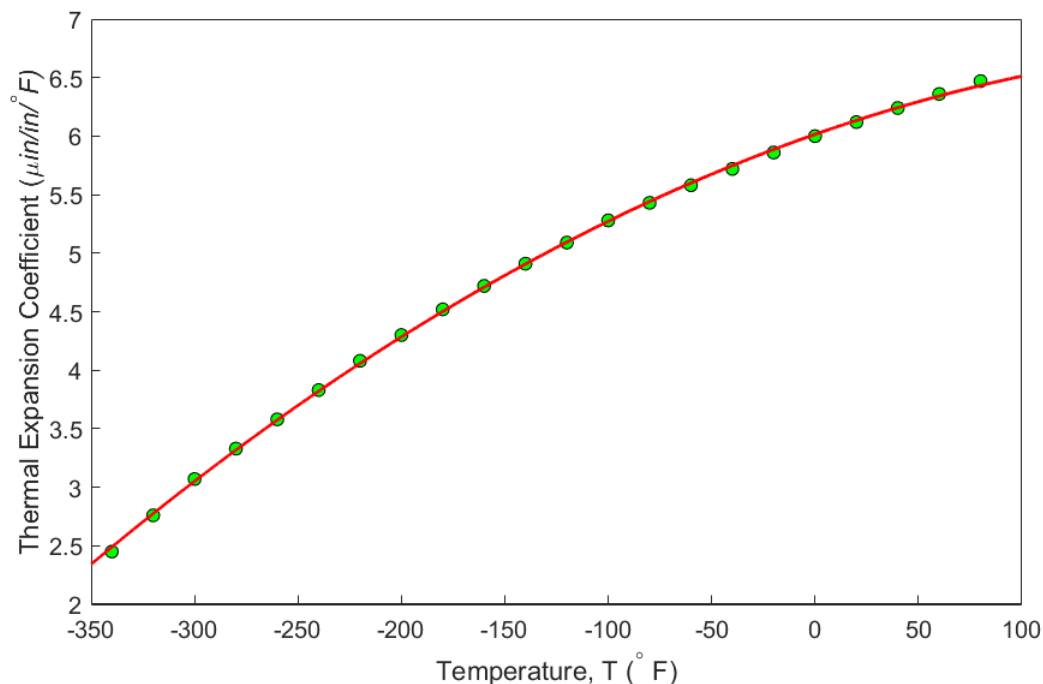


Figure 6.4.5.1(b). Polynomial regression model  $\alpha = -0.00001228T^2 + 0.006196T + 6.015$  for the linear coefficient of thermal expansion vs. temperature data for steel.

Visual observation of Figure 6.4.5.1(b) may make us believe that the second-order polynomial looks acceptable. However, we should be basing such decisions on quantitative measurements as we may not have the luxury of a visual inspection. Even if we did, the visual interpretation is speculative.

One may hence suggest using a polynomial order for which the sum of the squares of the residuals,  $S_r$ , is a minimum. For the data in Table 6.4.5.1, the sum of the square of the residuals,  $S_{rm}$  as a function of the order of the polynomial,  $m$  is shown in Table 6.4.5.2 Figure 6.4.5.2(a) and Figure 6.4.5.2(b)

Table 6.4.5.2. Sum of the square of the residuals as a function of the order of the polynomial.

Order of polynomial, $m$	$S_{rm}$
1	0.6912
2	0.007732
3	0.001063
4	0.001013
5	0.0009019
6	0.0006700

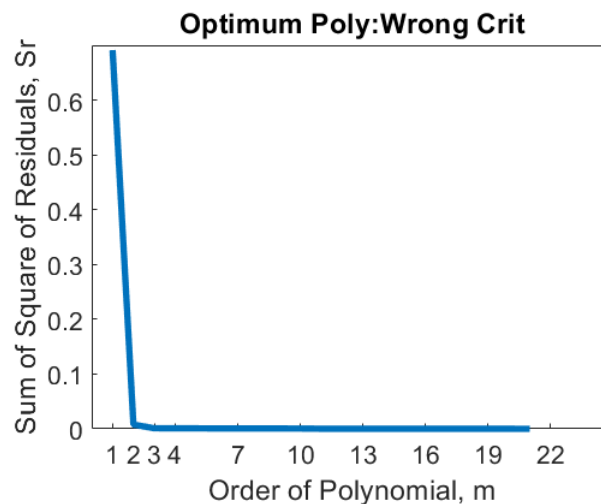


Figure 6.4.5.2(a). Sum of square of residuals as a function of the order of the polynomial. This graph starts at  $m = 1$

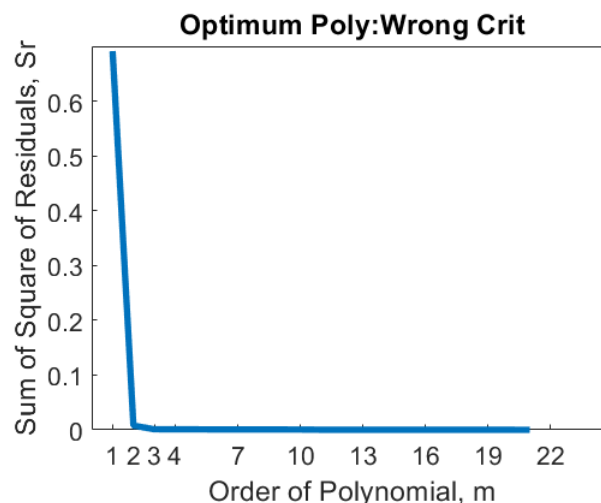


Figure 6.4.5.2(b). Sum of square of residuals as a function of the order of the polynomial. This graph is the same as Figure 6.4.5.2(a) but starts at  $m = 2$ .

The value of  $S_{rm}$  continues to decrease with the increase in the order of the polynomial (Figures \(\PageIndex{5.2(a)}\) and \(\PageIndex{5.2(b)}\)), and in fact, we will get  $S_{rm} = 0$  when the chosen polynomial order is one less than the number of data points (of course, we assume there is only one  $y$ -value for each  $x$ -value). In this case, the regression curve would go through all the points and be a perfect fit. In fact, it is polynomial interpolation for this extreme case. Using the criterion of minimizing  $S_{rm}$  with respect to the order of the polynomial is hence not acceptable.

Instead, the criterion suggested to use is as follows. Given  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  data points, choose the degree of the polynomial,  $m$  for which the variance as computed by

$$\text{Variance} = \frac{S_{rm}}{n - (m + 1)} \quad (6.4.5.2)$$

is a minimum or when there is no statistically significant decrease in its value as the degree of the polynomial is increased, where

$S_{rm}$  = sum of the square of the residuals for the polynomial of order  $m$ .

Note the reason  $m + 1$  is in the formula, as there are as many constants in the polynomial regression model of order,  $m$ . Also,  $S_{rm} = 0$ , when  $n = m + 1$ . As the order of the polynomial,  $m$  increases, both the numerator,  $S_{rm}$ , and the denominator,  $n - (m + 1)$ , decrease. These competing decreases would allow us to optimize the order of the polynomial.

For the data in Table 6.4.5.1, the variance is shown as a function of the order of the polynomial in Table 6.4.5.3 (shown only up to  $m = 6$ ), and Figures 6.4.5.3(a) and 6.4.5.3(b).

Table 6.4.5.3. Variance as a function of the order of the polynomial.

Order of polynomial, $m$	$\frac{S_{rm}}{n - (m + 1)}$
1	0.03455
2	0.0004069
3	0.00005906
4	0.00005961
5	0.00005637
6	0.00004467

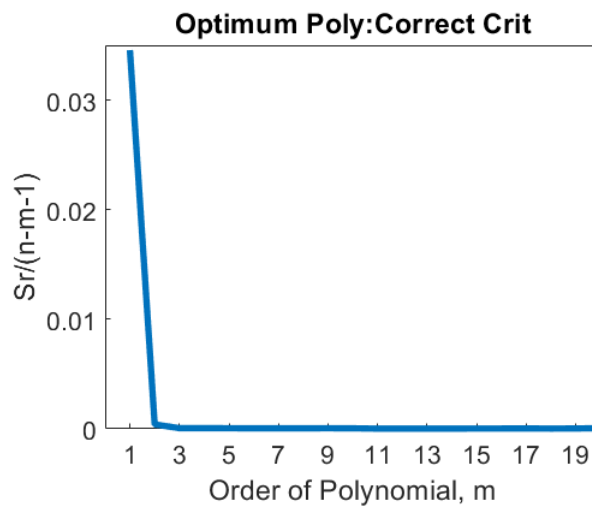


Figure 6.4.5.3(a). Variance as a function of the order of the polynomial. This graph starts at  $m = 1$ .

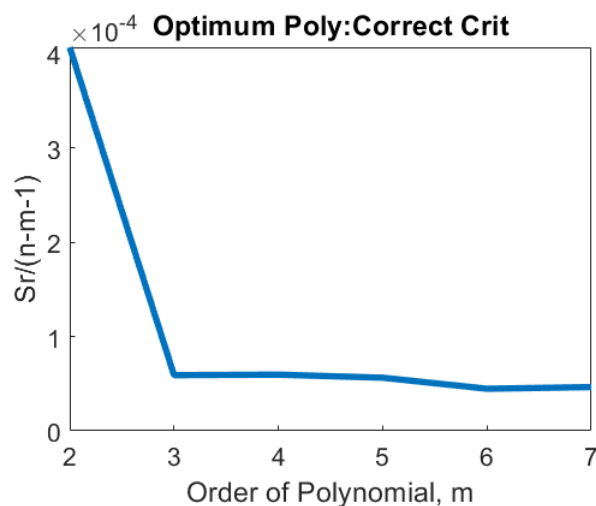


Figure 6.4.5.3(b). Sum of square of residuals as a function of the order of the polynomial. This graph is the same as Figure 6.4.5.3(a) but starts at  $m = 2$ .

So, what order of polynomial would you choose? A second- or third-order polynomial would be the right choice as little statistical change occurs in the variance value after  $m = 2$ .



## Audiovisual Lecture

**Title:** Optimum Order of Polynomial of Regression

**Summary:** This video discusses how you can find the optimum order of polynomial for regression



## Lesson 6: Other Nonlinear Regression Models

### Learning Objectives

After successful completion of this lesson, you should be able to:

- 1) derive constants of other popular nonlinear regression models
- 2) use the derived formula to find the constants of nonlinear regression models from given data with and without transformation.

### Introduction

In the previous lessons, we talked about several nonlinear regression models, such as exponential. In this lesson, we continue our discussion on some growth and power regression models.

### Growth model

Common growth models standard in scientific fields have been developed and are used successfully for specific situations. The growth models are used to describe how something grows with changes in the regressor variable (often the time). Examples in this category include the growth of thin films or population with time and are of the form

$$y = \frac{a}{1 + be^{-cx}} \quad (6.4.6.1)$$

where  $a$ ,  $b$  and  $c$  are the constants of the model.

At  $x = 0$ ,  $y = \frac{a}{1 + b}$  and as  $x \rightarrow \infty$ ,  $y \rightarrow a$ .

The residuals at each data point  $x_i$  are

$$E_i = y_i - \frac{a}{1 + be^{-cx_i}} \quad (6.4.6.2)$$

The sum of the square of the residuals is

$$\begin{aligned} S_r &= \sum_{i=1}^n E_i^2 \\ &= \sum_{i=1}^n \left( y_i - \frac{a}{1 + be^{-cx_i}} \right)^2 \end{aligned} \quad (6.4.6.3)$$

To find the constants  $a$ ,  $b$ , and  $c$ , we minimize  $S_r$  by differentiating  $S_r$  with respect to  $a$ ,  $b$  and  $c$ , and equating the resulting equations to zero.

$$\begin{aligned}\frac{\partial S_r}{\partial a} &= \sum_{i=1}^n \left( \frac{2e^{cx_i} [ae^{cx_i} - y_i (e^{cx_i} + b)]}{(e^{cx_i} + b)^2} \right) = 0, \\ \frac{\partial S_r}{\partial b} &= \sum_{i=1}^n \left( \frac{2ae^{cx_i} [by_i + e^{cx_i} (y_i - a)]}{(e^{cx_i} + b)^3} \right) = 0, \\ \frac{\partial S_r}{\partial c} &= \sum_{i=1}^n \left( \frac{-2abx_i e^{cx_i} [by_i + e^{cx_i} (y_i - a)]}{(e^{cx_i} + b)^3} \right) = 0. \quad (6.4.6.4a, b, c)\end{aligned}$$

One can use the Newton-Raphson method to solve the above set of simultaneous nonlinear equations for the constants of the regression model,  $a$ ,  $b$ , and  $c$ .

### ✓ Example 6.4.6.1

The height of a child is measured at different ages as follows.

Table 6.4.6.1. Height of the child at different ages.

$t$ (yrs)	0	5	8	12	16	18
$H$ (in)	20	36.2	52	60	69.2	70

Predict the height of the child as an adult of 30 years of age using the growth model

$$H = \frac{a}{1 + be^{-ct}}$$

### Solution

The saturation growth model of height,  $H$ , vs. age,  $t$ , is given as

$$H = \frac{a}{1 + be^{-ct}} \quad (6.4.6.E1.1)$$

where the constants  $a$ ,  $b$ , and  $c$  are the roots of the simultaneous nonlinear equation system

$$\begin{aligned}\sum_{i=1}^6 \left( \frac{2e^{ct_i} [ae^{ct_i} - H_i (e^{ct_i} + b)]}{(e^{ct_i} + b)^2} \right) &= 0 \\ \sum_{i=1}^6 \left( \frac{2ae^{ct_i} [bH_i + e^{ct_i} (H_i - a)]}{(e^{ct_i} + b)^3} \right) &= 0 \\ \sum_{i=1}^6 \left( \frac{-2abt_i e^{ct_i} [bH_i + e^{ct_i} (H_i - a)]}{(e^{ct_i} + b)^3} \right) &= 0 \quad (6.4.6.E1.2a, b, c)\end{aligned}$$

We need initial guesses of the roots to get the iterative process started to find the root of those equations. Suppose we use three of the given data points such as (0, 20), (12, 60) and (18, 70) to find the initial guesses of roots; we have

$$20 = \frac{a}{1 + be^{-c(0)}}$$

$$60 = \frac{a}{1 + be^{-c(12)}}$$

$$70 = \frac{a}{1 + be^{-c(18)}}$$

One can solve three unknowns  $a$ ,  $b$ , and  $c$  for the initial guesses from the three equations as

$$a = 7.5534 \times 10^1$$

$$b = 2.7767$$

$$c = 1.9772 \times 10^{-1}$$

Applying the Newton-Raphson method for simultaneous nonlinear equations with the above initial guesses, one can get the roots of Equations (6.4.6.E1.2a, b, c) as

$$a = 7.4321 \times 10^1$$

$$b = 2.8233$$

$$c = 2.1715 \times 10^{-1}$$

The saturation growth model of the height of the child then is

$$H = \frac{7.4321 \times 10^1}{1 + 2.8233e^{-2.1715 \times 10^{-1}t}}$$

The predicted height of the child as an adult of 30 years of age is

$$\begin{aligned} H &= \frac{7.4321 \times 10^1}{1 + 2.8233e^{-2.1715 \times 10^{-1} \times (30)}} \\ &= 74'' \end{aligned}$$

### Logistic Growth Model

In the logistic growth model, an example of a growth model in which a measurable quantity  $y$  varies with some quantity  $x$  is

$$y = \frac{ax}{b+x} \quad (6.4.6.5)$$

For  $x = 0$ ,  $y = 0$  while as  $x \rightarrow \infty$ ,  $y \rightarrow a$ . As noticed in the previous growth model, we had to solve three simultaneous nonlinear equations. Many times, one can transform the data and then use formulas derived for linear regression.

To transform the data for this model, we rewrite Equation (6.4.6.5) as

$$\begin{aligned} \frac{1}{y} &= \frac{b+x}{ax} \\ &= \frac{b}{a} \frac{1}{x} + \frac{1}{a} \end{aligned} \quad (6.4.6.6)$$

Let

$$z = \frac{1}{y}$$

$$w = \frac{1}{x}$$

$$a_0 = \frac{1}{a} \text{ implying that } a = \frac{1}{a_0}$$

$$a_1 = \frac{b}{a} \text{ implying that } b = a_1 \times a = \frac{a_1}{a_0}$$

Then

$$z = a_0 + a_1 w \quad (6.4.6.7)$$

The relationship between  $z$  and  $w$  is linear with the coefficients  $a_0$  and  $a_1$  found as follows.

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

$$a_0 = \frac{\sum_{i=1}^n z_i}{n} - a_1 \frac{\sum_{i=1}^n w_i}{n} \quad (6.4.6.8a, b)$$

Finding  $a_0$  and  $a_1$  then gives the constants of the original growth model as

$$\begin{aligned} a &= \frac{1}{a_0} \\ b &= \frac{a_1}{a_0} \end{aligned} \quad (6.4.6.9a, b)$$

### Logarithmic Functions

The form for the log regression models is

$$y = \beta_0 + \beta_1 \ln(x) \quad (6.4.6.10)$$

Equation (6.4.6.10) is a linear function between  $y$  and  $\ln(x)$  and the usual least-squares method applies in which  $y$  is the response variable and  $\ln(x)$  is the regressor.

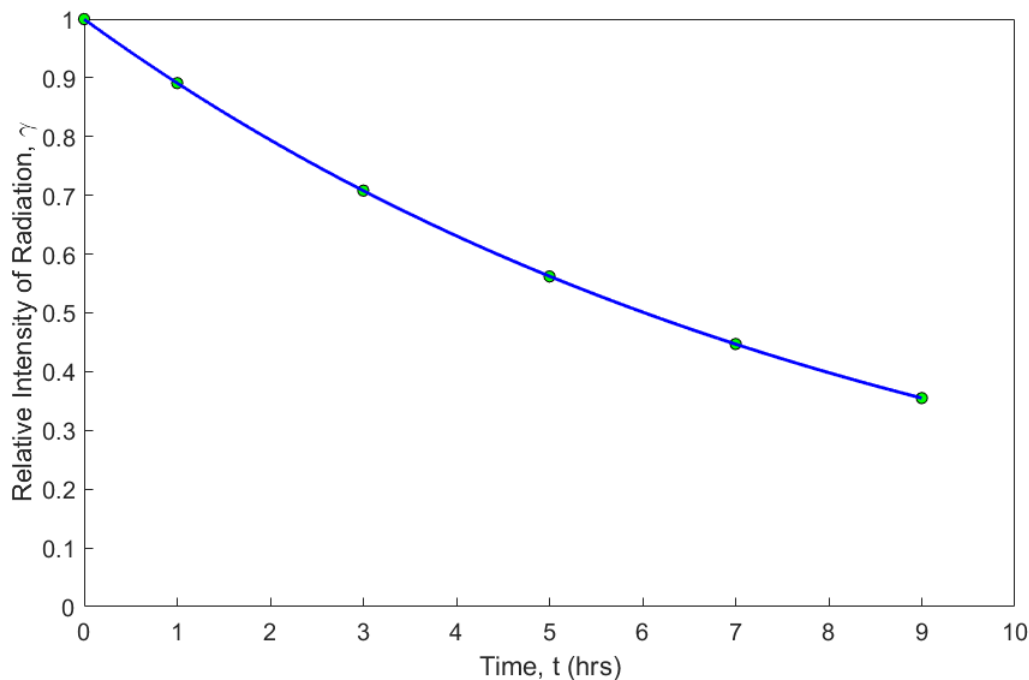


Figure 6.4.6.1. Exponential regression model with transformed data for relative intensity of radiation as a function of time.

#### ✓ Example 6.4.6.2

Sodium borohydride is a potential fuel for fuel cells. The following overpotential ( $\eta$ ) vs. current ( $i$ ) data was obtained in a study conducted to evaluate its electrochemical kinetics.

Table 6.4.6.2. Electrochemical kinetics of borohydride data.

$\eta$ (V)	-0.29563	-0.24346	-0.19012	-0.18772	-0.13407	-0.0861
$i$ (A)	<b>0.00226</b>	<b>0.00212</b>	<b>0.00206</b>	<b>0.00202</b>	<b>0.00199</b>	<b>0.00195</b>

At the conditions of the study, it is known that the relationship that exists between the overpotential ( $\eta$ ) and current ( $i$ ) can be expressed as

$$\eta = a + b \ln i$$

where  $a$  is an electrochemical kinetics parameter of borohydride on the electrode. Use the data in Table 6.4.6.2 to evaluate the values of  $a$  and  $b$ .

## Solution

Following the least-squares method, Table 6.4.6.3 tabulates the summations where

$$x = \ln i$$

$$y = \eta$$

We obtain

$$y = a + bx \quad (6.4.6.E2.1)$$

This is a linear relationship between  $y$  and  $x$ , and the coefficients  $b$  and  $a$  are found as follows:

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

$$a = \bar{y} - b\bar{x} \quad (6.4.6.E2.2a, b)$$

Table 6.4.6.3. Summation values for calculating constants of model.

#	$i$	$y = \eta$	$x = \ln(i)$	$x^2$	$xy$
1	0.00226	-0.29563	-6.0924	37.117	<b>1.8011</b>
2	0.00212	-0.24346	-6.1563	37.901	<b>1.4988</b>
3	0.00206	-0.19012	-6.1850	38.255	<b>1.1759</b>
4	0.00202	-0.18772	-6.2047	38.498	<b>1.1647</b>
5	0.00199	-0.13407	-6.2196	38.684	0.83386
6	0.00195	-0.08610	-6.2399	38.937	0.53726
$\sum_{i=1}^6$	0.012400	-1.1371	-37.098	229.39	<b>7.0117</b>

$$n = 6$$

$$\sum_{i=1}^6 x_i = -37.098$$

$$\sum_{i=1}^6 y_i = -1.1371$$

$$\sum_{i=1}^6 x_i y_i = 7.0117$$

$$\sum_{i=1}^6 x_i^2 = 229.39$$

$$b = \frac{6(7.0117) - (-37.098)(-1.1371)}{6(229.39) - (-37.098)^2}$$

$$= -1.3601$$

$$a = \frac{-1.1371}{6} - (-1.3601) \frac{-37.098}{6}$$

$$= -8.5990$$

Hence

$$\eta = -8.5990 - 1.3601 \times \ln i$$

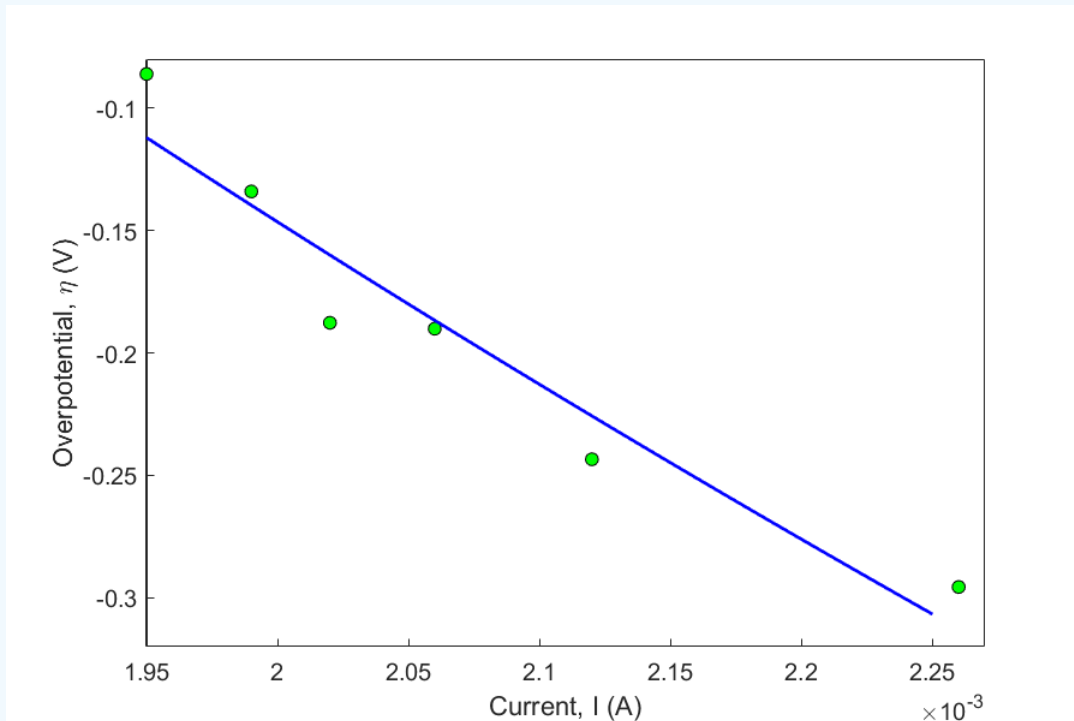


Figure 6.4.6.2. Overpotential as a function of current:  $\eta(V)$ .

### Power Functions

The power function equation describes many scientific and engineering phenomena. In chemical engineering, the rate of a chemical reaction is often written in power function form as

$$y = ax^b \quad (6.4.6.11)$$

The least-squares method is applied to the power function by first transforming the data (the assumption is that  $b$  is not known). If the only unknown is  $a$ , then a linear relation exists between  $x^b$  and  $y$ .

When both  $a$  and  $b$  are unknowns, the transformation of the data is as follows.

$$\ln(y) = \ln(a) + b \ln(x) \quad (6.4.6.12)$$

The resulting equation shows a linear relation between  $\ln y$  and  $\ln x$ .

Let

$$z = \ln y$$

$$w = \ln x$$

$$a_0 = \ln a \text{ implying } a = e^{a_0}$$

$$a_1 = b$$

we get

$$z = a_0 + a_1 w$$

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

$$a_0 = \frac{\sum_{i=1}^n z_i}{n} - a_1 \frac{\sum_{i=1}^n w_i}{n} \quad (6.4.6.13)$$

Since  $a_0$  and  $a_1$  can be found, the original constants of the model are

$$b = a_1$$

$$a = e^{a_0} \quad (6.4.6.14a, b)$$

### ✓ Example 6.4.1

The progress of a homogeneous chemical reaction is followed, and it is desired to evaluate the rate constant and the order of the reaction. The rate law expression for the reaction is known to follow the power function form

$$-r = kC^n \quad (6.4.6.E3.1)$$

Use the data provided in the table to obtain  $n$  and  $k$ .

Table 6.4.6.4. Chemical kinetics.

$C_A$ (gmol/l)	4	2.25	1.45	1.0	0.65	0.25	0.006
$-r_A$ (gmol/l·s)	0.398	0.298	0.238	0.198	0.158	0.098	0.048

### Solution

Taking the natural log of both sides of Equation (6.4.6.E3.1) we obtain

$$\ln(-r) = \ln(k) + n \ln(C) \quad (6.4.6.E3.2)$$

Let

$$z = \ln(-r)$$

$$w = \ln(C)$$

$$a_0 = \ln(k)$$

implying that

$$k = e^{a_0}$$

$$a_1 = n \quad (6.4.3.3a, b)$$

We get

$$z = a_0 + a_1 w$$

This is a linear relation between  $z$  and  $w$ , where

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

$$a_0 = \frac{\sum_{i=1}^m z_i}{m} - a_1 \frac{\sum_{i=1}^m w_i}{m} \quad (6.4.6.E3.4)$$

Table 6.4.6.5. Kinetics rate law using power function.

$i$	$C$	$-r$	$w$	$z$	$wz$	$w^2$
1	4	<b>0.398</b>	1.3863	-0.92130	-1.2772	<b>1.9218</b>
2	2.25	<b>0.298</b>	0.8109	-1.2107	-0.9818	<b>0.65761</b>
3	1.45	<b>0.238</b>	0.3716	-1.4355	-0.5334	<b>0.13806</b>
4	1	<b>0.198</b>	0.0000	-1.6195	0.0000	<b>0.00000</b>
5	0.65	<b>0.158</b>	-0.4308	-1.8452	0.7949	<b>0.18557</b>
6	0.25	<b>0.098</b>	-1.3863	-2.3228	3.2201	<b>1.9218</b>
7	<b>0.006</b>	<b>0.048</b>	-5.1160	-3.0366	15.535	<b>26.173</b>
$\sum_{i=1}^7$			-4.3643	-12.391	16.758	<b>30.998</b>

$$m = 7$$

$$\sum_{i=1}^7 w_i = -4.3643$$

$$\sum_{i=1}^7 z_i = -12.391$$

$$\sum_{i=1}^7 w_i z_i = 16.758$$

$$\sum_{i=1}^7 w_i^2 = 30.998$$

From Equation (E3.3)

$$\begin{aligned}
 a_1 &= \frac{7 \times (16.758) - (-4.3643) \times (-12.391)}{7 \times (30.998) - (-4.3643)^2} \\
 &= 0.31943 \\
 a_0 &= \frac{-12.391}{7} - (0.31943) \frac{-4.3643}{7} \\
 &= -1.5711
 \end{aligned}$$

From Equation (6.4.6.E3.3a) and (6.4.6.E3.2b) we obtain

$$k = e^{-1.5711} = 0.20782$$

$$n = a_1 = 0.31941$$

Finally, the model of the progress of that chemical reaction is

$$-r = 0.20782 \times C^{0.31941}$$



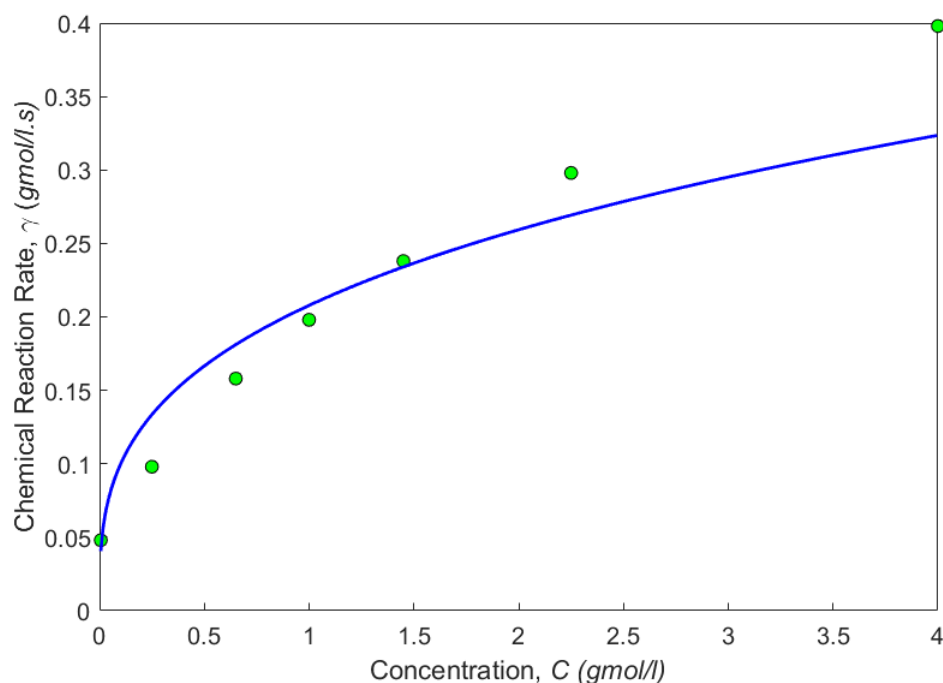


Figure 6.4.6.3. Kinetic chemical reaction rate as a function of concentration.

### Multiple Choice Test

(1). When using transformed data to find the constants of the regression model  $y = ae^{bx}$  to best fit  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , the sum of the square of the residuals that is minimized is

- (A)  $\sum_{i=1}^n (y_i - ae^{bx_i})^2$
- (B)  $\sum_{i=1}^n (\ln(y_i) - \ln(a) - bx_i)^2$
- (C)  $\sum_{i=1}^n (y_i - \ln(a) - bx_i)^2$
- (D)  $\sum_{i=1}^n (\ln(y_i) - \ln(a) - b \ln(x_i))^2$

(2). It is suspected from theoretical considerations that the rate of water flow from a firehouse is proportional to some power of the nozzle pressure. Assume pressure data is more accurate. You are transforming the data.

Flow rate, $F$ (gallons/min)	96	129	135	145	168	235
Pressure, $p$ (psi)	11	17	20	25	40	55

The exponent of the nozzle pressure in the regression model  $F = ap^b$  most nearly is

- (A) 0.49721
- (B) 0.55625
- (C) 0.57821
- (D) 0.67876

(3). The stress-strain curve is given as  $\sigma = k_1 \varepsilon e^{-k_2 \varepsilon}$  for concrete in compression, where  $\sigma$  is the stress and  $\varepsilon$  is the strain. To transform the data, one would use which of the following forms?

(A)  $\ln(\sigma) = \ln(k_1) + \ln(\varepsilon) - k_2\varepsilon$

(B)  $\ln\left(\frac{\sigma}{\varepsilon}\right) = \ln(k_1) - k_2\varepsilon$

(C)  $\ln\left(\frac{\sigma}{\varepsilon}\right) = \ln(k_1) + k_2\varepsilon$

(D)  $\ln(\sigma) = \ln(k_1\varepsilon) - k_2\varepsilon$

(4). In nonlinear regression, finding the constants of the model requires solving simultaneous nonlinear equations. However, in the exponential model  $y = ae^{bx}$  that is best fit to  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , the value of  $b$  can be found as a solution of a single nonlinear equation. That nonlinear equation is given by

(A)  $\sum_{i=1}^n y_i x_i e^{bx_i} - \sum_{i=1}^n y_i e^{bx_i} \sum_{i=1}^n x_i = 0$

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

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

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

(5). There is a functional relationship between the mass density  $\rho$  of air and the altitude  $h$  above sea level.

Altitude above sea level, $h$ (km)	0.32	0.64	1.28	1.60
Mass Density, $\rho$ (kg/m <sup>3</sup> )	1.15	1.10	1.05	0.95

In the regression model  $\rho = k_1 e^{-k_2 h}$ , the constant  $k_2$  is found as  $k_2 = 0.1315$ . Assume the mass density of air at the top of the atmosphere is  $1/1000^{th}$  of the mass density of air at sea level. The altitude in kilometers of the top of the atmosphere most nearly is

(A) 46.2

(B) 46.6

(C) 49.7

(D) 52.5

(6). A steel cylinder at 80°F of length 12'' is placed in a commercially available liquid nitrogen bath(−315°F). If the thermal expansion coefficient of steel behaves as a second-order polynomial function of temperature and the polynomial is found by regressing the data below,

Temperature, $T$ (°F)	Thermal expansion coefficient, $\alpha$ ( $\mu\text{in}/\text{in}^\circ\text{F}$ )
−320	2.76
−240	3.83
−160	4.72
−80	5.43

Temperature, $T$ ( $^{\circ}\text{F}$ )	Thermal expansion coefficient, $\alpha$ ( $\mu\text{in}/\text{in}^{\circ}\text{F}$ )
0	6.00
80	6.47

the reduction in the length of the cylinder in inches most nearly is

- (A) 0.0219
- (B) 0.0231
- (C) 0.0235
- (D) 0.0307

For complete solution, go to

[http://nm.mathforcollege.com/mcquizzes/06reg/quiz\\_06reg\\_nonlinear\\_solution.pdf](http://nm.mathforcollege.com/mcquizzes/06reg/quiz_06reg_nonlinear_solution.pdf)

### Problem Set

(1). It is suspected from theoretical considerations that the rate of flow from a fire hose is proportional to some power of the nozzle pressure. Determine whether the speculation is true. What is the exponent of the data? Assume pressure data is more accurate. You are allowed to transform the data.

Flow rate (gallons/min), $F$	94	118	147	180	230
Pressure (psi), $p$	10	16	25	40	60

**Answer**

$$30.213p^{0.49101}$$

(2). The following force vs. displacement data is given for a nonlinear spring.

Displacement, $x$ (m)	10	15	20
Force, $F$ (N)	100	200	400

Starting by minimizing the sum of the square of the residuals and without data transformation, the above  $F$  vs.  $x$  data is regressed to  $F = kx^2$ . Find the value of  $k$ .

**Answer**

$$0.97450 \text{ N/m}^2$$

(3). Data points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  is regressed to  $y = \frac{1}{(ax + b)^2}$ . The constants of the model,  $a$  and  $b$ , are solved by data transformation. Find the formulas for calculating  $a$  and  $b$ .

Hint: Take the inverse and square-root of both sides to transform the data

**Answer intentionally omitted** - follow the hint.

(4). Fit the regression model  $\sigma = K_1 \varepsilon e^{-K_2 \varepsilon}$  to the following stress-strain data of concrete. You are allowed to transform the data. Units of stress,  $\sigma$  are psi, and units of strain,  $\varepsilon$  are  $\mu\text{in}/\text{in}$ .

Stress, $\sigma$ (psi)	2250	3575	4250	4400	4200
Strain, $\varepsilon$ ( $\mu\text{in}/\text{in}$ )	500	1000	1500	2000	2375

**Answer**

$$K_1 = 5.8406$$

(note that the units for strain for which this  $K_2$  is given is  $\mu\text{in/in}$ ). In the final answer, strain is in  $\mu\text{in/in}$ , and stress in psi. The units of  $K_2$  are  $\text{in}/\mu\text{in}$ . The units of  $K_1$  are  $\text{psi}/(\mu\text{in/in})$  which is the same as  $\text{Msi}$ .

(5). It is desired to obtain a functional relationship between the mass density  $\rho$  of air and the altitude  $h$  above the sea level for the dynamic analysis of bodies moving within the earth's atmosphere. Use the regression model  $\rho = k_1 e^{-k_2 h}$  to fit the data given below. Find the constants  $k_1$  and  $k_2$ . You are allowed to transform the data.

Altitude (km)	Mass density ( $\text{kg/m}^3$ )
0.32	1.15
0.64	1.10
1.28	1.05
1.60	0.95

#### Answer

$k_1 = 1.2053$ ,  $k_2 = 0.13395$  where in the model,  $h$  is in kms, and  $\rho$  is in  $\text{kg/m}^3$

(6). You are working for Valdez SpillProof Oil Company as a petroleum engineer. Your boss is asking you to estimate the life of an oil well. The analysis used in the industry is called the *decline curve analysis*, where the barrels of oil produced per unit time are plotted against time, and the curve is extrapolated. One of the standard curves used is the harmonic decline model, that is,

$$q = \frac{b}{1 + at}$$

where  $q$  is the rate of production and  $t$  is the time,  $b$  and  $a$  are the constants of the regression model.

Time ( $t$ ), month	2	6	10	14	18
Rate of production ( $q$ ), barrels per day	260	189	120	87	75

- Find the constants of the regression model. Hint: You are allowed to transform the data, if possible.
- Find the total life of an oil field if 5 barrels per day is considered the production at which the field needs to be abandoned for further production.
- What does  $b$  stand for physically?

#### Answer

- $461.85/(1 + 0.29069t)$
- 314.30 months
- Answer intentionally omitted.

(7). From the physical understanding of a phenomenon, the velocity of a body is suspected to follow the relationship  $v = at^2$ , where  $v$  is the velocity and  $t$  is the time. Given  $n$  data points  $(t_1, v_1), (t_2, v_2), \dots, (t_n, v_n)$ , start from the fundamentals of minimizing the sum of the squares of the residuals to derive a single equation in terms of the time and velocity data to find the value of  $a$ . Simplify the equation. Show full derivation that includes that the derived value of  $a$  corresponds to an absolute minimum of the sum of the squares of the residuals. You are not allowed to transform the data.

#### Answer

$$a = \frac{\sum_{i=1}^n v_i t_i^2}{\sum_{i=1}^n t_i^4}$$

(8). The population for a small community is given as a function of time.

time, $t$ (years)	0	5	10
Population, $p$	100	165	314

By minimizing the sum of the square of the residuals and without data transformation, the model is regressed to  $p = ae^{bt}$ , where  $a$  and  $b$  are constants of the model. The value of  $b$  was found to be 0.1199. Find the value of  $a$ .

**Answer**

$$p = 94.136e^{0.1199t}$$

(9). The data given below is actually the weight (lbs) of a baby as a function of the age (months) of the baby

$t$	0	2	4	6	18
$W$	7.5	11.25	14.30	16.00	26.00

- a) Fit  $W = at^2 + bt + c$  to the data to find  $W(360)$ .  
b) We expect that the weight of the baby to saturate as the baby reaches adulthood. Suggest a different model and estimate  $W(360)$ . Compare your results with part (a).

**Answer**

a)  $W = -0.03642t^2 + 1.6659t + 7.7810$ ;  $W(360) = -4110.2$

b) Answer intentionally omitted

(10). The temperature of a copper sphere cooling in air is measured as a function of time to yield the following data.

Time, $t$ (s)	0.2	0.6	1.0	2.0
Temperature, $T$ (C)	146.0	129.5	114.8	85.1

From theoretical considerations, an exponential decrease of temperature is expected as a function of time. One can assume a regression model given by  $T = Ae^{-0.3t}$ . Starting from minimizing the sum of the squares of the residuals, find the constant of the model,  $A$ .

**Answer**

$$A = 155.02$$

(11). There is a functional relationship between the mass density  $\rho$  of air and altitude  $h$  above sea level, and this is found from the data below.

Altitude above sea level, $h$ (km)	0.32	0.64	1.28	1.60
Mass density of air, $\rho$ (kg/m <sup>3</sup> )	1.15	1.10	1.05	0.95

This functional relationship is found by regression using the model  $\rho = k_1 e^{-k_2 h}$ . The constant  $k_2$  is found as  $k_2 = 0.1315$ . Assuming the mass density of air at the top of the atmosphere is  $1/1000^{th}$  of the mass density of air at sea level, find the altitude above the sea level in kilometers of the top of the atmosphere.

**Answer** 52.53 km

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