Nonlinear Regression Without Transformation of Data

Nonlinear Regression

Popular nonlinear regression models. Given n data pairs (x_1, y_1), (x_2, y_2), . . . (x_n, y_n)

1. Exponential model: $y = ae^{bx}$
2. Power model: $y = ax^b$
3. Saturation growth model: $y = \frac{ax}{b+x}$
4. Polynomial model: $y = a_0 + a_1 x + a_2 x^2 + \cdots\cdots + a_m x^m$

Nonlinear Regression

Given (x_1, y_1), (x_2, y_2), . . . (x_n, y_n), best fit $y = f(x)$ to the data.

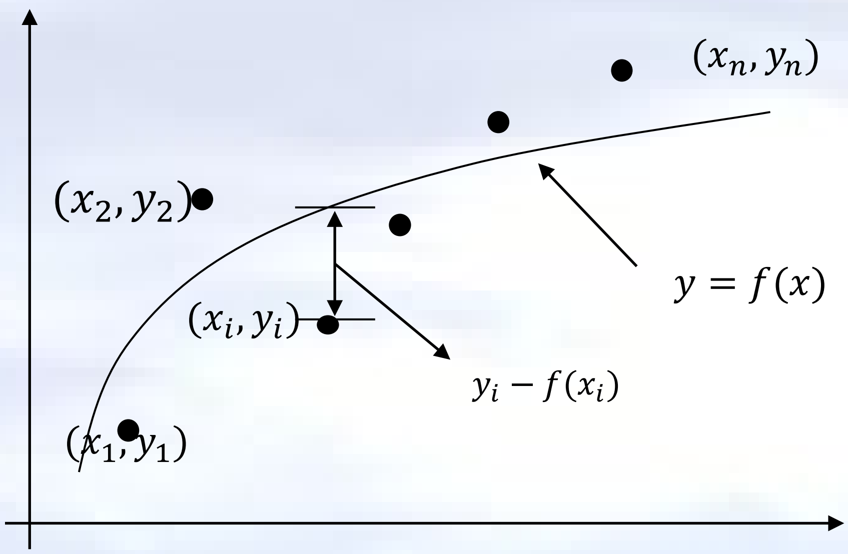


Figure. Nonlinear regression model for discrete y vs. x data

Exponential Model

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

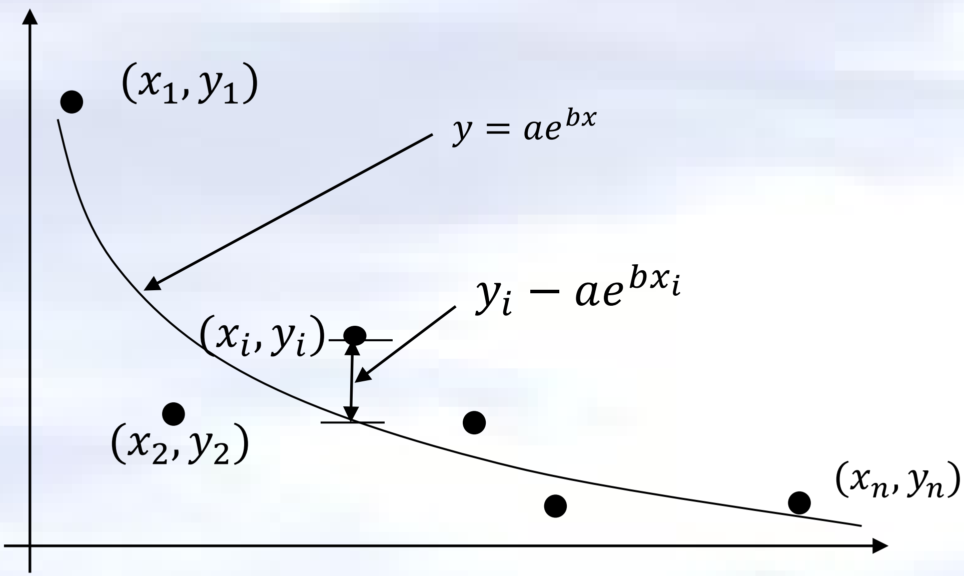


Figure. Exponential model of nonlinear regression for y vs. x data

Finding Constants of Exponential Model

The sum of the square of the residuals is defined as

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

Differentiate with respect to a and b, and put it equal to zero

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

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

Finding Constants of Exponential Model

Solving the first equation for a yields

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

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

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

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

Example - Exponential Model

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

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

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

Example - Exponential Model (contd)

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,

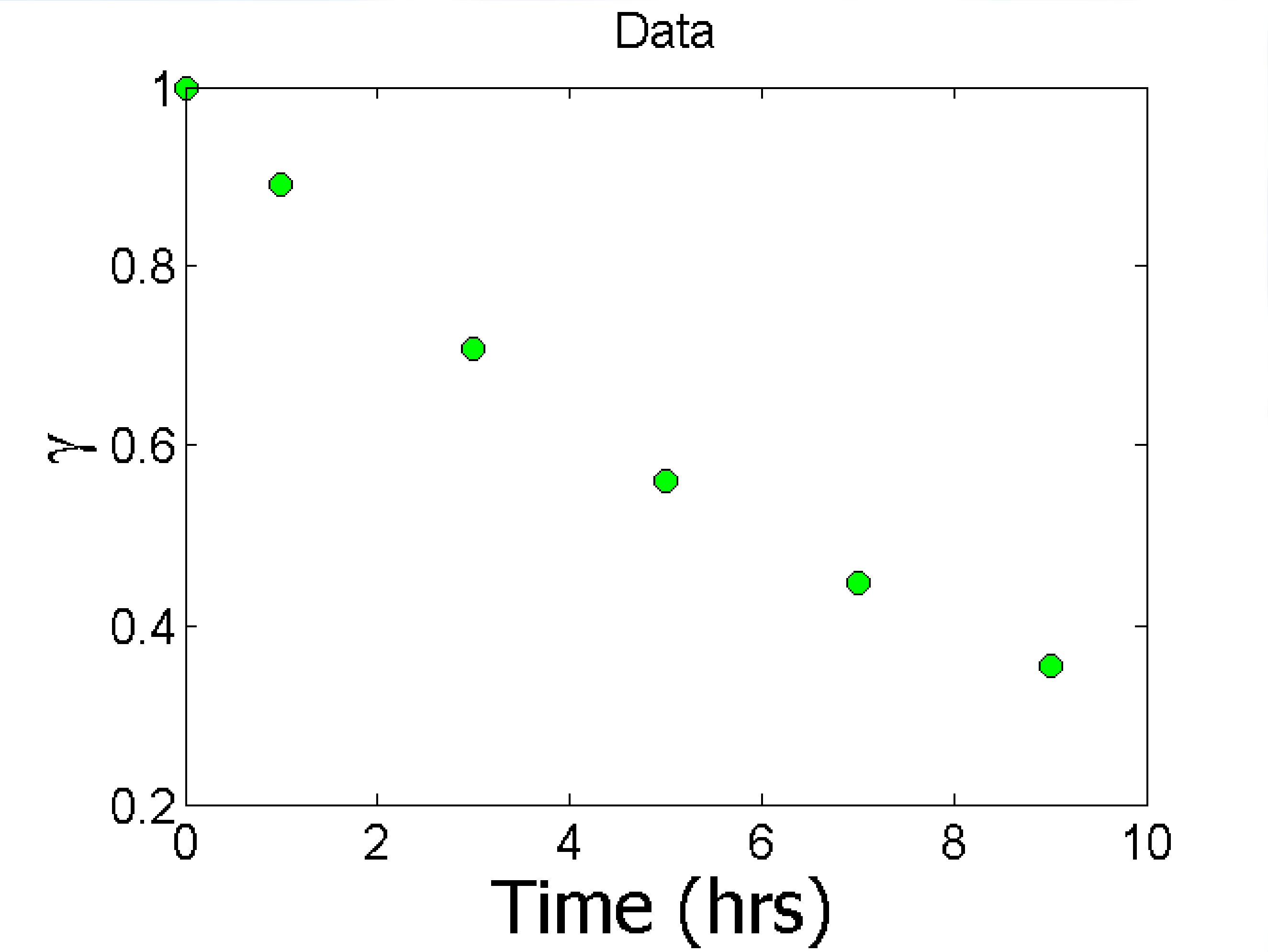
b) the half-life of Technium-99m, and

c) the radiation intensity after 24 hours.

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

t_i (hrs)	0	1	3	5	7	9
γ_i	1.000	0.891	0.708	0.562	0.447	0.355

Plot of data



Constants of the Model

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

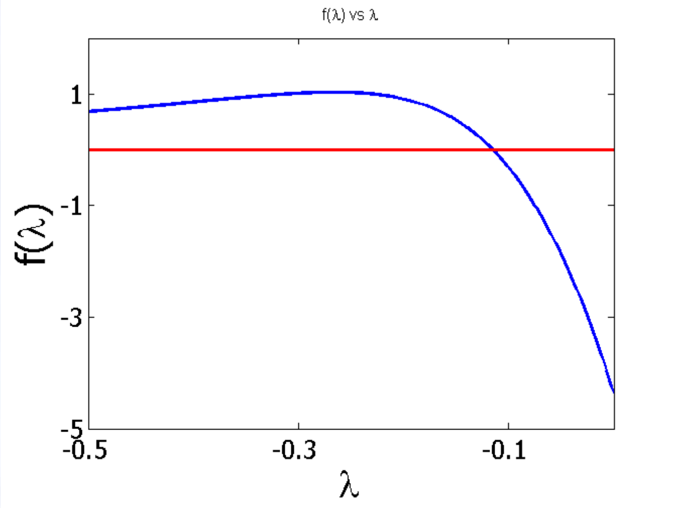
The value of λ is found by solving the nonlinear equation

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

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

Setting up the Equation in MATLAB

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



t_i (hrs)	0	1	3	5	7	9
γ_i	1.000	0.891	0.708	0.562	0.447	0.355

Setting up the Equation in MATLAB

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

$$\lambda = -0.1151$$

```
t=[0 1  3  5  7  9]
gamma=[1.000  0.891  0.708  0.562  0.447  0.355]
syms lamda
sum1=sum(gamma.*t.*exp(lamda*t));
sum2=sum(gamma.*exp(lamda*t));
sum3=sum(exp(2*lamda*t));
sum4=sum(t.*exp(2*lamda*t));
f=sum1-sum2/sum3*sum4;
```

Calculating the Other Constant

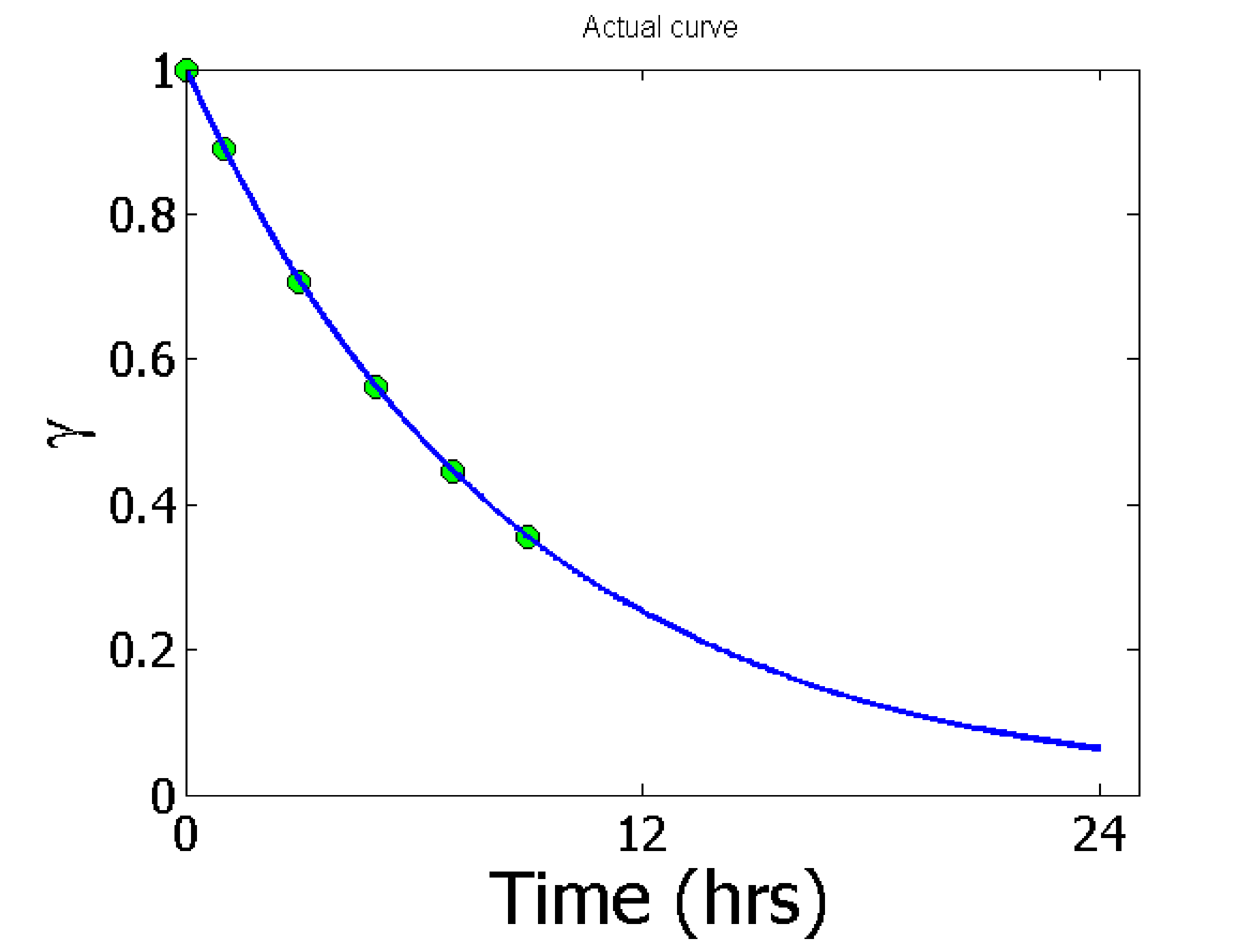
The value of A can now be calculated

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

The exponential regression model then is

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

Plot of data and regression curve



Relative Intensity After 24 hrs

Relative intensity of radiation after 24 hours

$$\gamma = 0.9998 \times e^{-0.1151(24)} = 6.3160 \times 10^{-2}$$

Percentage radioactive intensity left after 24 hours

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

Homework

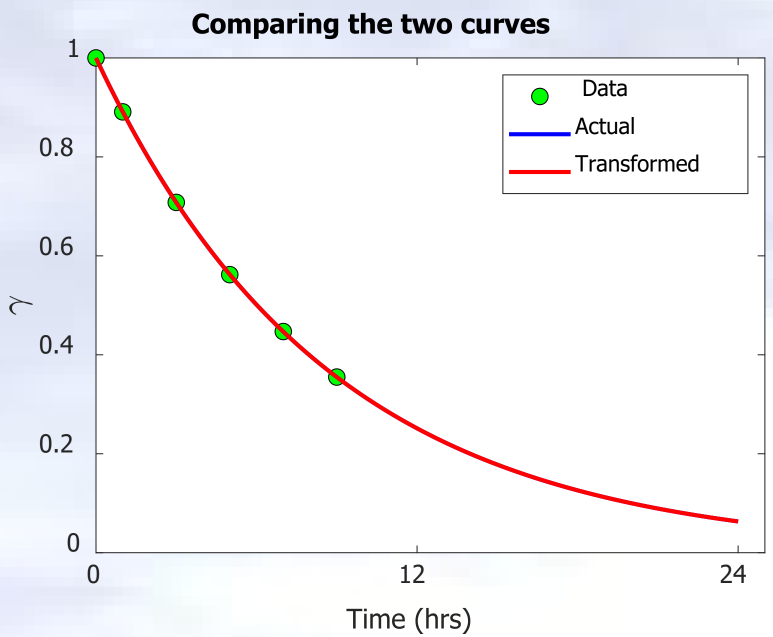
- What is the half-life of Technetium-99m isotope?
- Write a program in the language of your choice to find the constants of the model.
- Compare the constants of this regression model with the one where the data is transformed.
- What if the model was $\gamma = e^{\lambda t}$?

Without Transformation $\gamma = 0.9998\, e^{-0.1151t}$

With Transformation: $\gamma = 0.9997 e^{-0.1151t}$

Transformed vs Untransformed Data

t_i (hrs)	0	1	3	5	7	9
γ_i	1.000	0.891	0.708	0.562	0.447	0.355



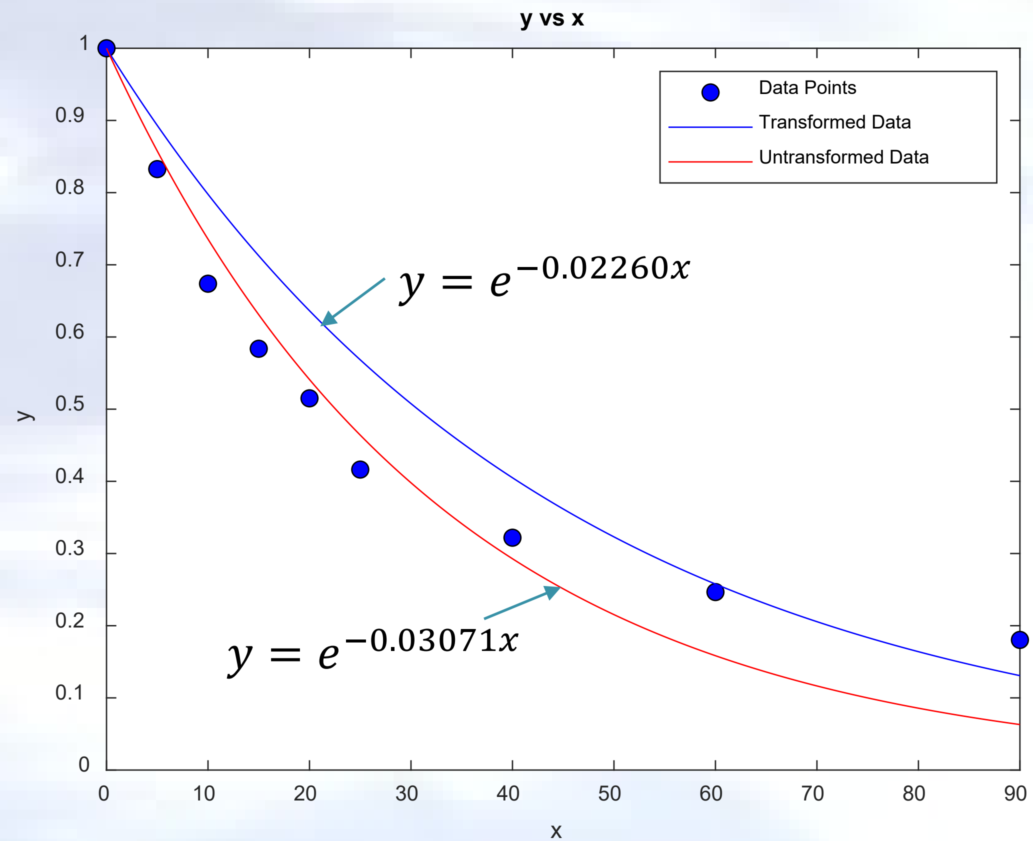
Without Transformation $\gamma = 0.9998\, e^{-0.1151t}$

With Transformation: $\gamma = 0.9997 e^{-0.1151t}$

Transformed vs Untransformed Data

$$y = e^{bx}$$

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



Without Transformation $y = e^{-0.03071t}$

With Transformation: $y = e^{-0.02260t}$

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