Nonlinear Regression: Untransformed Data

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Nonlinear Regression

Some popular nonlinear regression models:

1. Exponential model: $(y = ae^{bx})$
2. Power model: $(y = ax^{b})$
3. Saturation growth model: $\left(y = \dfrac{ax}{b + x}\right)$
4. Polynomial model: $(y = a_0 + a_1x + \ldots + amx^{m})$

Nonlinear Regression

Given *n* data points $(x_1,y_1), \ldots\ldots (x_n,y_n)$, best fit $y = f(x)$ to the data, where $f(x)$ is a nonlinear function of x

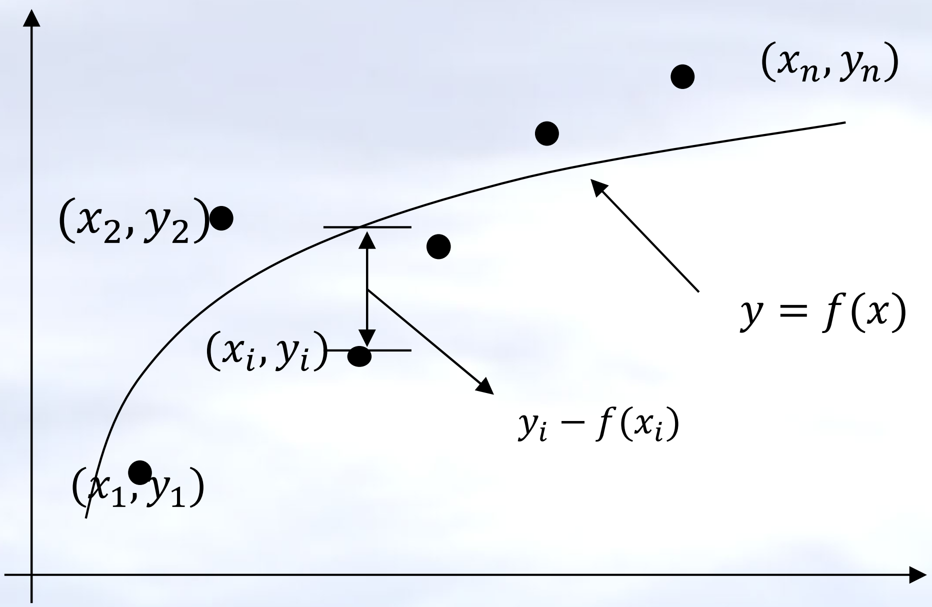


Figure. Nonlinear regression model for discrete y vs. x data

Exponential Model

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

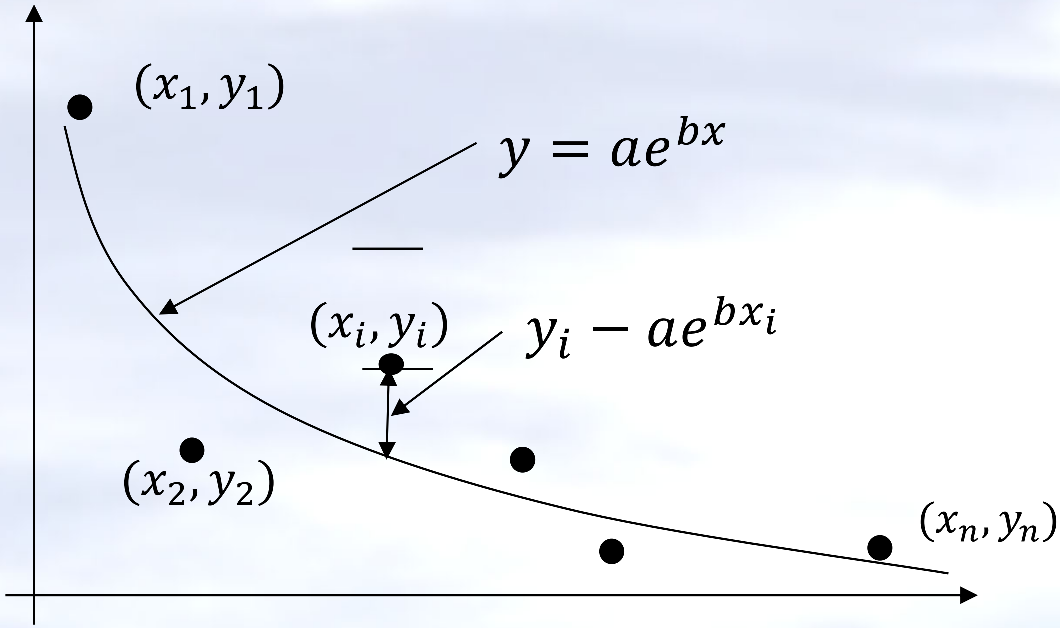


Figure. Exponential model of nonlinear regression for y vs. x data

Finding Constants of Exponential Model

The sum of the square of the residuals is defined as

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

Differentiate with respect to *a* and *b*

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

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

Finding Constants of Exponential Model

Rewriting the equations, we obtain

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

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

Finding constants of Exponential Model

Solving the first equation for a yields

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

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

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

Example 1-Exponential Model

Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the 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 1-Exponential Model cont.

The relative intensity is related to time by the equation

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

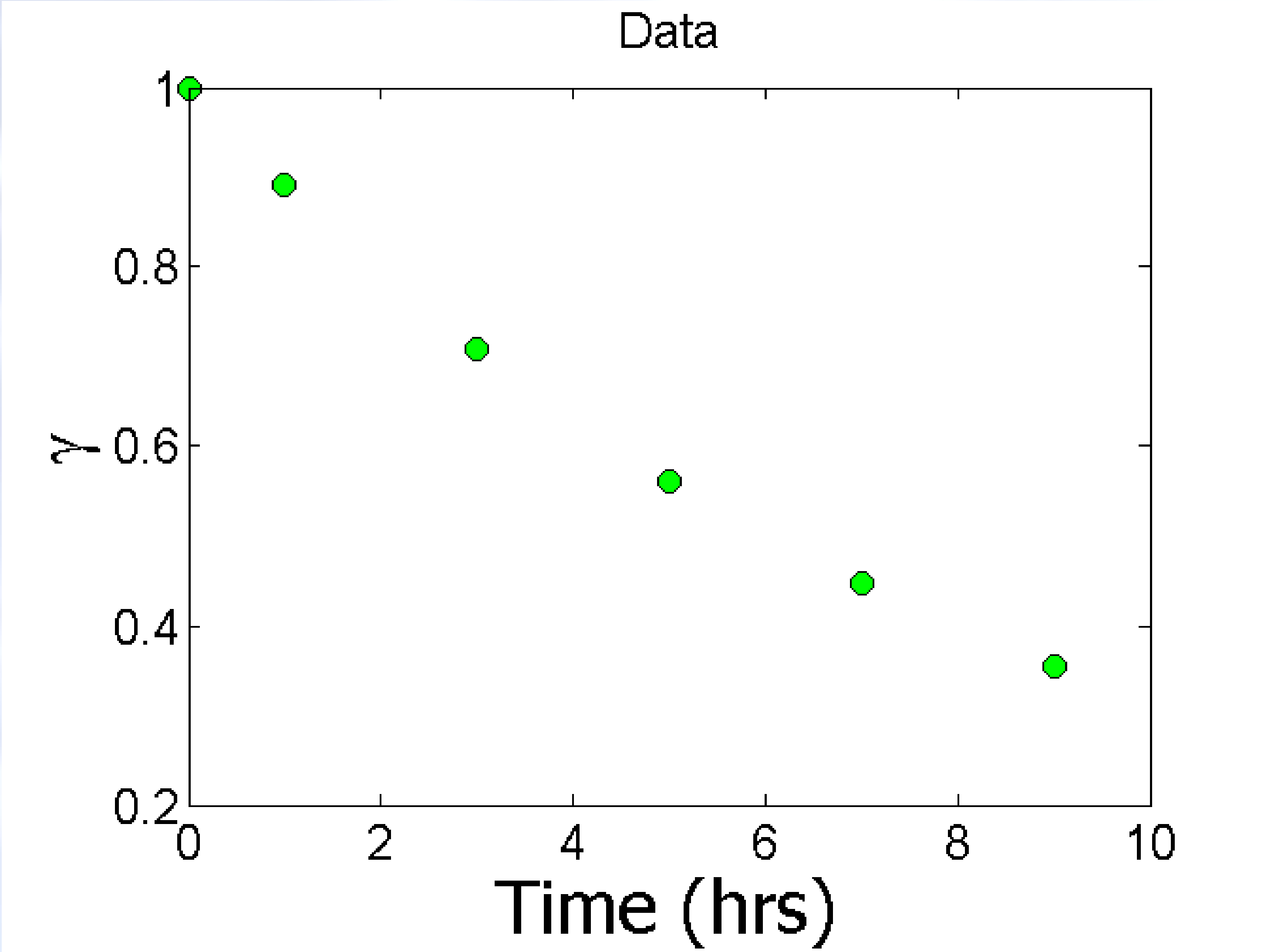
Find:

a) The value of the regression constants A and λ

b) The half-life of Technetium-99m

c) Radiation intensity after 24 hours

Plot of data



Constants of the Model

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

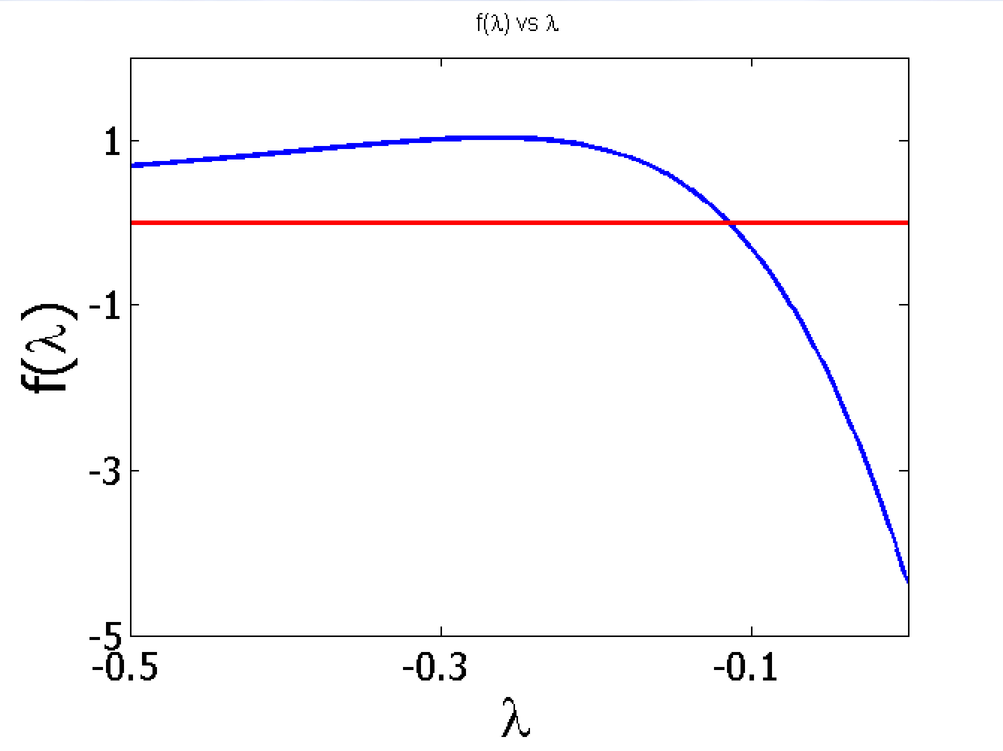
The value of λ is found by solving the nonlinear equation

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

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

Plotting the Equation in MATLAB

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



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

Setting up the Equation in MATLAB

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

$$\lambda = -0.1151$$

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

Calculating the Other Constant

The value of *A* can now be calculated

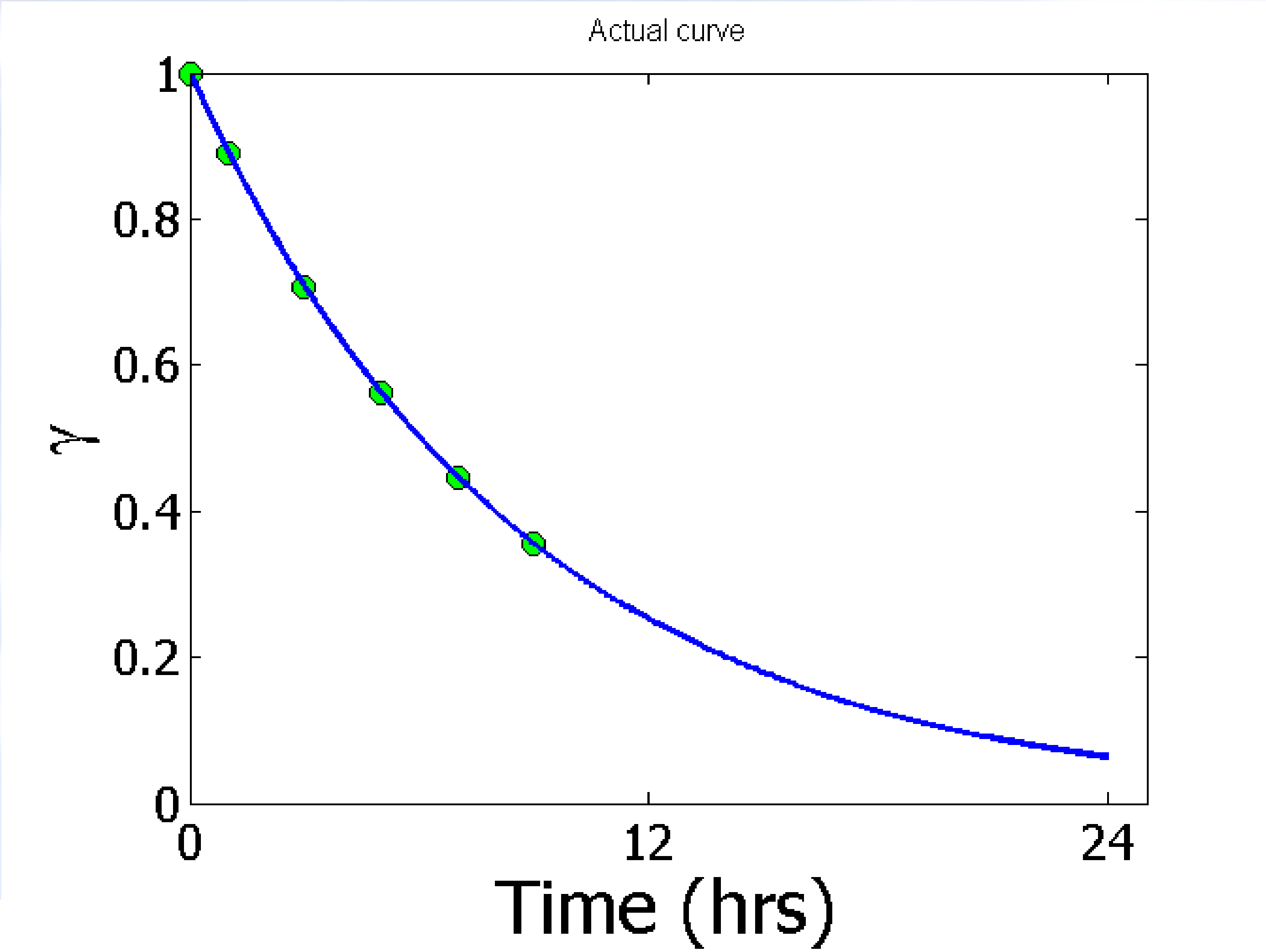
$$A = \frac{\sum_{i=1}^{6} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{6} e^{2\lambda t_i}}$$

$$= 0.9998$$

The exponential regression model then is

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

Plot of data and regression curve



Relative Intensity After 24 hrs

The relative intensity of radiation after 24 hours

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

$$= 6.3160 \times 10^{-2}$$

This result implies that only

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

radioactive intensity is left after 24 hours.

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