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Research Paper

Linear modeling and regression for exponential engineering functions by a generalized ordinary least squares method

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Abstract

Linear transformations are performed for selected exponential engineering functions. The Optimum values of parameters of the linear model equation that fits the set of experimental or simulated data points are determined by the linear least squares method. The classical and matrix forms of ordinary least squares are illustrated.

Keywords: *Exponential Functions; Linear Modeling; Ordinary Least Squares; Parametric Estimation; Regression Steps.*

1. Introduction

Many engineering processes and systems (physical, chemical, nuclear, or biochemical) are considered first- order systems which can be described by a first-order ordinary differential equation (ODE). The solution of this differential equation is often expressed by an exponential function that may be linearized into a straight line equation with a slope and an intercept. The best fit (the optimum values of a slope and an intercept) for an experimental or simulated set of data points can be obtained by using the least squares method, which is the most widely used criterion. It has been a common practice to plot the data points on a graph paper and draw the best straight line through them. However, the method of least squares gives a more reliable way to obtain a better functional relationship.

The linearization of a function is the first order term of its Taylor power series expansion around the point of interest [9]. Francis Galton (1822-1911), a scientist and polymath, was the first who studied linear statistical models (regression) [10]. Linear regression is the study of linear (straight-line) relationships between variables, usually under an assumption of normally distributed errors. Gauss is credited with developing the fundamentals of the basis for the least- squares analysis in 1795 at the age of eighteen [11]. However, Legendre was the first to publish the method. Mosconi and Solonnikov [12] prove a general linearization principle which gives existence of a global solution of the associated system and exponential convergence of the latter to the stationary one. Naudot and Yang [13] studied normalization and quasi-linearization of a family of germs of hyperbolic vector fields at the origin. Ali et al. [14] design and linearize concurrent dual-band doherty power amplifier with frequency-dependent power ranges.

Chubich and Chernikova [15] studied Gaussian nonlinear discrete systems based on the time domain linearization and optimal control. Denisov et al. [16] used a statistical linearization to obtain stochastic continuous-discrete models and estimated the parameters of these mathematical models. Cao et al. [17] proposed a nonlinear least squares method to estimate the time-varying coefficients in an ODE that models an HIV dynamic system. Cai and Chen [18] proposed finite iteration steps for the least squares method to obtain a least norm solution for an initial linear matrix. Kwong et al. [19] used fuzzy least-squares regression (FLSR) to model the relationships in QFD (quality function deployment) considering both fuzziness and randomness into account. Kadalbajoo and Arora [20] proposed a stabilized finite-element method (Galerkin least-squares) to determine the parameters of the devection-diffusion equation.

Lu et al. [21] investigated the dual regularized total least squares (dual RTLS), and proposed a strategy for finding two regularization parameters in the resulting equation. Bensic [22] illustrated the way of using a generalized nonlinear regression method for the purpose of parameter estimation in the classical parametric independent and identically distributed sample model. Quan et al. [23] proposed a weighted least square support vector machine (WLS-SVM) for the prediction of nonlinear time series. Zhou et al. [24] proposed gradient based iterative algorithms (based on weighted least squares) to solve the general coupled Sylvester matrix equations.

The objective of this paper is to illustrate the executive steps of linearization and optimization by the ordinary least squares method applying on the exponential engineering functions in order to determine the optimum parameters in a linear regression model that govern the investigated system (physical, chemical, or biochemical). The least squares method may be used as a classical form or as a matrix form. Moreover, it can either be used separately, or within algorithms in computer programs.

The concept of the linear least squares method is to determine the constants (a slope and an intercept) of the linear equation by minimizing the sum of the squares of the differences (residuals) between the measured values (y_1, y_2, …, y_n) and the values of the fitting linear function ($y = a\,x + b$) [8].

That is,

$a\,x_1 + b - y_1 = r_1$

$a\,x_2 + b - y_2 = r_2$

$\vdots$

$a\,x_n + b - y_n = r_n$

So that

$\sum_{i=1}^{n} r_i^2$ = minimum

Which can be solved by performing the following:

$$\frac{\partial}{\partial a}\sum_{i=1}^{n} r_i^2 = 0$$

And

$$\frac{\partial}{\partial b}\sum_{i=1}^{n} r_i^2 = 0$$

Solving these partial differential equations for a and b give

$$a = \frac{n(\sum xi\,yi) - (\sum x_i)(\sum y_i)}{n(\sum x_i^2) - (\sum x_i)^2}$$

And

$$b = \frac{(\sum y_i)(\sum x_i^2) - (\sum xi\,yi)(\sum x_i)}{n(\sum x_i^2) - (\sum x_i)^2}$$

2. Linearization procedures

The following are selected exponential engineering functions that may be linearized:

a) For atomic solid diffusion [1],

$$D = D_o\, \boldsymbol{e}^{-q_d/RT} \quad (1)$$

Or

$\ln D = \ln D_o - \frac{q_d}{RT}$

Which becomes

$y = b + a\,x$, $y = \ln D$, $a = \frac{-q_d}{R}$, $b = \ln D_o$, $x = \frac{1}{T}$

b) For gas dynamic viscosity [2],

$$\mu = \mu_o\, \boldsymbol{e}^{-q_v/RT} \quad (2)$$

Or

$\ln \mu = \ln \mu_o - \frac{q_v}{RT}$

So

$y = b + a\,x$, $y = \ln \mu$, $a = \frac{-q_v}{R}$, $b = \ln \mu_o$, $x = \frac{1}{T}$

c) For chemical reaction rate constant [3],

$$k = k_o\, \boldsymbol{e}^{-E/RT} \quad (3)$$

$\ln k = \ln k_o - \frac{E}{RT}$

Becomes

$y = b + a\,x$, $y = \ln k$, $a = \frac{-E}{R}$, $b = \ln k_o$, $x = \frac{1}{T}$

d) For nuclear decay [4],

$$N = N_o\, \boldsymbol{e}^{-\lambda t} \quad (4)$$

$\ln N = \ln N_o - \lambda\, t$

Thus

$y = b + a\,x$, $y = \ln N$, $a = -\lambda$, $b = \ln N_o$, $x = t$

e) For biochemical oxygen demand [5],

$$BOD = L\,(1 - \boldsymbol{e}^{-k\,t}) \quad (5)$$

$1 - (\frac{BOD}{L}) = e^{-k\,t}$
Or
$\ln(1 - (\frac{BOD}{L})) = -k\,t$
And so
y = a x , $y = \ln(1 - (\frac{BOD}{L}))$, a = - k , x = t

f) For heating dynamic response to a step input [6],

$$(T - T_o) = (T_f - T_o)(1 - e^{-t/\tau}) \qquad (6)$$

$1 - \left[\frac{(T - T_o)}{(T_f - T_o)}\right] = e^{-t/\tau}$
Or
$\ln\left[1 - \left[\frac{(T - T_o)}{(T_f - T_o)}\right]\right] = \frac{-t}{\tau}$
Hence
y = a x , $y = \ln\left[1 - \left[\frac{(T - T_o)}{(T_f - T_o)}\right]\right]$, $a = \frac{-1}{\tau}$, x = t

g) For a stress-strain relation of concrete compression [7],

$$\sigma = k_1 \epsilon\, e^{-k_2 \epsilon} \qquad (7)$$

Or
$\ln\left(\frac{\sigma}{\epsilon}\right) = \ln k_1 - k_2\,\epsilon$
Thus
y = a + b x , $y = \ln\left(\frac{\sigma}{\epsilon}\right)$, $a = \ln k_1$, $b = -k_2$, $x = \epsilon$

Nomenclature:
D—diffusion coefficient, m^2/s;
D_o—temperature independent preexponential, m^2/s;
q_d—activation energy for diffusion, J/mol;
R—universal gas constant, 8.314 J/mol.K°
T—absolute temperature, K°
μ—dynamic viscosity coefficient, cP;
μ_o—preexponential factor, cP;
q_v—activation energy for viscosity, J/mol;
k—chemical or biochemical reaction rate constant, min^{-1};
k_o—frequency factor, min^{-1};
E—activation energy for the reaction, J/mol;
N_o—original number of unstable nuclei present at the initial time (t = 0);
N—number of nuclei present at some subsequent time (t);
λ—decay constant ($\lambda = \ln 2 / t_{1/2}$);
BOD—biochemical oxygen demand, mg of O_2/L;
L—initial level of oxygen, mg of O_2/L;
τ—time constant of the process, s;
T_o—initial temperature of the process, K°;
T_f—final temperature of the process, K°;
σ—applied stress, psi;
ϵ—strain ($\epsilon = \Delta L/L_o$);
k_1 & k_2—compression constants;

3. Regression approaches

The undetermined constants (the slope and intercept) of the straight line equation that best fit the experimental or simulated data points can be determined by the least squares method which can be performed by either of the following forms (the classical or matrix) [8]:

A) y = a x + b
Let

$S_x = \frac{1}{n}\sum x_i = \frac{1}{n}(x_1 + x_2 + \cdots + x_n)$

$S_y = \frac{1}{n}\sum y_i = \frac{1}{n}(y_1 + y_2 + \cdots + y_n)$

$S_{xy} = \frac{1}{n}\sum x_i y_i = \frac{1}{n}(x_1 y_1 + x_2 y_2 + \cdots + x_n y_n)$

$S_{xx} = \frac{1}{n}\sum x_i^2 = \frac{1}{n}(x_1^2 + x_2^2 + \cdots + x_n^2)$

Then

$$a = \frac{S_{xy} - S_x\, S_y}{S_{xx} - (S_x)^2}$$

And

$$b = \frac{S_{xx}\, S_y - S_{xy}\, S_x}{S_{xx} - (S_x)^2}$$

B) $y = c_1 + c_2\, x$

$f_1(x) = 1$

$f_2(x) = x$

The matrix equation for the data points (a set of simultaneous linear algebraic equations) can be formulated as:

$F\,\{c\} = [y]$

Or

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{Bmatrix} c_1 \\ c_2 \end{Bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Multiplication both sides with F^T (transpose of the function matrix) yield the following:

$F^T\, F\,\{c\} = F^T\,[y]$

Or

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{Bmatrix} c_1 \\ c_2 \end{Bmatrix} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Now, matrix multiplication will yield two equations with two unknowns (c_1 and c_2) that can be solved simultaneously.

4. Conclusions

From this applying math to engineering research, we can derive the following conclusions:

1) There are different approaches and mechanisms that can be used to transform a nonlinear function into a linear (a straight line) equation.
2) Nonlinear least squares method is used to model nonlinear functions (such as quadratic, polynomials, or exponential functions that are difficult to be linearized).
3) From an engineering practice, it is desirable to deal with linear forms of equations, hence, transforming the exponential engineering functions into linear equations and then applying the linear least squares method on the data points to determine the best values of parameters and coefficients.
4) The resulting math model is considered the specific equation for the investigated system and is used to predict new processing values.
5) When using the linear least squares method, either approach (the classical or matrix form) will give identical values of parameters and coefficients.
6) The linear least squares method is more reliable, in comparison to the graphical method (which is based on eye vision), for determining the constants (the slope and intercept) of the linear equation.

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