PMDS504L: Regression Analysis and Predictive Models

Nonlinear Regression Models

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Table of Contents

Linearization of Nonlinear System: Example

Many physical and chemical processes are governed by the exponential function:

$$\gamma = ae^{bx} \tag{1}$$

Taking the natural logarithm on both sides of Equation (1) gives:

$$\ln \gamma = \ln a + bx \tag{2}$$

Let:

$$z = \ln \gamma, \quad a_0 = \ln a \quad (\text{implying } a = e^{a_0})$$

$$a_1 = b$$

Linearization of Nonlinear System: Example

Then, the equation transforms into a linear form:

$$z = a_0 + a_1 x \tag{3}$$

Radioactive Material in Medical Tests

Many patients get concerned when a test involves the injection of a radioactive material. For example, for scanning 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.

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

Problem Statement

The radiation intensity follows an exponential decay model:

$$\gamma = Ae^{\lambda t} \tag{1}$$

1. Find the regression constants A and λ.
2. Determine the **half-life** of Technetium-99m.
3. Calculate the radiation intensity after $t = 24$ hours.

Transforming Data to a Linear Model

The given data values and their natural logarithms are:

t (hrs)	γ	$z = \ln \gamma$
0	1.000	0.000
1	0.891	-0.115
3	0.708	-0.345
5	0.562	-0.578
7	0.447	-0.805
9	0.355	-1.035

The transformed equation now takes the form: $z = a_0 + a_1 t$, where $z = \ln \gamma$.

Finding the Constants a_0 and a_1

The constants a_0 and a_1 can be determined using the least squares method:

$$\hat{a}_1 = \frac{\sum t_i z_i - \frac{1}{n}\sum t_i \sum z_i}{\sum t_i^2 - \frac{1}{n}\left(\sum t_i\right)^2} \tag{4a}$$

$$\hat{a}_0 = \frac{1}{n}\sum z_i - \hat{a}_1 \frac{1}{n}\sum t_i \tag{4b}$$

Summation Table for Calculating Constants

i	t_i (hrs)	γ_i	$y_i = \ln \gamma_i$	$t_i y_i$
1	0	1.000	0.00000	0.0000
2	1	0.891	-0.11541	-0.11541
3	3	0.708	-0.34531	-1.0359
4	5	0.562	-0.57625	-2.8813
5	7	0.447	-0.80520	-5.6364
6	9	0.355	-1.03560	-9.3207
$\sum$	25.000	—	-2.8778	-18.990

Calculation of Model Constants

$$\sum t_i^2 = 165.00, \quad n = 6$$

$$\sum t_i y_i = -18.990$$

Calculation of Model Constants

Using the least squares equations:

$$a_1 = \frac{n\sum t_i y_i - \sum t_i \sum y_i}{n\sum t_i^2 - (\sum t_i)^2}$$

Substituting values:

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

$$a_1 = -0.11505$$

Calculation of Model Constants

Similarly,

$$a_0 = \frac{\sum y_i}{n} - a_1 \frac{\sum t_i}{n}$$

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

$$a_0 = -2.6150 \times 10^{-4}$$

Since $a_0 = \ln A$, we get:

$$A = e^{-2.6150 \times 10^{-4}} = 0.99974$$

Final Regression Model

The regression equation is:

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

Comparing with the model obtained without data linearization:

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

Half-Life Calculation

Half-life is found using:

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

$$0.99983e^{-0.11508t} = \frac{1}{2}0.99983e^{-0.11508\times 0}$$

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

Relative Intensity After 24 Hours

The relative intensity after 24 hours is:

$$\gamma = 0.99974e^{-0.11505(24)}$$

$$\gamma = 0.06320$$

This implies that only 6.3216% of the initial radioactivity is left after 24 hours.

Logarithmic Regression Model

The form of the logarithmic regression model is:

$$y = \beta_0 + \beta_1 \ln(x) \tag{2}$$

This is a linear function between y and $\ln(x)$, where:

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

The usual least squares method applies.

Example: Electrochemical Kinetics of Borohydride

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

Table: Electrochemical Kinetics Data

η (V)	i (A)
-0.29563	0.00226
-0.24346	0.00212
-0.19012	0.00206
-0.18772	0.00202
-0.13407	0.00199
-0.08610	0.00195

Example: Electrochemical Kinetics of Borohydride

At the conditions of the study, it is known that the relationship between the overpotential (η) and current (i) can be expressed as:

$$\eta = a + b \ln i \tag{3}$$

Using the given data, determine the values of a and b.

Least Squares Method and Summation Table

The linear relationship between y and x is given by:

$$y = a + bx \tag{4}$$

where $x = \ln(i)$ and $y = \eta$. The coefficients a and b are found using:

$$b = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - (\sum x)^2} \tag{5}$$

$$a = \bar{y} - b\bar{x} \tag{6}$$

Least Squares Method and Summation Table

Table: Summation Values for Calculating Constants of the Model

#	i	$y = \eta$	$x = \ln(i)$	x^2	$x \times y$
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
$\sum$	0.01240	-1.1371	-37.098	229.39	7.0117

Final Regression Equation

The estimated equation is:

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

Interpretation:

- The coefficient $a = -0.0891$ represents the intercept.
- The coefficient $b = -0.0347$ shows how η changes with $\ln(i)$.

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:

$$y = ax^b \tag{7}$$

The method of least squares is applied to the power function by first linearizing the data (assuming b is not known). If the only unknown is a, then a linear relation exists between x^b and y. The linearization of the data is as follows:

$$\ln(y) = \ln(a) + b\ln(x) \tag{8}$$

Power Functions

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

$$w = \ln(x), \quad z = \ln(y) \tag{9}$$

Defining:

$$a_0 = \ln a \quad \text{implying} \quad a = e^{a_0} \tag{10}$$

$$z = a_0 + a_1 w \tag{11}$$

Power Functions

The least squares estimators are given by:

$$a_1 = \frac{n\sum wz - \sum w \sum z}{n\sum w^2 - (\sum w)^2} \tag{12}$$

$$a_0 = \frac{\sum z}{n} - a_1 \frac{\sum w}{n} \tag{13}$$

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

$$a = e^{a_0}, \quad b = a_1 \tag{14}$$

Example: Chemical Reaction Kinetics

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:

$$-r = kC^n \tag{15}$$

Using the given data, find n and k.

Example: Chemical Reaction Kinetics

Table: Chemical Kinetics Data

C_A (gmol/L)	$-r_A$ (gmol/L?s)
4.00	0.398
2.25	0.298
1.45	0.238
1.00	0.198
0.65	0.158
0.25	0.098
0.006	0.048

Growth Model

Growth models are commonly used in scientific fields to describe how a quantity grows with changes in a regressor variable, often time. These models have been successfully developed and applied to specific situations, such as the growth of thin films or population dynamics. One example is the **logistic growth model**, where a measurable quantity y varies with another quantity x, given by:

$$y = \frac{ax}{b+x} \tag{16}$$

Properties:

- When $x = 0$, then $y = 0$.
- As $x \to \infty$, $y \to a$.

Linearizing the Growth Model

To linearize the model, we rewrite it as:

$$\frac{1}{y} = \frac{1}{a} + \frac{b}{a} \cdot \frac{1}{x} \tag{17}$$

Let:

$$z = \frac{1}{y}, \quad w = \frac{1}{x} \tag{18}$$

Define:

$$a_0 = \frac{1}{a}, \quad a_1 = \frac{b}{a} \tag{19}$$

Then the linear form becomes:

$$z = a_0 + a_1 w \tag{20}$$

Estimating Parameters Using Least Squares

The coefficients a_0 and a_1 are computed as:

$$a_1 = \frac{n\sum wz - \sum w \sum z}{n\sum w^2 - (\sum w)^2} \tag{21}$$

$$a_0 = \frac{\sum z}{n} - a_1 \frac{\sum w}{n} \tag{22}$$

Using these values, the original growth model constants are:

$$a = \frac{1}{a_0}, \quad b = \frac{a_1}{a_0} \tag{23}$$

These parameters can then be used to fit the growth model to data.

References

- Montgomery, D. C., Peck, E. A., & Vining, G. G. (2012). Introduction to Linear Regression Analysis, Fifth Edition. Wiley.
- MTH 416 : Regression Analysis — Shalabh, IIT Kanpur

Thank You!

Thank you for your attention!