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Research Article

Parameter Estimation for a Class of Lifetime Models

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Our purpose in this paper is to present a better method of parametric estimation for a bivariate nonlinear regression model, which takes the performance indicator of rubber aging as the dependent variable and time and temperature as the independent variables. We point out that the commonly used two-step method (TSM), which splits the model and estimate parameters separately, has limitation. Instead, we apply the Marquardt's method (MM) to implement parametric estimation directly for the model and compare these two methods of parametric estimation by random simulation. Our results show that MM has better effect of data fitting, more reasonable parametric estimates, and smaller prediction error compared with TSM.

1. Introduction

In the study of fatigue lifetime evaluation of rubber materials, accelerated aging test is widely used as an effective procedure for obtaining the data on performance indicators (y), aging time (t), and aging temperature (T). In order to investigate the relationships among them, Dakin [1, 2] proposed the kinetic equation for aging; that is,

$$y = Be^{-Kt^{\alpha}}, \tag{1}$$

where y is the performance indicator of rubber, t is the aging time, K is an aging rate constant depending on the temperature T, B is a constant, and α is a constant in $(0, 1)$.

Mott and Roland [3] and Wise et al. [4] interpreted that the K in (1) can be expressed in the Arrhenius form. In this paper, we also assume the convention that the K for rubber can be described by the Arrhenius type

$$K = Ae^{-C/T}, \tag{2}$$

where T is aging temperature and A and C are constants.

By (2) and (1), we obtain the model

$$y = Be^{-Ae^{-C/T}t^{\alpha}}, \tag{3}$$

which is called the y-t-T bivariate nonlinear regression model in this paper. Here, B, A, C, and α are model parameters. In the past, one (see, e.g., [5–7]) usually split (3) into (1) and (2) to estimate the parameters in (3).

The constant α is determined by successive approximation method, which is to minimize (4) to two decimal places:

$$I = \sum_{i=1}^{l}\sum_{j}^{n}\left(y_{ij} - \widehat{y_{ij}}\right)^2, \tag{4}$$

where y_{ij} and $\widehat{y_{ij}}$ denote the experimental measurements and predicted values of the performance indicators of rubber when the aging temperature index is i and the experiment serial number is j, respectively. When α is assigned a value, (1) can be converted into the following linear form through logarithm transformation:

$$Y = a + bX, \tag{5}$$

where $Y = \ln y$, $a = \ln B$, $b = -K$, and $X = t^{\alpha}$.

The values of a and b are determined by the least squares method:

$$\widehat{b_i} = \frac{\sum XY - \left(\sum X \sum Y\right)/n}{\sum X^2 - \left(\sum X\right)^2/n}, \qquad \widehat{a_i} = \frac{\sum Y}{n} - b_i\frac{\sum X}{n}. \tag{6}$$

The B is given by $\widehat{B} = \sum \widehat{B_i}/l$, where l is the maximum index of aging temperature.

The K is given by $\widehat{K_i} = -\widehat{b_i}$ and used as the known value in (2). Similarly, (2) can be converted into the following linear form through logarithm transformation:

$$W = D + EZ, \tag{7}$$

where $W = \ln K$, $D = \ln A$, $E = -C$, and $Z = T^{-1}$.

The values of D and E are also determined by the least squares method:

$$\widehat{E} = \frac{\sum WZ - \left(\sum W \sum Z\right)/l}{\sum W^2 - \left(\sum W\right)^2/l}, \qquad \widehat{D} = \frac{\sum W}{l} - E\frac{\sum Z}{l}. \tag{8}$$

The estimated values of A and C are given by $\widehat{A} = e^{\widehat{D}}$ and $\widehat{C} = -\widehat{E}$.

At last, the final estimates of the parameters are substituted into (3) to form the regression forecast model.

However, the above-mentioned TSM has the following limitation.

First, the estimates of the parameters in (1) and (2), obtained by the logarithm regression method, are generally not the least squares solution of the original variables [8].

Second, substituting the estimates of the parameters $\widehat{K_i}$ in (1) into (2) may lead to large errors. This is because the estimates of the parameters A and C in (3) highly rely on the precision of $\widehat{K_i}$, if $\widehat{K_i}$ has a small change that will lead to considerable change of the values of A and C. Furthermore, TSM is a tedious calculation method.

Finally, the parameter B in (3) is the average of $\widehat{B_i}$, whose goodness needs verifying.

Regarding the limitation above, the purpose of this paper is to adopt MM to estimate the four parameters in (3).

2. Marquardt's Method

The general form of the nonlinear regression model is

$$Y = \varphi\left(x_1, x_2, \ldots, x_p; \beta_1, \beta_2, \ldots, \beta_r\right) + \xi, \tag{9}$$

where φ is a known nonlinear function, $x_1, x_2, \ldots, x_p$ are a set of p independent variables, $\beta_1, \beta_2, \ldots, \beta_r$ are a set of r unknown parameters to be estimated, and ξ is the random error. If y and $x_1, x_2, \ldots, x_p$ are observed for n times, n sets of observations $((x_{i1}, x_{i2}, \ldots, x_{ip}, y_i),\ i = 1, 2, \ldots, n)$ can be obtained.

Substituting the ith set of observations of the independent variables into the model (9), we see that

$$\varphi\left(x_{i1}, x_{i2}, \ldots, x_{ip}; \beta_1, \beta_2, \ldots, \beta_r\right) = \varphi\left(x_i, \beta\right). \tag{10}$$

Since $x_{i1}, x_{i2}, \ldots, x_{ip}$ are known values, we deduce that $\varphi(x_i, \beta)$ is a function of $\beta_1, \beta_2, \ldots, \beta_r$. For a given initial value $\beta^{(0)} = (\beta_1^{(0)}, \beta_2^{(0)}, \ldots, \beta_r^{(0)})$, we expand $\varphi(x_i, \beta)$ using Taylor's formula at $\beta^{(0)}$ and omit the quadratic and above terms. The expansion is as follows:

$$\begin{aligned}\varphi\left(x_i, \beta\right) \approx{}& \varphi\left(x_i, \beta^{(0)}\right) \\ &+ \left.\frac{\partial \varphi}{\partial \beta_1}\right|_{\beta=\beta^{(0)}} \left(\beta_1 - \beta_1^{(0)}\right) + \left.\frac{\partial \varphi}{\partial \beta_2}\right|_{\beta=\beta^{(0)}} \left(\beta_2 - \beta_2^{(0)}\right) \\ &+ \cdots + \left.\frac{\partial \varphi}{\partial \beta_r}\right|_{\beta=\beta^{(0)}} \left(\beta_r - \beta_r^{(0)}\right).\end{aligned} \tag{11}$$

All the numbers in (11) except the parameters $\beta_1, \beta_2, \ldots, \beta_r$ are known. It is clear that the right-hand side of (11) is a linear function of $\beta_1, \beta_2, \ldots, \beta_r$. Thus, we apply the least squares method to (11) and set

$$\begin{aligned}Q = {}& \sum_{i=1}^{n} \left\{ y_i - \left[\varphi\left(x_i, \beta^{(0)}\right) + \sum_{j=1}^{r} \left.\frac{\partial \varphi}{\partial \beta_j}\right|_{\beta=\beta^{(0)}} \left(\beta_j - \beta_j^{(0)}\right) \right] \right\}^2 \\ &+ d\sum_{j=1}^{r} \left(\beta_j - \beta_j^{(0)}\right)^2,\end{aligned} \tag{12}$$

where $d \geq 0$ is called the damping factor. When $d = 0$, this method of linearization becomes the Gauss-Newton method [9] which is a special case of MM. Even worse, the selection of initial values of iteration for the Gauss-Newton method is harder than that for MM.

In order to minimize Q, the first partial derivatives of Q with respect to $\beta_1, \beta_2, \ldots, \beta_r$ should be zero; that is,

$$\begin{aligned}0 = \frac{\partial Q}{\partial \beta_k} &= 2\sum_{i=1}^{n} \left[y_i - \varphi\left(x_i, \beta^{(0)}\right) \right. \\ &\qquad \left. + \sum_{j=1}^{r} \left.\frac{\partial \varphi\left(x_i, \beta\right)}{\partial \beta_j}\right|_{\beta=\beta^{(0)}} \left(\beta_j - \beta_j^{(0)}\right) \right] \\ &\qquad \times \left.\frac{\partial \varphi\left(x_i, \beta\right)}{\partial \beta_k}\right|_{\beta=\beta^{(0)}} \\ &\quad + 2d\left(\beta_k - \beta_k^{(0)}\right), \quad k = 1, 2, \ldots, r.\end{aligned} \tag{13}$$

The equality (13) can be turned into the following form:

$$\begin{aligned}
&(a_{11}+d)\left(\beta_1-\beta_1^{(0)}\right)+a_{12}\left(\beta_2-\beta_2^{(0)}\right)\\
&\quad+\cdots+a_{1r}\left(\beta_r-\beta_r^{(0)}\right)=a_{1y},\\
&a_{21}\left(\beta_1-\beta_1^{(0)}\right)+(a_{22}+d)\left(\beta_2-\beta_2^{(0)}\right)\\
&\quad+\cdots+a_{2r}\left(\beta_r-\beta_r^{(0)}\right)=a_{2y},\\
&\qquad\vdots\\
&a_{r1}\left(\beta_1-\beta_1^{(0)}\right)+a_{r2}\left(\beta_2-\beta_2^{(0)}\right)\\
&\quad+\cdots+(a_{rr}+d)\left(\beta_r-\beta_r^{(0)}\right)=a_{my},
\end{aligned}\tag{14}$$

where

$$\begin{aligned}
a_{jk}&=\sum_{i=1}^{n}\left.\frac{\partial\varphi}{\partial\beta_j}\right|_{\beta=\beta^{(0)}}\cdot\left.\frac{\partial\varphi}{\partial\beta_k}\right|_{\beta=\beta^{(0)}}=a_{kj},\\
a_{jy}&=\sum_{i=1}^{n}\left(y_i-\varphi\left(x_i-\beta^{(0)}\right)\right)\cdot\left.\frac{\partial\varphi}{\partial\beta_j}\right|_{\beta=\beta^{(0)}},\\
&\qquad j=1,2,\ldots,r;\quad k=1,2,\ldots,r.
\end{aligned}\tag{15}$$

Thus

$$\begin{aligned}
\beta&=\begin{bmatrix}\beta_1\\ \beta_2\\ \vdots\\ \beta_r\end{bmatrix}\\
&=\begin{bmatrix}\beta_1^{(0)}\\ \beta_2^{(0)}\\ \vdots\\ \beta_r^{(0)}\end{bmatrix}\\
&\quad+\begin{bmatrix}a_{11}+d^{(0)} & a_{12} & \cdots & a_{1r}\\ a_{21} & a_{22}+d^{(0)} & \cdots & a_{2r}\\ \vdots & \vdots & \vdots & \vdots\\ a_{r1} & a_{r2} & \cdots & a_{rr}+d^{(0)}\end{bmatrix}^{-1}\begin{bmatrix}a_{1y}\\ a_{2y}\\ \vdots\\ a_{ry}\end{bmatrix}.
\end{aligned}\tag{16}$$

Obviously, this solution depends on the initial values $\beta_1^{(0)},\beta_2^{(0)},\ldots,\beta_r^{(0)}$, and $d^{(0)}$. If all the absolute values $|\beta_j-\beta_j^{(0)}|$ for $i=1,2,\ldots,r$ are quite small, the estimation will be considered successful. On the contrary, if each $|\beta_j-\beta_j^{(0)}|$ is rather large, we will insert β_j calculated in the previous step into (14) as a new $\beta_j^{(0)}$. Then we compute the updated values of β_j from (14) and insert them back to (14) as the new $\beta_j^{(0)}$. Iterate this process until all the absolute values $|\beta_j-\beta_j^{(0)}|$ can be ignored. Since $a_{1y},a_{2y},\ldots,a_{ry}$ are fixed in (14), the larger the value of d is, the smaller the absolute values of $\beta_1-\beta_1^{(0)},\beta_2-\beta_2^{(0)},\ldots,\beta_r-\beta_r^{(0)}$ are. Therefore, the value of d should not be too large; otherwise the times of iteration will be increased. The boundary for selecting the value of d depends on whether the residual sum of squares is decreasing.

2.1. Steps for Calculating the Parameters in (3). There are two independent variables (aging time t and aging temperature T) and four unknown parameters (B, A, C, and α) in (3). The steps for solving the nonlinear equations for the four parameters are as follows.

(a) Calculate the partial derivatives of y in (3) with respect to B, A, C, and α, respectively; and we obtain

$$\begin{aligned}
\frac{\partial y}{\partial B}&=e^{-Ae^{-C/T}t^{\alpha}},\\
\frac{\partial y}{\partial A}&=-Be^{-Ae^{-C/T}t^{\alpha}+e^{-C/T}t^{\alpha}},\\
\frac{\partial y}{\partial C}&=\frac{BA^2t^{\alpha}}{T}e^{-Ae^{-C/T}t^{\alpha}-C/T},\\
\frac{\partial y}{\partial \alpha}&=-BAt^{\alpha}\ln te^{-Ae^{-C/T}t^{\alpha}-C/T}.
\end{aligned}\tag{17}$$

(b) Select the initial iteration values of the parameters; that is, $\beta^{(0)}=(B^{(0)},A^{(0)},C^{(0)},\alpha^{(0)})$. Whether the selection of initial values is appropriate will determine the amount of calculation and the convergence of iteration process. This paper uses TSM to estimate the initial values of the parameters according to the aging data in the related paper [6]. These values are also considered the initial values of the parameters in the process of random simulation in Section 3.

(c) Insert the n sets of observations $((y_i,t_i,T_i),\ i=1,2,\ldots,n)$ and the partial derivatives in (17) and $\beta^{(0)}$ into (15), and obtain each of the coefficient values in (14). For the first iteration, set the initial value; that is, $d=d^{(0)}=0.01a_{11}$, calculate from (14) the β in (16), and then insert the estimate of β into the original expression (12) to calculate the residual sum of squares: $Q^{(0)}=\sum_{i=1}^{n}[y_i-y(T_i,t_i;B,A,C,\alpha)]^2$. Obviously, the smaller the value of $Q^{(0)}$ is, the better it is.

(d) For the second iteration, set $\beta^{(0)}=\beta$, and $d=10^md^{(0)}$ for $m=-1,0,1,2,\ldots$.

(i) First, set $m=-1$; that is, $d=0.1d^{(0)}$, and then obtain the new values $\beta=(B^{(1)},A^{(1)},C^{(1)},\alpha^{(1)})$. Next, calculate the new residual sum of squares: $Q^{(1)}=\sum_{i=1}^{n}[y_i-y(T_i,t_i;B^{(1)},A^{(1)},C^{(1)},\alpha^{(1)})]^2$.

(ii) If $Q^{(1)}<Q^{(0)}$, the second iteration is done. But if $Q^{(1)}\geq Q^{(0)}$, set $m=0$; that is, $d=d^{(0)}$, recalculate β, and recalculate the residual sum of squares $Q^{(1)}$.

(iii) If $Q^{(1)}<Q^{(0)}$, the second iteration is done. But if $Q^{(1)}\geq Q^{(0)}$, set $m=1$; that is, $d=10d^{(0)}$, and recalculate β and $Q^{(1)}$.

Table 1: Data for y-t-T by random simulation.

$T_1 = 380$		$T_2 = 390$		$T_3 = 400$		$T_4 = 410$		$T_5 = 420$	
t_1	y_1	t_2	y_2	t_3	y_3	t_4	y_4	t_5	y_5
2	0.90164	2	1.06520	2	0.97163	14	0.74929	6	0.95249
5	0.96176	7	0.86762	6	0.90061	15	0.77756	12	0.70445
7	0.87269	14	0.88055	11	0.94456	21	0.85007	14	0.81271
9	0.84975	19	0.86093	16	0.89346	25	0.74324	15	0.8594
15	0.83473	28	0.90947	23	0.81057	27	0.65854	27	0.59827
21	0.84506	31	0.84498	23	0.81645	28	0.81902	38	0.61045
22	0.90798	35	0.84552	30	0.87126	29	0.68834	43	0.52327
38	0.90154	41	0.85828	32	0.81683	37	0.66011	46	0.62483
46	0.85955	47	0.76119	41	0.68749	43	0.62437	49	0.53331
49	0.87239	51	0.89269	49	0.67741	52	0.66685	52	0.47344
58	0.80548	60	0.72179	60	0.63145	52	0.66147	55	0.48434
61	0.87837	65	0.76753	64	0.70384	56	0.70915	56	0.48452
65	0.75141	66	0.75146	65	0.76225	59	0.57080	63	0.55642
73	0.82056	67	0.76682	73	0.62422	63	0.57548	65	0.49338
74	0.91427	77	0.65527	75	0.57640	66	0.62424	78	0.39203
79	0.77127	87	0.82239	76	0.59947	72	0.67121	79	0.51148
80	0.80846	92	0.63481	80	0.65660	76	0.58539	80	0.54383
93	0.85508	93	0.72213	84	0.72900	78	0.60945	82	0.38676
98	0.74497	94	0.75969	87	0.72015	79	0.60864	85	0.43803
99	0.82579	95	0.74208	88	0.74480	89	0.64069	98	0.40408

(iv) If $Q^{(1)} < Q^{(0)}$, the second iteration is done. But if $Q^{(1)} \geq Q^{(0)}$, set $m = 2$; that is, $d = 100d^{(0)}$, and recalculate β and $Q^{(1)}$. If $Q^{(1)} < Q^{(0)}$, the second iteration is done. Keep on increasing the values of β until $Q^{(1)} < Q^{(0)}$, and the fourth step is finished.

(e) For the third iteration, take the terminal values at the second iteration of d, β, and $Q^{(1)}$ as the new $d^{(0)}$, $\beta^{(0)}$, and $Q^{(0)}$, respectively. Repeat the whole process of the second iteration until a new $Q^{(1)} < Q^{(0)}$.

(f) Iterate the procedure as in processes (d) and (e) until $\max_{1\leq j\leq r}|\beta_j - \beta_j^{(0)}| \leq$ eps (tolerance) is satisfied. But we have to notice that the value of d should not be too large at this time; otherwise $\max_{1\leq j\leq r}|\beta_j - \beta_j^{(0)}| \leq$ eps would hold even though the actual iteration failed.

3. Random Simulation and Result Analysis

3.1. Random Simulation and Data Processing. Random simulation is a method which uses random numbers to conduct computer simulation. The sample observations obtained by random sampling were utilized to estimate the parameters of the models (see, e.g., [10, 11]).

This paper uses MatLab programming to simulate the data. Follow the steps below.

(1) Determine the model and initial values of the parameters.

(2) Select a constant T randomly to compute $T_i = T + 10i$ $(i = 1, 2, \ldots, n)$.

(3) Assume that t follows the uniform distribution on the interval $(1, 100)$ and generates the random numbers from $(1, 100)$ as t. The number of times of simulations is N.

(4) After obtaining all the simulated values, insert them into the model and add to y by a random number following the uniform distribution on $(-0.1, 0.1)$. We can simulate n sets of subsamples eventually.

In this paper, $T = 370$, $n = 5$, and $N = 20$. The initial values of the parameters are $B = 1$, $A = 8000$, $C = 5000$, and $\alpha = 0.6$. Then we can simulate 5 sets of data (each with 20 numbers) in Table 1.

According to the simulated data, we first use MatLab programming to figure out that the approximate value of α is 0.80 and then calculate the values of B, A, C, and α by TSM using SPSS software. The results are displayed in Table 2.

Then we estimate the parameters in the bivariate nonlinear model (3) by MM using SPSS software (the initial values of the parameters here are the same as those used in random simulation). The results are displayed in Table 3.

3.2. Result Analysis. (1) In regression analysis, the coefficient of determination $R^2 = 1 -$ (residual sum of squares)/(total sum of squares of deviations) is a statistic that measures the goodness of fit of the model under consideration. Specifically, the coefficient of determination is a statistical measure of how well the regression line fits the real data points. The closer to 1 the R^2 is, the closer the points of practical observations to the sample line and the better the goodness of fit of the model are. From Tables 2 and 3, it can be seen that the R^2 of MM is

Table 2: Analysis for two-step method.

Statistics	T_1	T_2	T_3	T_4	T_5
R^2	0.335	0.643	0.671	0.564	0.809
Sig.	0.008	0.000	0.000	0.000	0.000
$\widehat{B_i}$	0.906	0.973	0.955	0.831	0.917
$\widehat{K_i}$	0.003	0.008	0.011	0.01	0.022
Residual sum of squares	0.056	0.098	0.149	0.107	0.231
$\widehat{B} = (\sum \widehat{B_i})/5 = 0.916 = 0.916$, $\widehat{A} = 193493.655$, and $\widehat{C} = 6746.318$.					
The total residuals sum of squares = 0.641.					

Table 3: Analysis for Marquardt's method.

	Sum of squares	DF	Mean square
Regression	55.235	4	13.809
Residuals	0.325	96	0.003
Total	**55.5602**	**100**	
$R^2 = 1 -$ (residual sum of squares)/(total) = 0.843.			
$\widehat{B} = 0.973$, $\widehat{A} = 35616.923$, $\widehat{C} = 5689.481$, and $\widehat{\alpha} = 0.633$.			

larger than that of TSM, which indicates that the prediction model of MM is more suitable for fitting the simulated data.

(2) Comparing the estimates of the parameters obtained by the two methods, we can easily find out that the estimates of the parameters of MM are closer to the initial values, which indicates that using MM to estimate the parameters in the y-t-T model is more reasonable.

(3) We compare their residual sum of squares. The residual sum of squares for MM is 0.325, and that for TSM is 0.641. The former is only half of the latter. Obviously, the prediction error of the y-t-T model resulting from using MM is smaller, and the precision of its fitted equation is higher.

4. Conclusion

In this paper, we demonstrate that the MM is more suitable for estimating the parameters of the aging lifetime model by the theoretical analysis and random simulation. Our method not only avoids a plenty of tedious calculation in TSM but also adds the damping factor, which loosens the limitation of selecting the initial values. Furthermore, compared with TSM, MM greatly decreases the fitting error between the predicted values and the practical observed values, and we obtain the best-fit parameters. In addition, the model estimated by MM has higher fitting precision than that by TSM.

We note that the parametric estimation in this paper can also be used in the prediction of lifetime of other materials, such as composite materials (see [12]).

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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