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Parameter Estimation for the Weibul distribution model Using Least-Squares Methodin conjunction with Simplex and Quasi-Newton Optimization Methods

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Abstract: We find Survival rate estimates, parameter estimates for the Weibulldistribution model using least-squares estimation method for the case when partial derivatives were not available, the Simplex optimization Methods (Nelder and Mead, and Hooke and Jeeves were used, and for the case when first partial derivatives were available, the Quasi – Newton Methods(Davidon-Fletcher-Powel (DFP) and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) optimization methods)were applied.The medical data sets of 21 Leukemiacancer patients with time span of 35 weeks were used.

Key Words: Weibull Distribution model, Nelder and Mead, and Hooke and Jeeves, DFP and BFGS optimization methods, Parameter estimation, Least Square method, Kaplan-Meier estimates, Survival rate Estimates, Variance-Covariance matrix.

1. Introduction

The Methods (Nelder and Mead ([1]) and Hooke and Jeeves ([2]) do not require first partial derivatives and the function values are compared to find the optimal value of the objective function. Whereas, the Quasi –Newton Methods (DFP and BFGS) require first partial derivatives for the function ([3], [4]). In this paper, we find the parameter estimates, optimal function values and other information using simplex optimization methods and Quasi-Newton optimization methods. These optimization methods were applied using medical data sets of cancer patients ([5]).

The method of linear least-squares requires that a straight line be fitted to a set of data points such that the sum of squares of the vertical deviations from the points to be minimized ([6], [7]).

Adrien Merie Legendre(1752-1833) is generally credited for creating the basic ideas of the method of least squares. Some people believe that the method was discovered at the same time by Karl F. Gauss (1777-1855), Pierre S. Laplace (1749-1827) and others. Furthermore, Markov's name is also included for further development of these ideas. In recent years, ([8],[9],[10])an effort have been made to find better methods of fitting curves or equations to data, but the least-squares method remained dominant, and is used as one of the important methods of estimating the parameters. The least-squares method ([7], [11]) consists of finding those parametersthat minimize a particular objective function based on squared deviations.

It is to be noted that for the least-squares estimation method, we are interested to minimize some function of the residual, that is, we want to find the best possible agreement between the observed and the estimated values. To define the objective function F, we set up a vector of residuals

$$r_i = y_i^{obs} - y_i^{est} , i = 1,2,\cdots,m . \quad (1)$$

Then the objective function is a sum of squared residuals - the term 'least-squares' derives from the function:

$$F = \sum_{i=1}^{m} r_i^2 = \sum_{i=1}^{m} (y_i^{obs} - y_i^{est})^2 . \quad (2)$$

The objective function is the sum of the squares of the deviations between the observed values and the corresponding estimated values ([7], [11]). The maximum absolute discrepancy between observed and estimated values is minimized using optimization methods.We usednon parametric Kaplan-Meier estimates ($KM(t_i)$) ([12],[13]) as the observed values (y_i^{obs}) of the objective functionand the survivor rate estimates ($S(t_i)$) of

Weibull([14], [19]) model as the estimated value (y_i^{est}) of the objective function*F* ([10]). We considered the objective function for the model of the form

$$F = \sum_{i=1}^{m} f_i \left(KM(t_i) - S(t_i)\right)^2 \qquad (3)$$

where f_i is the number of failures at time t_i and *m* is the number of failure groups ([19]).

We used the following procedure:

- Note that the Kaplan-Meier method ([12]) is independent of parameters, so for a particular value of time t_i, we find the value of the Kaplan-Meier estimate $KM(t_i)$ of the survival function.
- We suppose that the survivor function of Weibulldistribution modelat time t_i is $S(t;\alpha,\beta) = exp\left(-\left(\frac{t}{\alpha}\right)^{\beta}\right)$, andat thestartingpoint (α_0, β_0) , it is $S(t_i;\alpha_0,\beta_0)$.
- From the numerical values of the Kaplan-Meier estimates $KM(t_i)$, and the survivor function $S(t_i;\alpha_0,\beta_0)$ of theWeibulldistribution model at time t_i, we can evaluate errors $\left|S(t_i;\alpha_0,\beta_0) - KM(t_i)\right|$.
- The function value with a suitable starting point (α_0, β_0) is given by $F(t_i;\alpha_0,\beta_0) = \max_i \left|S(t_i;\alpha_0,\beta_0) - KM(t_i)\right|$.
- We find numerical value of the function (objective function, *F*) at initial point (α_0, β_0) and this function value can be used in numerical optimizationsearch methods (Simplex or Quasi) to find the optimalpoint (α^*, β^*) (parameter estimates or optimal point).

For practical applications of least square method, we considered some medical data sets ([5]). The drug 6-mercaptopurine (6-MP) was compared to a placebo to maintain remission in acute leukemia patients. The following table gives remission times for two groups of twenty one patients each; one group was given the placebo and was given the other the drug 6-MP.

	Length of remission (in weeks) of leukemia patients
6-MP for 21 patients	6,6,6,6* ,7,9*,10,10*, 11*, 13,16,17*,19*, 20*, 22,23,25*, 32*, 32*, 34*, 35*
Placebo for 21 patients	1, 1, 2, 2, 3, 4, 4, 5, 5, 8, 8, 8, 8, 11, 11, 12, 12, 15, 17, 22, 23

*Censored observations

We considered only the data of twenty one patients who were given 6-MP drug and there were 7 failures at times 6, 7, 10, 13, 16, 22 and 23; and 12 of the 21 patients were censored. The data of twentyone leukemia patients were used for assessing the adequacy of Weibull model to find the survivor rate estimates. The results of each Weibull model are demonstrated by giving the values of the variance-covariance matrices, parameter estimates and other related information in tables 1, table 2 and table 3.

2. Weibull distribution model using Least-Squares Methods and Applying Simplex Methods (Nelder and Mead and Hooke and Jeeves Search Methods)

For a practical application of the least-squares estimation method when assuming that partial derivatives of the objective function *F* were not available.

Nelder and Mead ([15], [16], [17]) and Hooke and Jeeves ([2], [18]) are simplex methods and are useful for optimizing the nonlinear programming problems. These are numerical methods without calculating the derivatives of the objective function. These methods do not require first partial derivatives (gradients) so may converge very slow or even may diverge at all ([15], [18]). The numerical results of Weibull distribution modelusing Nelder and Mead and Hooke and Jeeves search methods have been presented in this paper. The results include function values, parameter estimates, survivor-rate estimates; Kaplan-Meier estimates ([12], [13]) and other information have been presented in Table-1 and Table-2.

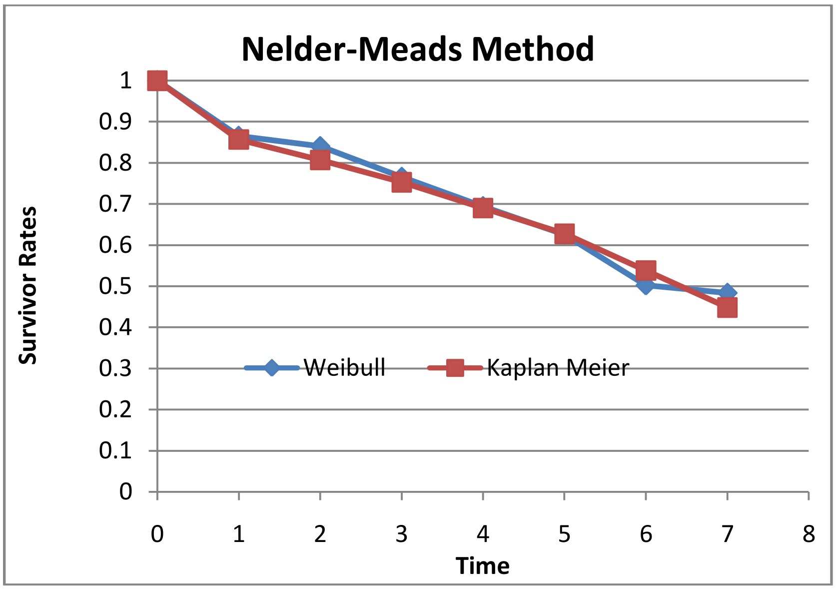
Numerical Results for WeibullProbability Distribution Model using Least-Squares Methods and Applying Nelder and Mead(NM) and Hooke and Jeeves(HJ) Methods

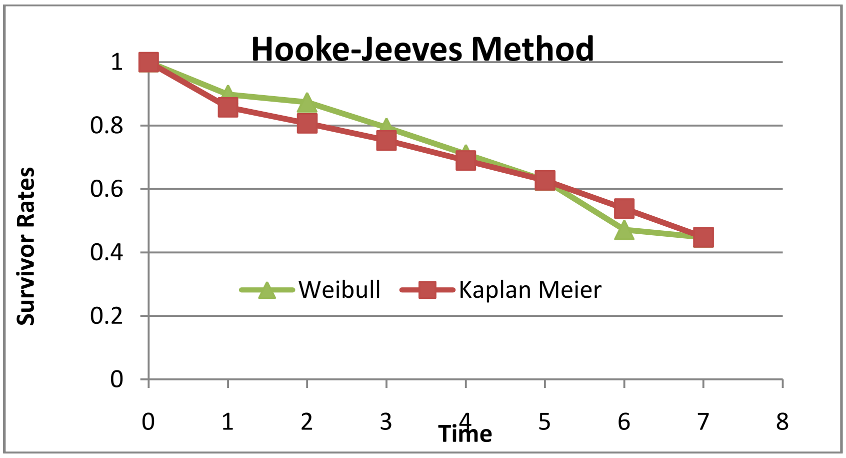
Table-1: Comparison of Survival Rate estimates for WeibullDistribution Model

Failure Time (Weeks)	Number of Failures	Nelder and MeadMethod		Hooke and Jeeves Method	
		Weibull Model	Kaplan Meier	Weibull Model	Kaplan Meier
0	0	1	1	1	1
6	3	0.865732620474	0.85714	0.898006594306	0.85714
7	1	0.840664386549	0.80722	0.873278953618	0.80722
10	1	0.765987437822	0.75294	0.793650282790	0.75294
13	1	0.693815454854	0.69019	0.710143126567	0.69019
16	1	0.625439373884	0.62745	0.626834808323	0.62745
22	1	0.502360228474	0.53815	0.471258856942	0.53815
23	1	0.483713394792	0.44817	0.447484072603	0.44817

Table-2: Parameter Estimates and Optimal Function Value for WeibullDistribution Model

	Nelder and Mead Method	Hooke and Jeeves Method
Parameters Estimates	30.003363883834738 1.2032546182868922	26.605853270000018 1.4969669700000001
Optimal Functional value	0.003355341230836913	0.06655626910885548





3. Weibull distribution model using Least-Squares Methods and Applying Quasi-Newton Optimization Methods (DFP and BFGS Methods)

We know that the survivor function for the two-parameter Weibull distribution ([9], [10]) is

$$S(t) = \exp\left(-(\frac{t}{\alpha})^{\beta}\right), \tag{4}$$

where α is the scale parameter and β is the shape parameter. To find the parameter estimates for the Weibull distribution model using least-squares estimation procedures, we consider the objective function F as

$$F = \sum_{i=1}^{m} f_i (S(t_i) - KM(t_i))^2 , \tag{5}$$

where $KM(t)$ is the Kaplan-Meier estimate for the failure time t.

To apply DFP and BFGS optimization methods, we find first partial derivatives of the objective function F using eq.(4) and eq.(5), we have

$$\frac{\partial F}{\partial \alpha} = 2\sum_{i=1}^{m} f_i\left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial \alpha} \tag{6}$$

and

$$\frac{\partial F}{\partial \beta} = 2\sum_{i=1}^{m} f_i\left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial \beta} , \tag{7}$$

where

$$\frac{\partial S(t)}{\partial \alpha} = \left(\frac{\beta}{\alpha}\right)\left(\frac{t}{\alpha}\right)^{\beta} S(t)$$

and

$$\frac{\partial S(t)}{\partial \alpha} = -\ln\left(\frac{t}{\alpha}\right) \left(\frac{t}{\alpha}\right)^{\beta} S(t) .$$

Using the objective function eq.(5), and the first partial derivatives eq.(6) and eq.(7) in the DFP and the BFGS optimization method, we can find the estimated value of the parameters for which the least-squares function gives the minimum value for Weibull distribution model and the results are presented in the table-3

Numerical Results forWeibullProbability Distribution Model using Least-Squares Methods and ApplyingQuasi Newton Methods

Table-3

Quasi Methods	Parameters Estimates	Optimal Functional value	Gradient at Optimal (α^*, β^*)	The Variance-Covariance at Optimal (α^*, β^*)
DFP Model	30.75038 1.12722	0.0032110996832	-0.27132E-05 -0.21420E-04	1737.012994 -73.958416 -73.958416 4.270356701
BFGS Model	30.75490 1.12708	0.00321109491	0.10014E-07 0.16052E-05	2253.579391 -83.711796 -83.711796 4.460812438

III. CONCLUSION

The Survival rate estimates for the 21 Leukemia patients for the period of 35 week under observations with drug 6-MP ([5], [19]) were compared using parametricWeibull distribution modeland non-parametric Kaplan Meier Model ([12]). We found that the results like parameter estimates, optimal function value, variance covariance matrix, gradient vector at the optimal point $\left(\alpha^*, \beta^*\right)$ using theWeibull distribution model were approximately samefor both the cases when the derivatives of an objective function wereavailable (using Quasi-Newton method (DFP and BFGS methods))and when first partial derivatives of the objective function werenot available (using the Hooke and Jeeves, and Nelder and Mead method). We also noted that the parameter estimates for the Nelder and Mead methodare very close to the Quasi-Newton methods (DFP or BFGS).

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