Math 4543: Numerical Methods

Lecture 11 — Nonlinear Regression

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Lecture Plan

The agenda for today

- Recap the concept of Regression Analysis
- What is Nonlinear Regression?
- Know about different types of nonlinear regression models and their utility
- Exponential Model
- Polynomial Model
- Growth Model
- Logarithmic Model
- Power Model

Regression Analysis

Recall the idea of a regression model

In statistical modeling, regression analysis is a set of statistical processes for ***estimating*** the relationships between a dependent variable and one or more independent variables.

The problem statement for a regression model is as follows. Given n data pairs $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, best fit $y = f(x)$ to the data (Figure 1).

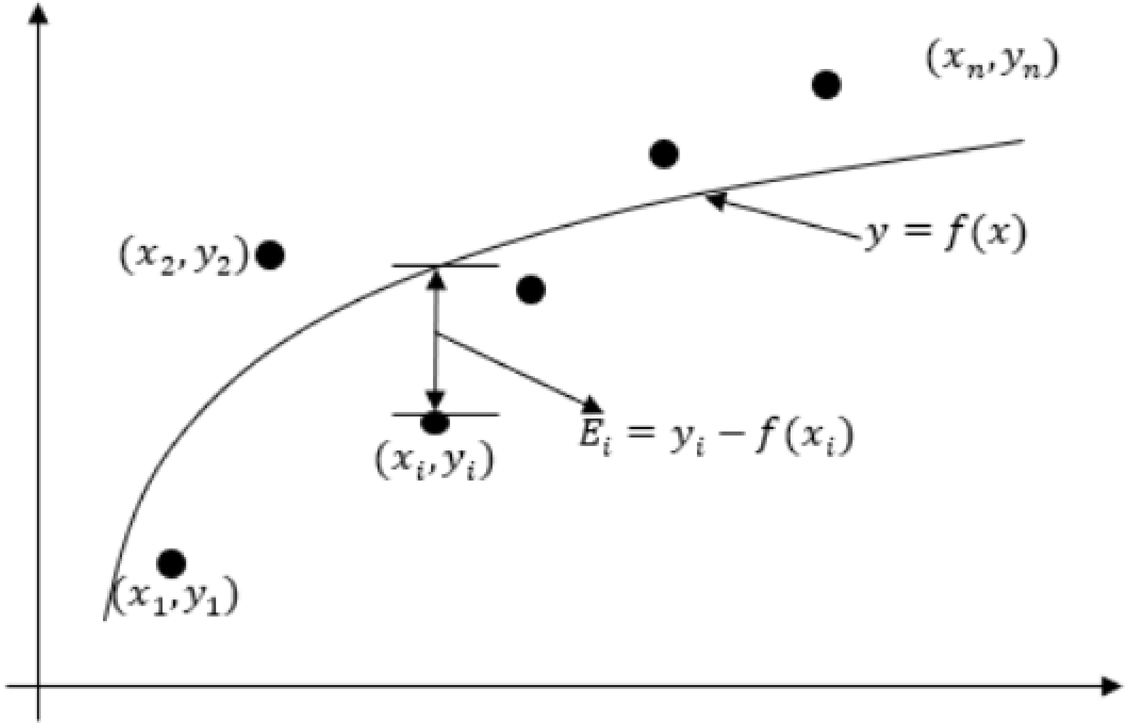


Figure 1. A general regression model for discrete y vs. x data

Nonlinear Regression

What is it?

In nonlinear regression, the relationships are modeled using ***nonlinear predictor functions*** which are nonlinear combinations of the model parameters.

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

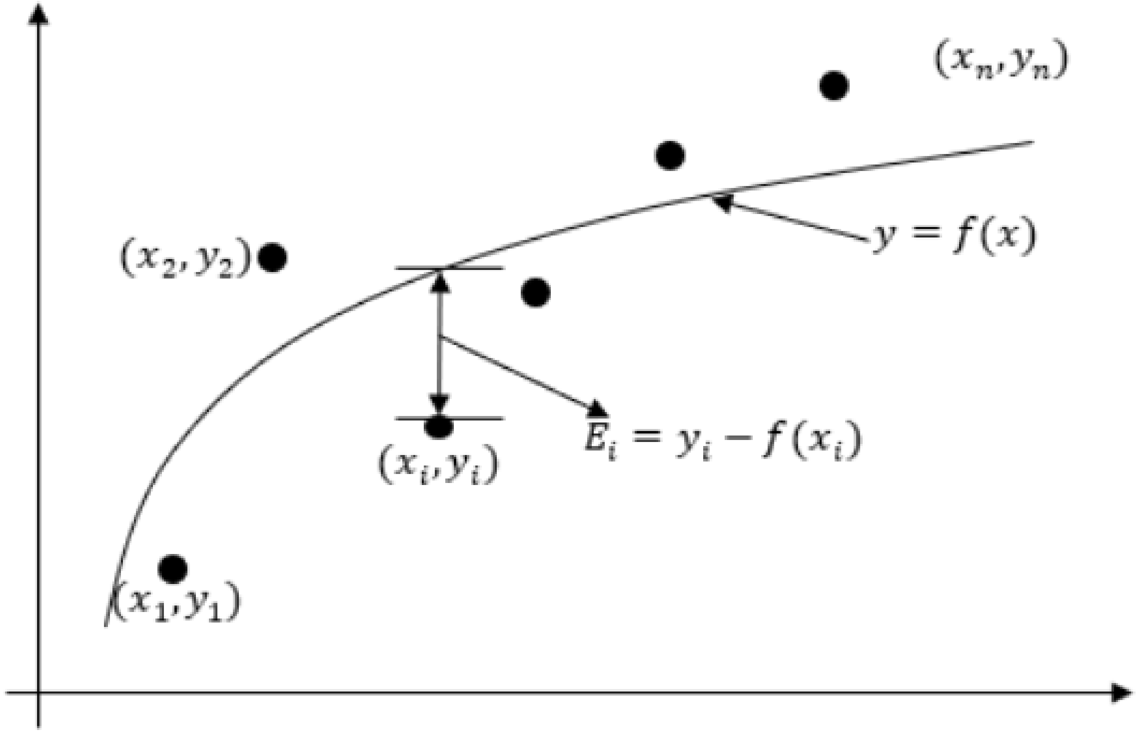


Figure 1. Nonlinear regression model for discrete y vs. x data

Nonlinear Regression

How to quantify the *goodness* of fit?

A measure of goodness of fit, that is, how well $y = f(x)$ predicts the response variable y is the magnitude of the residual E_i at each of the n data points.

The residual at each data point x_i is found

$$E_i = y_i - f(x_i) \qquad (1)$$

to get the sum of the square of the residuals as

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

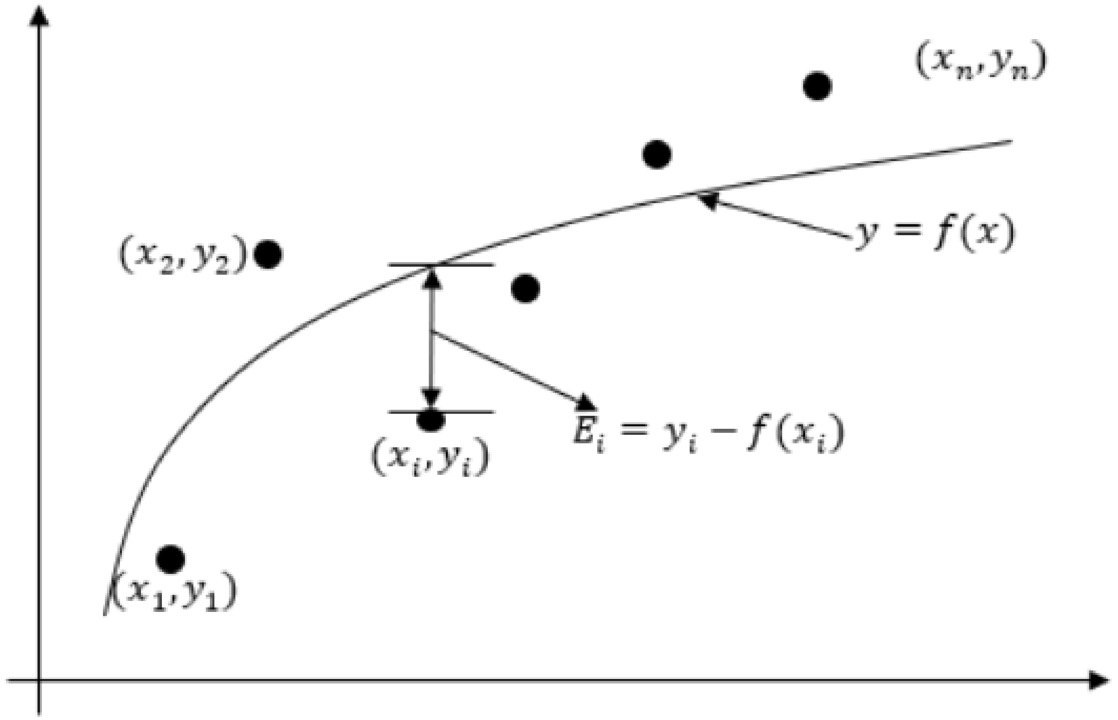


Figure 1. Nonlinear regression model for discrete y vs. x data

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

Nonlinear Regression

Exponential Model

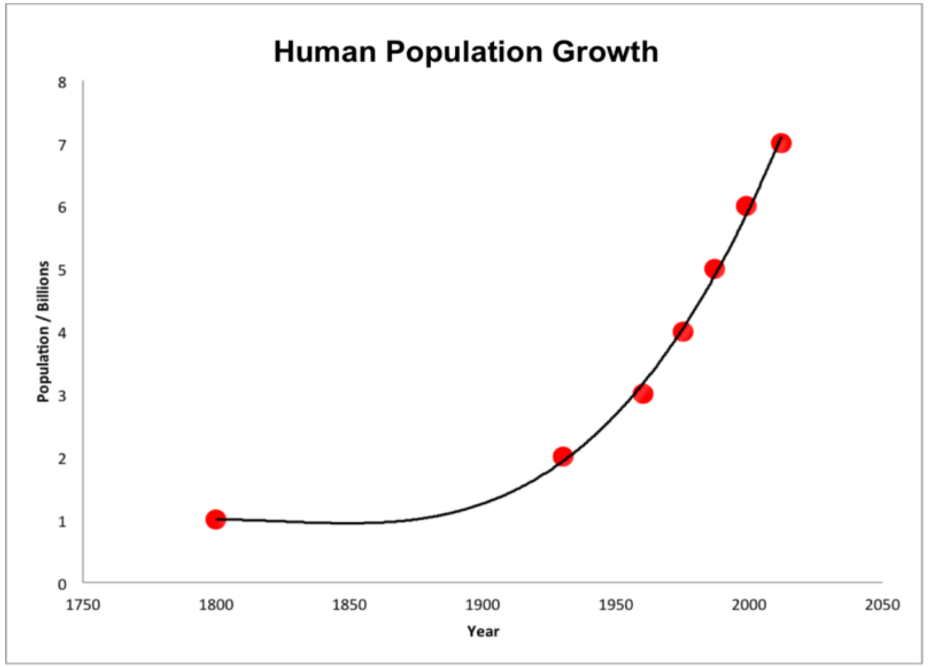
Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, best fit $y = ae^{bx}$ to the data. In this model, the constants of the regression model are a and b.

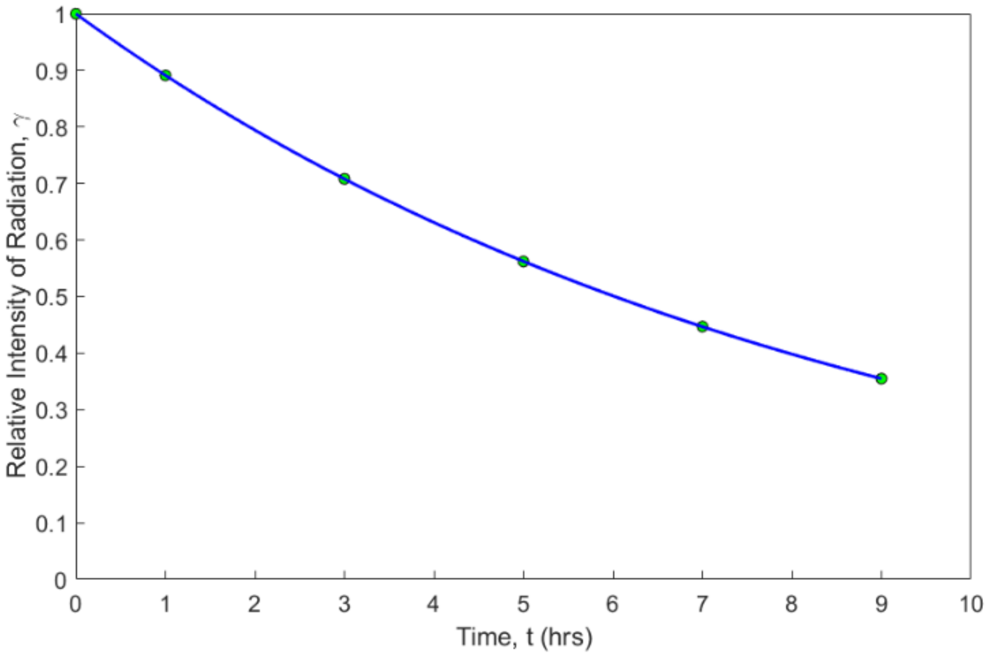
- ✓ For modeling ***exponentially*** *increasing* processes, *e.g.* Population growth formula

$$P_t = P_0 e^{kt}$$

- ✓ For modeling ***exponentially*** ***decaying*** processes, *e.g.* Radioactivity of Tc-99 isotope

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



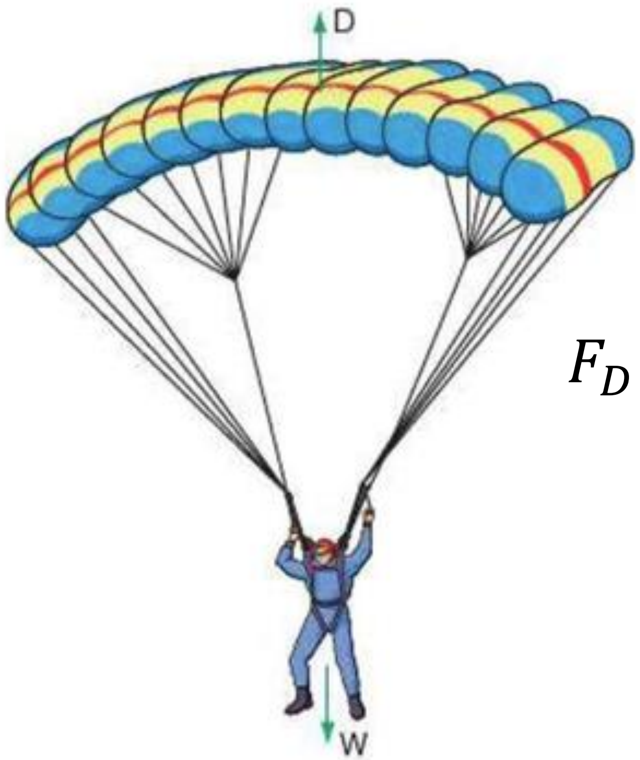


Nonlinear Regression

Power Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, best fit $y = ax^b$ to the data. In this model, the constants of the regression model are a and b.

e.g. Drag force of a parachute



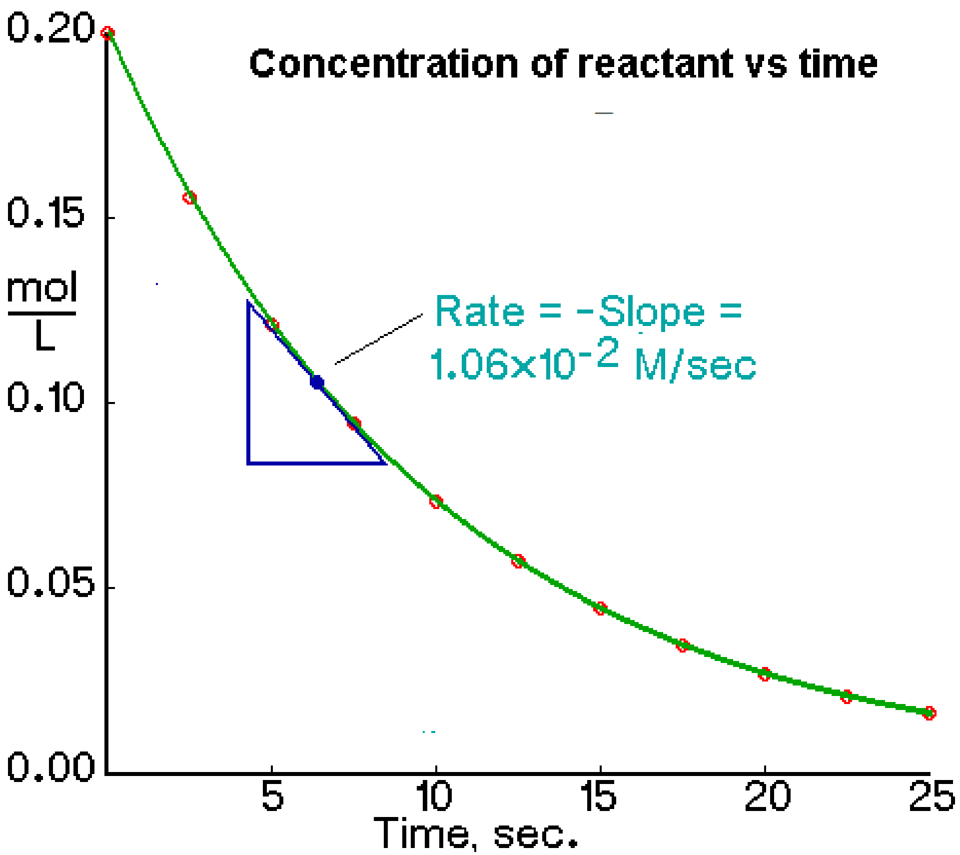
$$F_D = \frac{1}{2}\rho v^2 C_D A$$

e.g. Reaction rate of chemicals

$$-r = k[A]^n[B]^m$$

for the reaction

$$\text{n}\mathbf{A} + \text{m}\mathbf{B} \longrightarrow \text{Product}$$



Nonlinear Regression

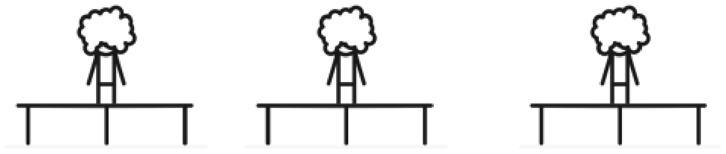
Saturation/Logistic Growth Model

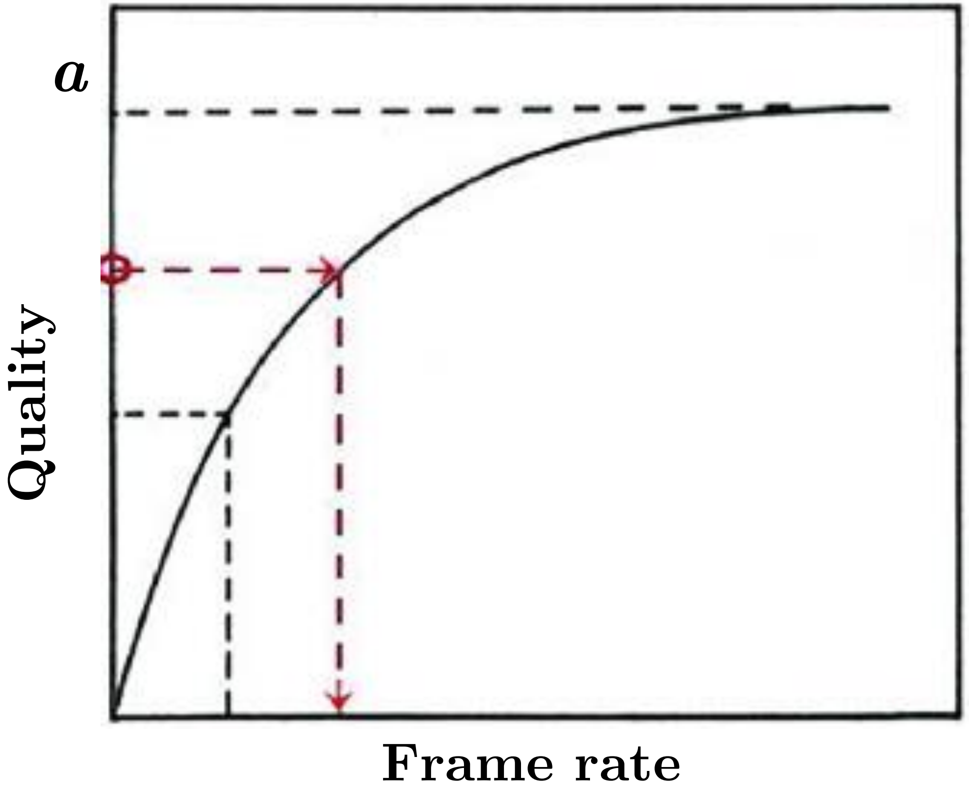
Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, best fit $y = \dfrac{ax}{b+x}$ to the data. In this model, the constants of the regression model are a and b.

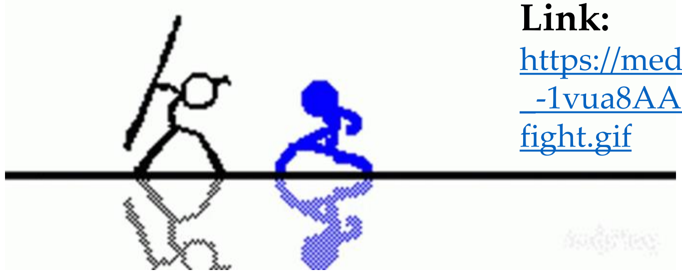
Link:
https://www.reddit.com/media?url=https%3A%2F%2Fexternal-preview.redd.it%2FmRiiz7nxj2FOTqi43MMF4G_eliE7zp1z8kctYQ5g8dI.gif%3Fformat%3Dmp4%26s%3D98e2e6b56258afa45427e47a5f346c54ecf193e1

e.g. goodness of an animated scene

How good an animation looks is measured by a variable called performance and is a function of the frame rate. 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 (60 FPS).







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https://media.tenor.com/l16K_-1vua8AAAAd/everybody-fight.gif

Nonlinear Regression

Other models

- **Growth Model**

$$y = \frac{a}{1 + be^{-cx}}$$

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

At $x = 0$, $y = \dfrac{a}{1+b}$ and

as $x \to \infty$, $y \to a$.

- **Polynomial Model**

$$y = a_0 + a_1x + a_2x^2 + \cdots\cdots + a_mx^m,\ 0 \le m \le n-1$$

to regress the data to an m^{th} order polynomial.

- **Logarithmic Model**

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

y is the response variable and $\ln(x)$ is the regressor.

And many more…

Exponential Model

What is it?

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, best fit $y = ae^{bx}$ to the data (Figure 1).

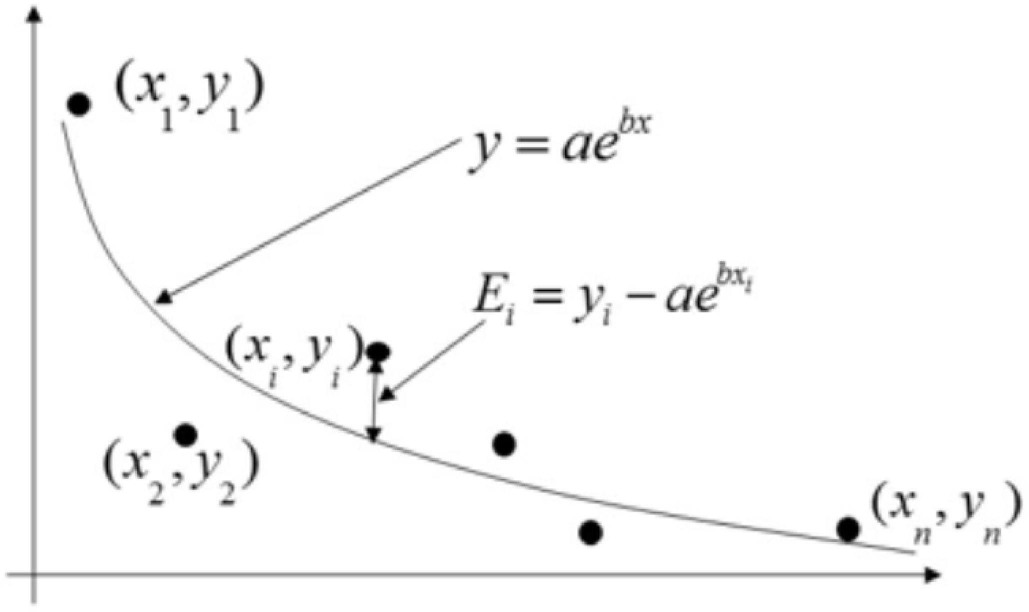


Figure 1. Exponential regression model for *y* vs. *x* data

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

$$E_i = y_i - ae^{bx_i} \qquad (1)$$

The sum of the square of the residuals is

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

Exponential Model

Deriving the parameters

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

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

$$\frac{\partial S_r}{\partial b} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i}\right)\left(-ax_i e^{bx_i}\right) = 0 \qquad (3a, b)$$

Expanding Equations (3a,b) gives

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

$$-2a\sum_{i=1}^{n} y_i x_i e^{bx_i} + 2a^2\sum_{i=1}^{n} x_i e^{2bx_i} = 0 \qquad (4a, b)$$

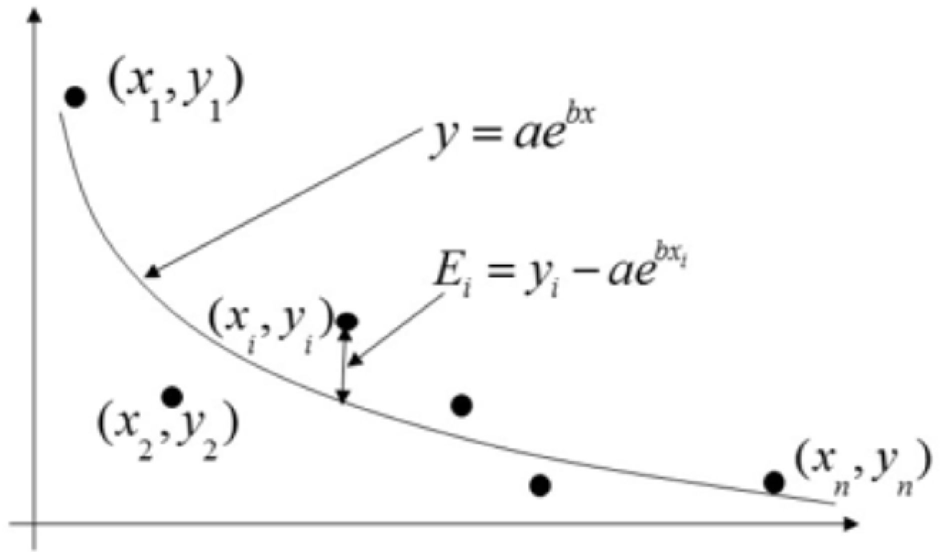


Figure 1. Exponential regression model for *y* vs. *x* data

Simplifying Equation (4a,b) gives

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

$$-\sum_{i=1}^{n} y_i x_i e^{bx_i} + a\sum_{i=1}^{n} x_i e^{2bx_i} = 0 \qquad (5a, b)$$

Exponential Model

Deriving the parameters

$$a = \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \qquad (6)$$

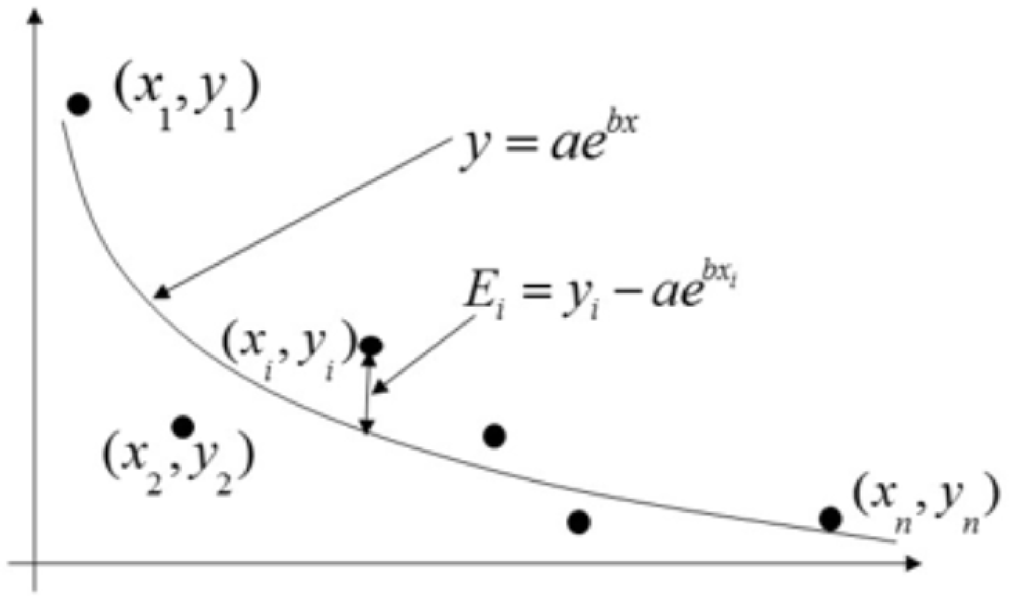


Figure 1. Exponential regression model for y vs. x data

Substituting Equation (6) in (5b) gives

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \sum_{i=1}^{n} x_i e^{2bx_i} = 0 \qquad (7)$$

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

Exponential Model

An example

Table 1 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

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

a). the value of the regression constants A and λ,

Exponential Model

An example

Solution

a) The value of λ is given by solving

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

Then the value of A from Equation (6) takes the form,

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

Solve equation $(E1.1)$ using the **Bisection Method** with initial guesses $\lambda=-0.120$ and $\lambda=-0.110$.

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 2 Summation value for calculation of constants of the model

i	t_i	γ_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

Need 3 tables for each iteration! (2 new)

Exponential Model

An example

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

Similarly

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

Since

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

the value of λ 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 $\boxed{\lambda = -0.11508}$. This value of the root was obtained after 20 iterations with an absolute relative approximate error of less than 0.000008%.

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

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

$$= \frac{2.9373}{2.9378}$$

$$\boxed{= 0.99983}$$

The regression formula is hence given by

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

Exponential Model

Avoiding the hassle with Data Transformation

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

$$y = ae^{bx} \qquad (5)$$

Taking the natural log of both sides of Equation (5) gives

$$\ln y = \ln a + bx \qquad (6)$$

Let

$$z = \ln y$$

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

$$a_1 = b \qquad (7)$$

then

$$z = a_0 + a_1 \qquad (8)$$

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

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

$$a_0 = \bar{z} - a_1\bar{x} \qquad (9a, b)$$

When the constants a_0 and a_1 are found, the original constants of the exponential model are found as given in Equation (7)

$$b = a_1$$
$$a = e^{a_0}$$

Exponential Model

The same example (now with data transformation)

Table 1 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

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

a). the value of the regression constants A and λ,

Exponential Model

The same example (now with data transformation)

Solution

a)

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

Taking the natural logarithm on both sides,

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

Assuming

$$y = \ln \gamma$$

$$a_0 = \ln(A) \qquad (E1.3)$$

$$a_1 = \lambda \qquad (E1.4)$$

we get

$$y = a_0 + a_1 t$$

This is a linear relationship between y and t.Then

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

$$a_0 = \bar{y} - a_1 \bar{t} \qquad (1.5a, b)$$

Exponential Model

The same example (now with data transformation)

Table 2 shows the summations one would need for calculating a_0 and a_1.

Table 2 Summations of data to calculate constants of the model.

i	t_i	γ_i	$y_i = ln\gamma_i$	$t_i y_i$	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	25.0000
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

$$n = 6$$

$$\sum_{i=1}^{6} t_i = 25.000 \qquad \sum_{i=1}^{6} t_i y_i = -18.990$$

$$\sum_{i=1}^{6} y_i = -2.8778 \qquad \sum_{i=1}^{6} t_i^2 = 165.00$$

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

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

$$a_0 = \ln(A) \qquad \lambda = a_1 = -0.11505$$

$$A = e^{a_0}$$
$$= e^{-2.6150\times10^{-4}}$$
$$= 0.99974$$

The regression formula then is

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

Exponential Model

Effect of data transformation

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

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

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.

Exponential Model

An example (with vs without data transformation)

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
90	0.1803

Exponential Model

An example

Solution

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

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

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

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

$$\ln(y) = bx \qquad (E2.3)$$

Assuming

$$z = \ln y \qquad (E2.4)$$

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

$$z = bx \qquad (E2.5)$$

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

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

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

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

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

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

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

Exponential Model

An example

Without transforming the data

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

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

The sum of the square of the residuals is

$$\begin{aligned} S_r &= \sum_{i=1}^{n} E_i^2 \\ &= \sum_{i=1}^{n} \left(y_i - e^{bx_i}\right)^2 \qquad (E2.8) \end{aligned}$$

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

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

Expanding and simplifying Equation (E2.9) gives

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

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

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

Exponential Model

An example

Clearly, the two models are not close, and you can see this in Figure 2 as well.

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

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

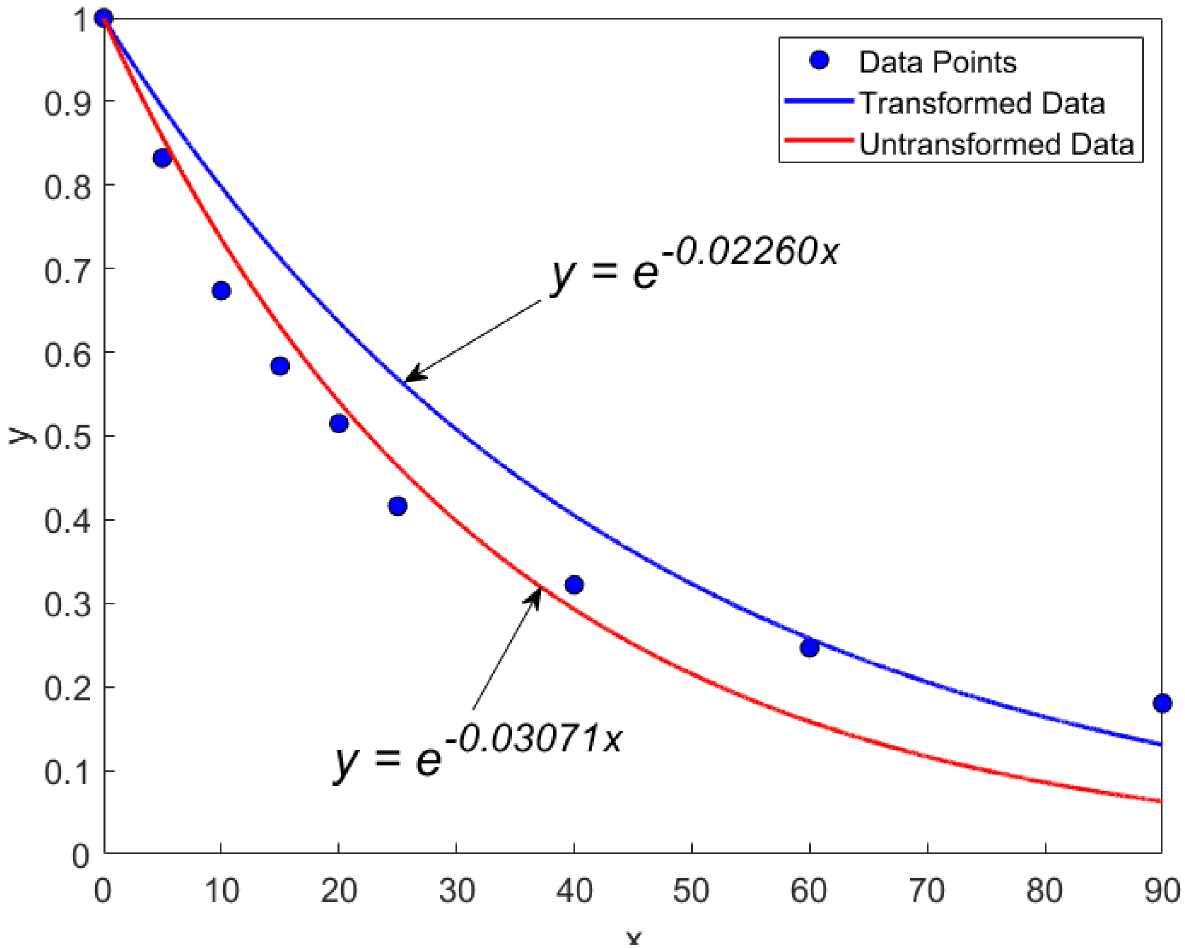
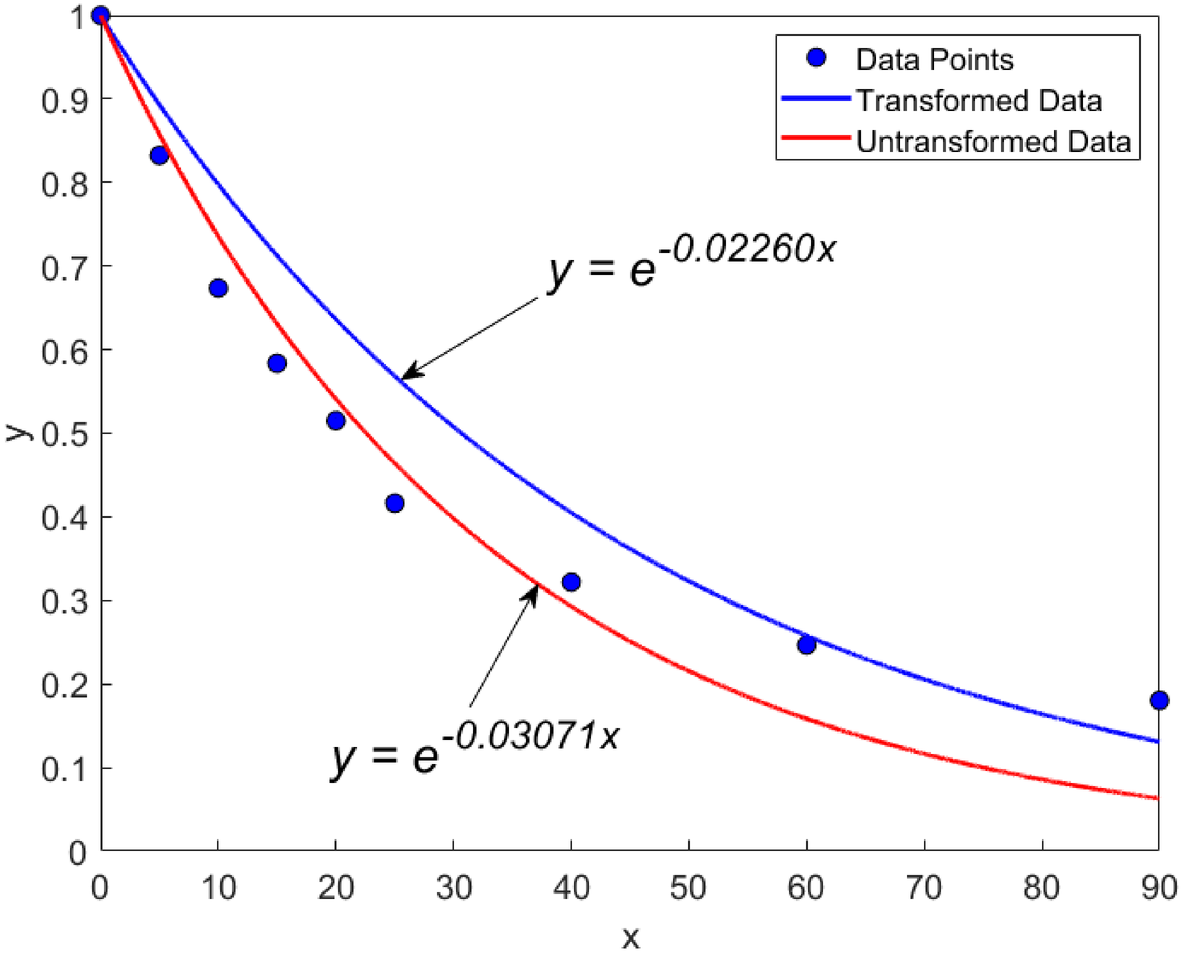


Figure 2. Comparing an exponential regression model with and without data transformation

Mini Quiz

The difference in the models



$$y = e^{-0.03071x} \quad \text{vs.} \quad y = e^{-0.02260x}$$

We were supposed to get the ***best-fit*** curve.

But why are these regression curves different?

Polynomial Model

What is it?

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

$$y = a_0 + a_1 x + a_2 x^2 + \cdots\cdots + a_m x^m,\; m < n \qquad (1)$$

The residual at each data point is given by

$$E_i = y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m \qquad (2)$$

The sum of the square of the residuals is given by

$$\begin{aligned} S_r &= \sum_{i=1}^{n} E_i^2 \\ &= \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m\right)^2 \qquad (3) \end{aligned}$$

For optimal value of *m*, perform ***Bias-Variance*** tradeoff.

Polynomial Model

Deriving the coefficients

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

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

Setting these equations in matrix form gives

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

$$XA = Y$$

or, $A = X^{-1}Y$

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

Polynomial Model

An example

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

Temperature, T (°F)	Coefficient of thermal expansion, $\alpha(\mathrm{in/in/^\circ F})$
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}

Table 1 Coefficient of linear thermal expansion at given different temperatures

Regress the above data to $\alpha = a_0 + a_1 T + a_2 T^2$

Polynomial Model

An example

Solution

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

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

Polynomial Model

An example

Table 2 Summations for calculating constants of the model

i	$T(^\circ\mathrm{F})$	$\alpha(\mathrm{in/in/^\circ F})$	T^2	T^3
1	80	6.4700×10^{-6}	6.4000×10^{3}	5.1200×10^{5}
2	40	6.2400×10^{-6}	1.6000×10^{3}	6.4000×10^{4}
3	-40	5.7200×10^{-6}	1.6000×10^{3}	-6.4000×10^{4}
4	-120	5.0900×10^{-6}	1.4400×10^{4}	-1.7280×10^{6}
5	-200	4.3000×10^{-6}	4.0000×10^{4}	-8.0000×10^{6}
6	-280	3.3300×10^{-6}	7.8400×10^{4}	-2.1952×10^{7}
7	-340	2.4500×10^{-6}	1.1560×10^{5}	-3.9304×10^{7}
$\sum_{i=1}^{7}$	-8.6000×10^{2}	3.3600×10^{-5}	2.5800×10^{5}	-7.0472×10^{7}

Polynomial Model

An example

Table 2 (cont)

i	T^4	$T \times \alpha$	$T^2 \times \alpha$
1	4.0960×10^{7}	5.1760×10^{-4}	4.1408×10^{-2}
2	2.5600×10^{6}	2.4960×10^{-4}	9.9840×10^{-3}
3	2.5600×10^{6}	-2.2880×10^{-4}	9.1520×10^{-3}
4	2.0736×10^{8}	-6.1080×10^{-4}	7.3296×10^{-2}
5	1.6000×10^{9}	-8.6000×10^{-4}	1.7200×10^{-1}
6	6.1466×10^{9}	-9.3240×10^{-4}	2.6107×10^{-1}
7	1.3363×10^{10}	-8.3300×10^{-4}	2.8322×10^{-1}
$\sum_{i=1}^{7}$	2.1363×10^{10}	-2.6978×10^{-3}	8.5013×10^{-1}

$$n = 7$$

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

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

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

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

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

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

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

Polynomial Model

An example

From Equation (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

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

Growth Model

What is it?

The core ***growth model*** regression curve is of the form —

$$y = \frac{a}{1 + be^{-cx}}$$

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

At $x = 0$, $y = \dfrac{a}{1+b}$ and

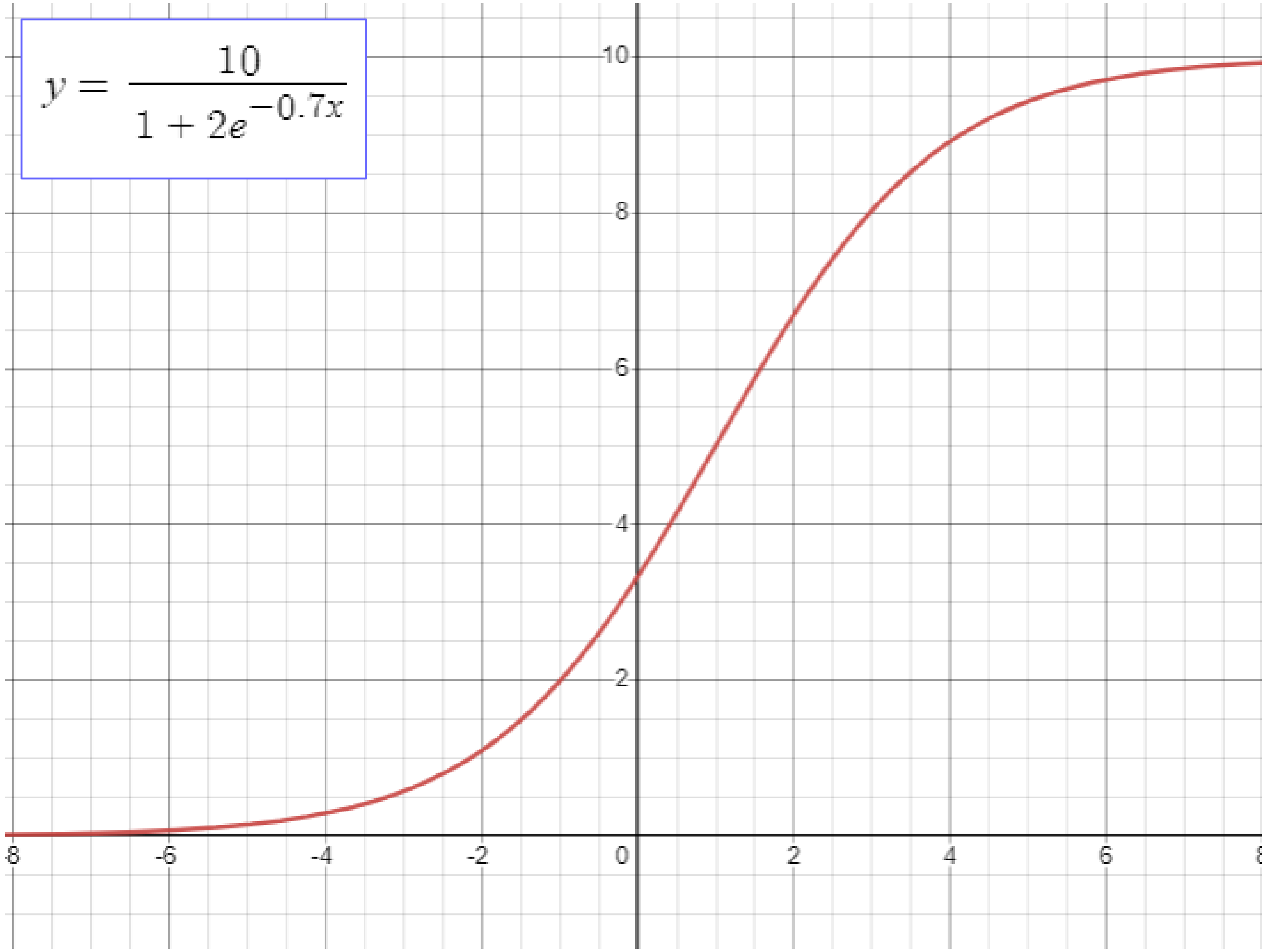
as $x \to \infty$, $y \to a$.

The residuals at each data point x_i, are

$$E_i = y_i - \frac{a}{1 + be^{-cx_i}}$$

The sum of the square of the residuals is

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



Growth Model

Deriving the parameters

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.

$$\frac{\partial S_r}{\partial a} = \sum_{i=1}^{n} \left(\frac{2e^{cx_i}\left[ae^{cx_i} - y_i\left(e^{cx_i} + b\right)\right]}{\left(e^{cx_i} + b\right)^2} \right) = 0,$$

$$\frac{\partial S_r}{\partial b} = \sum_{i=1}^{n} \left(\frac{2ae^{cx_i}\left[by_i + e^{cx_i}\left(y_i - a\right)\right]}{\left(e^{cx_i} + b\right)^3} \right) = 0,$$

$$\frac{\partial S_r}{\partial c} = \sum_{i=1}^{n} \left(\frac{-2abx_i e^{cx_i}\left[by_i + e^{cx_i}\left(y_i - a\right)\right]}{\left(e^{cx_i} + b\right)^3} \right) = 0. \qquad (4a, b, c)$$

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.

Growth Model

An example

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

Table 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,

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

Growth Model

An example

Solution

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

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

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

$$\sum_{i=1}^{6}\left(\frac{2e^{ct_i}\left[ae^{ct_i}-H_i\left(e^{ct_i}+b\right)\right]}{\left(e^{ct_i}+b\right)^2}\right)=0$$

$$\sum_{i=1}^{6}\left(\frac{2ae^{ct_i}\left[bH_i+e^{ct_i}\left(H_i-a\right)\right]}{\left(e^{ct_i}+b\right)^3}\right)=0$$

$$\sum_{i=1}^{6}\left(\frac{-2abt_ie^{ct_i}\left[bH_i+e^{ct_i}\left(H_i-a\right)\right]}{\left(e^{ct_i}+b\right)^3}\right)=0$$

$$(E1.2a,b,c)$$

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

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

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

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

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

$$b = 2.7767$$

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

Applying the Newton-Raphson method for simultaneous nonlinear equations with the above initial guesses, one can get the roots of Equations (1.2a,b,c)

$$a = 7.4321\times 10^1 \qquad b = 2.8233 \qquad c = 2.1715\times 10^{-1}$$

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

$$H=\frac{7.4321\times 10^1}{1+2.8233e^{-2.1715\times 10^{-1}t}}=\frac{7.4321\times 10^1}{1+2.8233e^{-2.1715\times 10^{-1}\times(30)}}$$

$$=74''$$

Growth Model

The logistic/saturated version

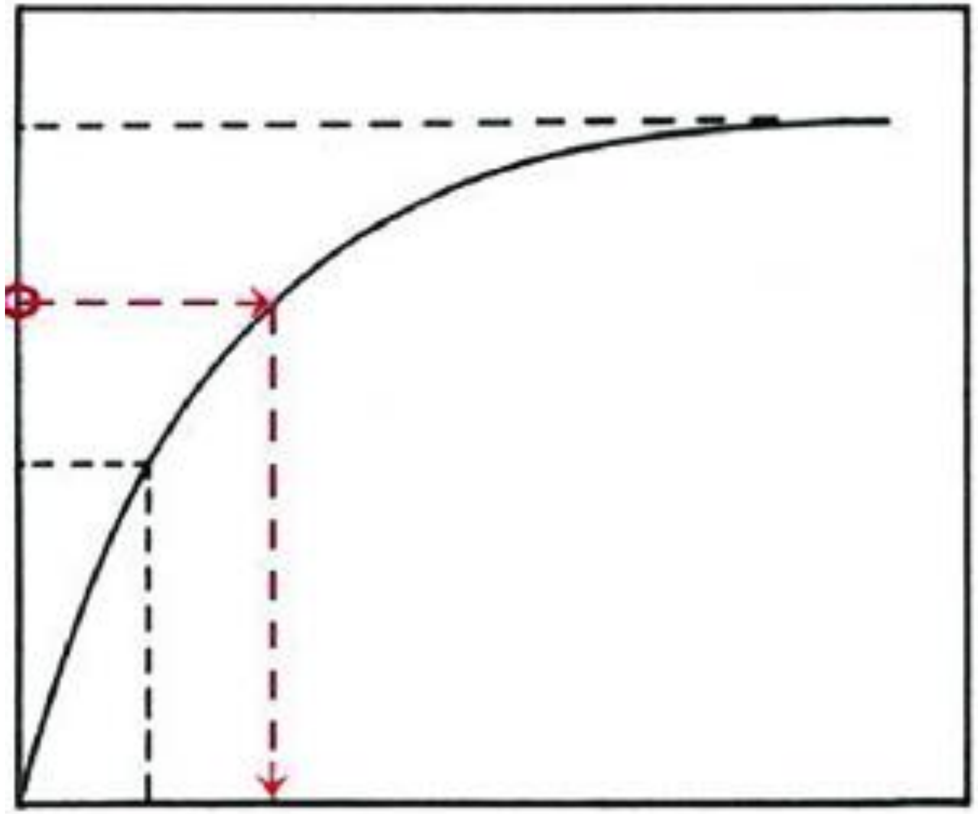
In the logistic growth model, an example of a growth model in which a measurable quantity y varies with some quantity x is

$$y = \frac{ax}{b+x} \qquad (5)$$

For $x = 0$, $y = 0$ while as $x \to \infty$, $y \to a$. 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 (5) as

$$\begin{aligned} \frac{1}{y} &= \frac{b+x}{ax} \\ &= \frac{b}{a}\frac{1}{x} + \frac{1}{a} \qquad (6) \end{aligned}$$



Growth Model

The logistic/saturated version (with Data Transformation)

To transform the data for this model, we rewrite Equation (5) as

$$\frac{1}{y} = \frac{b+x}{ax} = \frac{b}{a}\frac{1}{x} + \frac{1}{a} \qquad (6)$$

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

$$z = a_0 + a_1 w \qquad (7)$$

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

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

$$a_0 = \frac{\sum_{i=1}^{n} z_i}{n} - a_1 \frac{\sum_{i=1}^{n} w_i}{n} \qquad (8a, b)$$

$$\boxed{a = \frac{1}{a_0} \qquad b = \frac{a_1}{a_0}}$$

Mini Quiz

What about the original growth model?

Can we linearize the ***original Growth Model*** regression curve?

If so, how? If not, why?

$$y = \frac{a}{1 + be^{-cx}}$$

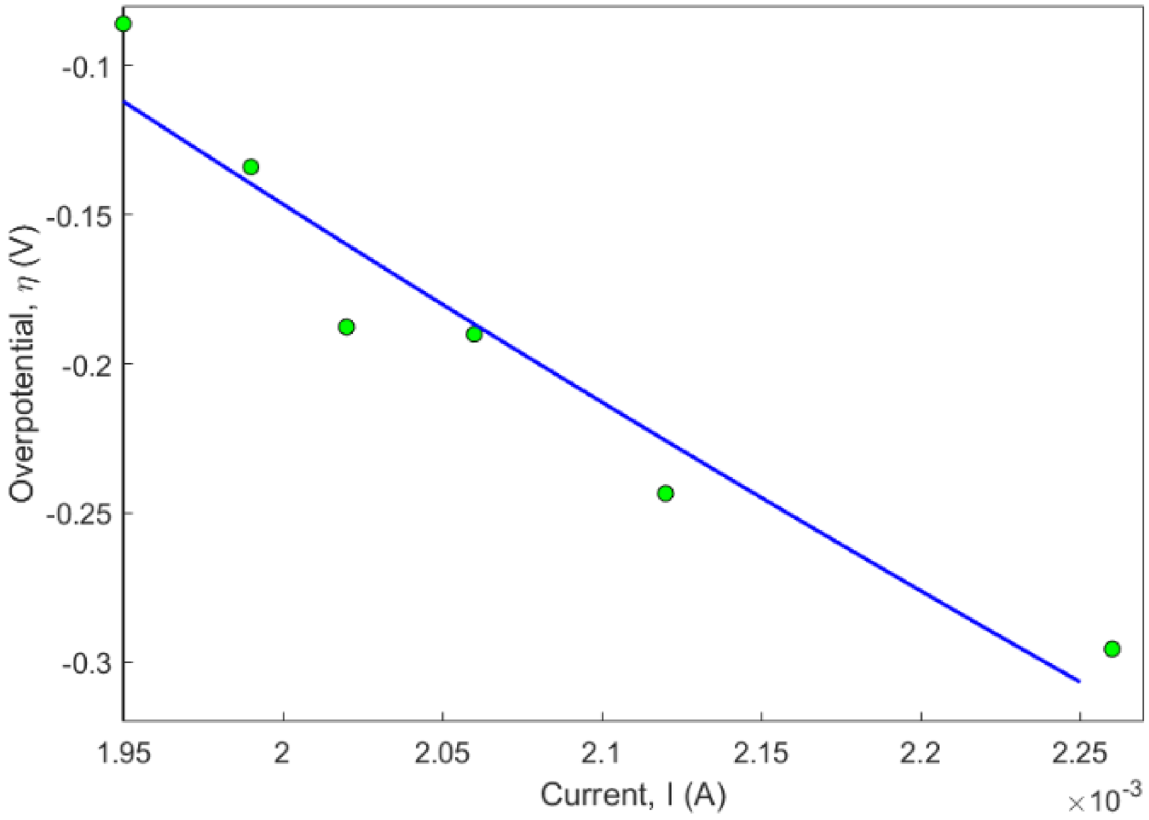
Logarithmic Model

What is it?

The form for the log regression models is

$$y = \beta_0 + \beta_1 \ln(x) \qquad (10)$$

Equation (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.



Derivation of the parameters left as an exercise.

Logarithmic Model

An example

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

Table 2 Electrochemical Kinetics of borohydride data.

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

At the conditions of the study, it is known that the relationship that exists between the overpotential (η) 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 2 to evaluate the values of a and b.

Logarithmic Model

An example

Solution

Following the least-squares method, Table 3 tabulates the summations where

$$x = \ln i$$
$$y = \eta$$

We obtain $y = a + bx \qquad (E2.1)$

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

$$b = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_1^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

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

Table 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	1.8011
2	0.00212	−0.24346	−6.1563	37.901	1.4988
3	0.00206	−0.19012	−6.1850	38.255	1.1759
4	0.00202	−0.18772	−6.2047	38.498	1.1647
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	7.0117

$n = 6 \qquad \sum_{i=1}^{6} x_i = -37.098 \qquad \sum_{i=1}^{6} y_i = -1.1371$

$\sum_{i=1}^{6} x_i y_i = 7.0117 \qquad \sum_{i=1}^{6} x_i^2 = 229.39$

Logarithmic Model

An example

$$b = \frac{6\left(7.0117\right) - \left(-37.098\right)\left(-1.1371\right)}{6\left(229.39\right) - \left(-37.098\right)^2}$$
$$= -1.3601$$

$$a = \frac{-1.1371}{6} - \left(-1.3601\right)\frac{-37.098}{6}$$
$$= -8.5990$$

Hence

$$\boxed{\eta = -8.5990 - 1.3601 \times \ln i}$$

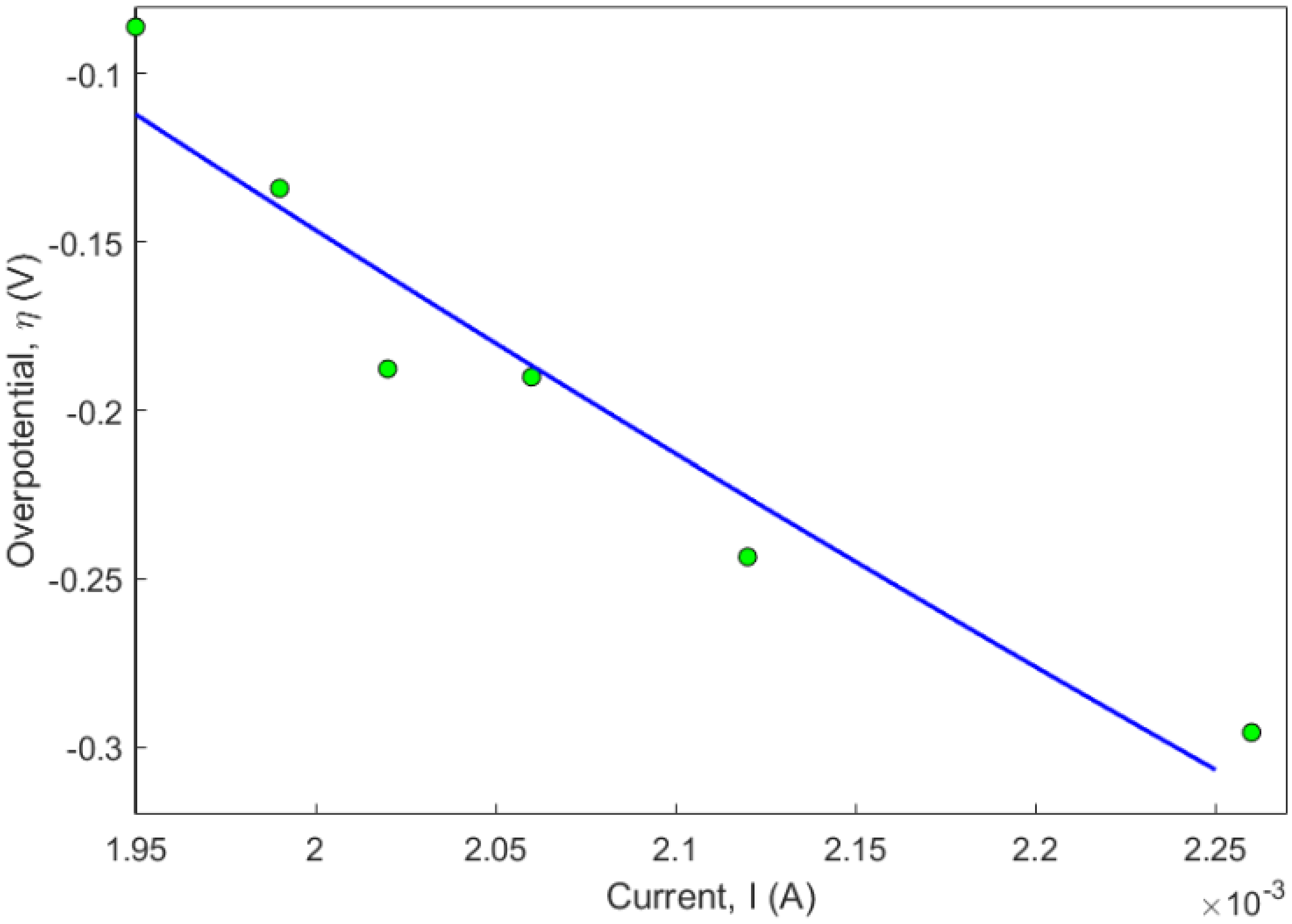


Figure 2 Overpotential as a function of current.$\eta(V)$

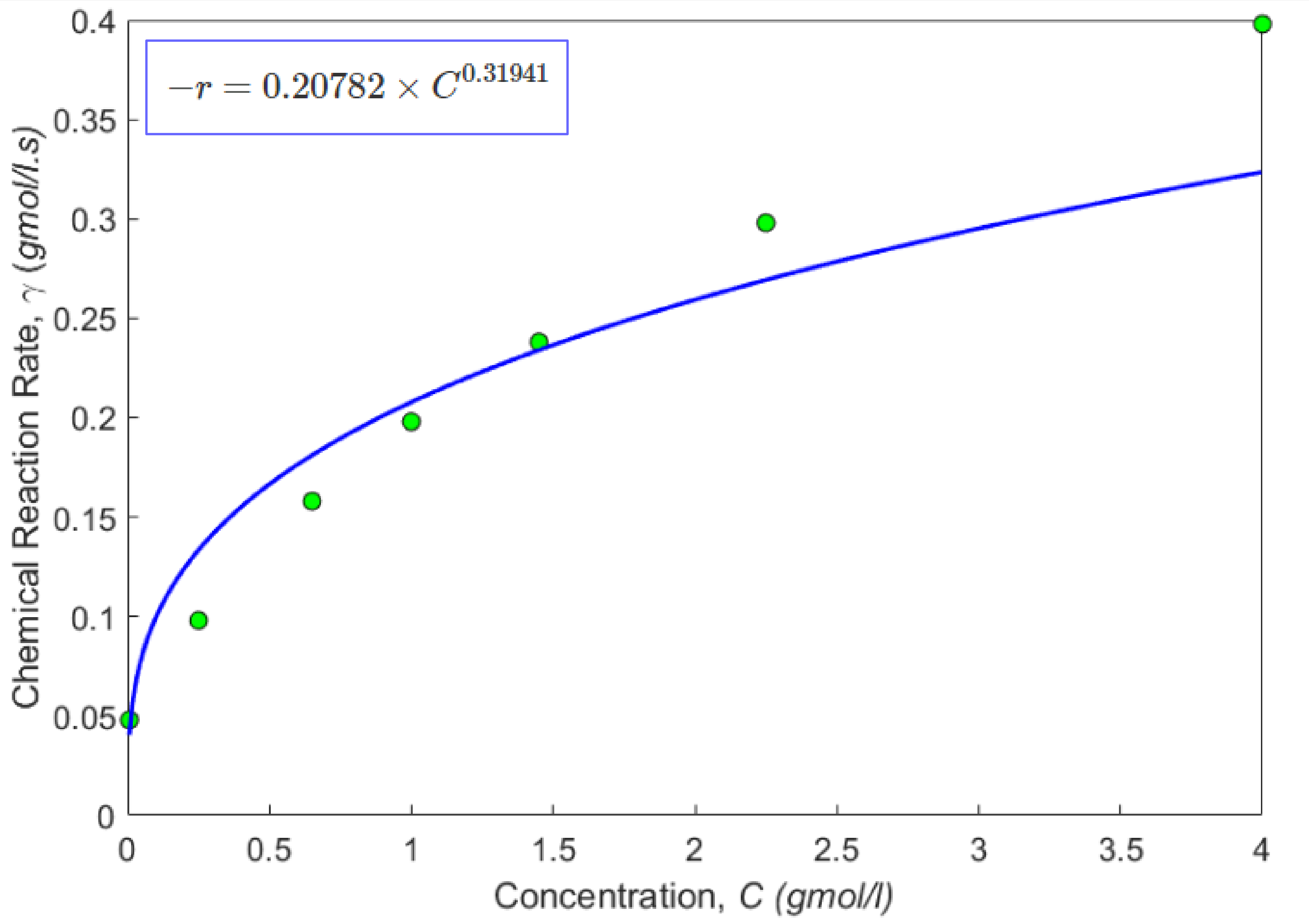
Power Model

What is it?

The ***power model*** regression curve is of the form —

$$y = ax^b$$

Derivation of the parameters left as an exercise.



Power Model

Applying data transformation

$$y = ax^b$$

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.

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

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

Let

$$z = \ln y$$

$$w = \ln(x)$$

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

$$a_1 = b$$

$$z = a_0 + a_1 w$$

$$a_1 = \frac{n\sum_{i=1}^{n} w_i z_i - \sum_{i=1}^{n} w_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} w_i^2 - \left(\sum_{i=1}^{n} w_i\right)^2} \qquad a_0 = \frac{\sum_{i=1}^{n} z_i}{n} - a_1\frac{\sum_{i=1}^{n} w_i}{n}$$

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

$$\boxed{\begin{aligned} b &= a_1 \\ a &= e^{a_0} \end{aligned}}$$

Power Model

An example

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

$$-r = kC^n$$

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

Table 4 Chemical kinetics.

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

Power Model

An example

Solution

Taking the natural log of both sides of Equation (35), we obtain

$$\ln(-r) = \ln(k) + n\ln(C) \qquad (E3.1)$$

Let

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

$$w = \ln(C)$$

$$a_0 = \ln(k)$$

implying that

$$k = e^{a_0}$$

$$a_1 = n \qquad (3.2a, b)$$

We get

$$z = a_0 + a_1 w$$

This is a linear relation between z and w, where

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

$$a_0 = \frac{\sum_{i=1}^{m} z_i}{m} - a_1 \frac{\sum_{i=1}^{m} w_i}{m} \qquad (E3.3)$$

Power Model

An example

Table 5 Kinetics rate law using power function

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

$$m = 7$$

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

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

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

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

From Equation (E3.3)

$$a_1 = \frac{7 \times (16.758) - (-4.3643) \times (-12.391)}{7 \times (30.998) - (-4.3643)^2}$$
$$= 0.31943$$

$$a_0 = \frac{-12.391}{7} - (0.31943)\frac{-4.3643}{7}$$
$$= -1.5711$$

Power Model

An example

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

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

$$n = a_1 = 0.31941$$

Finally, the model of progress of that chemical reaction is

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