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Parameter Estimation for the Logistic and Log-logistic Distribution Models Using Simplex and Quasi-Newton Optimization Methods

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Abstract

We find Survival rate estimates, parameter estimates, variance-covariance matrices for the Logistic and Log-logistic probability distribution models using least-squares estimation methods without having partial derivatives, namely the simplex optimization Methods (Nelder and Meads ([15]), and Hooke and Jeeves ([18])) and having partial derivatives namely, the Quasi – Newton optimization Methods (Davidon-Fletcher-Powel (DFP, ([7,8])) and the Broyden-Fletcher-Goldfarb-Shanno (BFGS, ([4,8,19])). The medical data sets of 21 Leukemia cancer patients with time span of 35 weeks ([5, 10]) were used.

Key Words: Logistic, Log-logistic probability distribution Models, Nelder and Meads, Hooke and Jeeves Simplex Methods, DFP, BFGS optimization methods, Parameter estimations, Least Square method, non-parametric model Kaplan-Meier estimates method, Survival rate Estimates, Variance-Covariance, parameter estimates.

Introduction

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 ([16]).
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, ([3],[6]) an effort have been made to find better methods of fitting curves to the given 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 ([3]) consists of finding those parameters that minimize a particular objective function based on squared deviations.

It is to be noted that for the least-squares estimation method, ([6]), 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

$$r_i = y_i^{obs} - y_i^{est}, i = 1,2,\cdots,m. \quad (1.1)$$

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

$$F = \sum_{i=1}^{m} r_i^2 = \sum_{i=1}^{m} (y_i^{obs} - y_i^{est})^2. \quad (1.2)$$

The objective function is the sum of the squares of the deviations between the observed values and the corresponding estimated values ([6]). The maximum absolute discrepancy between observed and estimated values is minimized using quasi Newton optimization methods.

We treated Kaplan-Meier estimates ($KM(t_i)$) ([13]) as the observed values (y_i^{obs}) of the objective function and the survivor rate estimates ($S(t_i)$) of Logistic ([12],[20]) and Log-logistic ([1,2,14]), probability distribution models as the estimated value (y_i^{est}) of the objective function F ([3]). We considered the objective function for the models of the form

$$F = \sum_{i=1}^{m} f_i (KM(t_i) - S(t_i))^2 \quad (1.3)$$

where f_i is the number of failures at time t_i and m is the number of failure groups.

We used the following procedure:

- Note that the Kaplan-Meier ([13]) method 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 Logistic and Log-logistic probability distribution models at time t_i are $S(t_i; a, b)$, and with the starting value of the parameters (a_0, b_0), we can find the value of the survivor function $S(t_i; a_0, b_0)$.
- From the numerical values of the Kaplan-Meier estimates $KM(t_i)$, and the survivor function $S(t_i; a, b)$ of the Logistic and Log-logistic probability distribution models at time t_i, we can evaluate errors $|S(t_i; a, b) - KM(t_i)|$.
- The function value with a suitable starting point (a_0, b_0) is given by

$$F(t_i; a_0, b_0) = \max_i |S(t_i; a_0, b_0) - KM(t_i)|.$$

- We find numerical value of the function at initial point (a_0, b_0) and this function value can be used in numerical optimization search methods to find the minimum point $\left(a^*, b^*\right)$ (optimal value of the parameters).

For practical applications of least square method, we considered some medical data sets ([8]). 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 twenty-one leukemia patients were used for assessing the appropriateness of Logistic model to find the survivor rate estimates. The results of each Logistic and Log-logistic probability distribution models using Least-Squares method and applying simplex methods and Quasi-Newton methods are presented by giving the values of the variance-covariance matrices, parameter estimates and other related information in tables 1, table 2 and table 3.

Logistic and Log-logistic Probability Distribution Models using Least-Squares Methods and Applying Nelder and Meads and Hooke and Jeeves Search Methods

Nelder and Meads ([15]) and Hooke and Jeeves ([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 optimization methods do not require first partial derivatives (gradients), so may converge very slow or even may diverge at all ([16], [17]). The numerical results of Logistic and Log-logistic distribution models using Nelder and Mead's 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 ([5], [13]) and other information have been presented in Table-1 and Table-2.

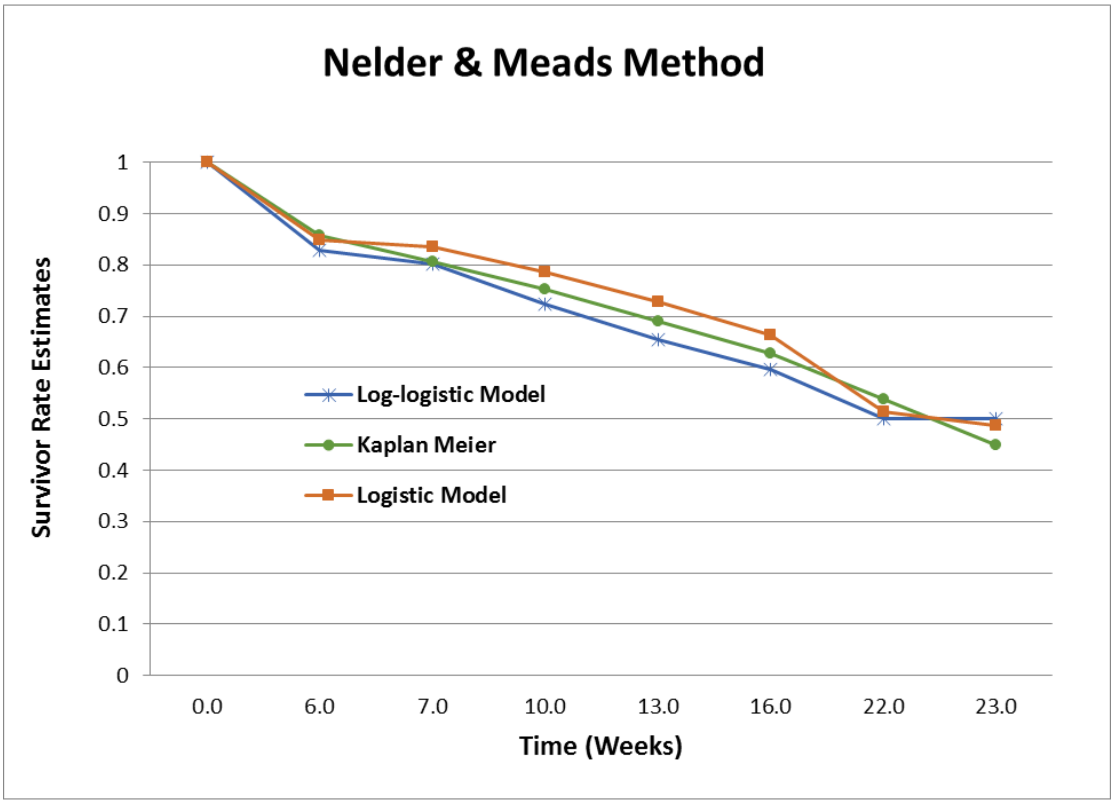
Numerical Results for Logistic and Log-logistic Probability Distribution Models using Least-Squares Methods and Applying Nelder and Mead's (NM) and Hooke and Jeev's (HJ) Methods

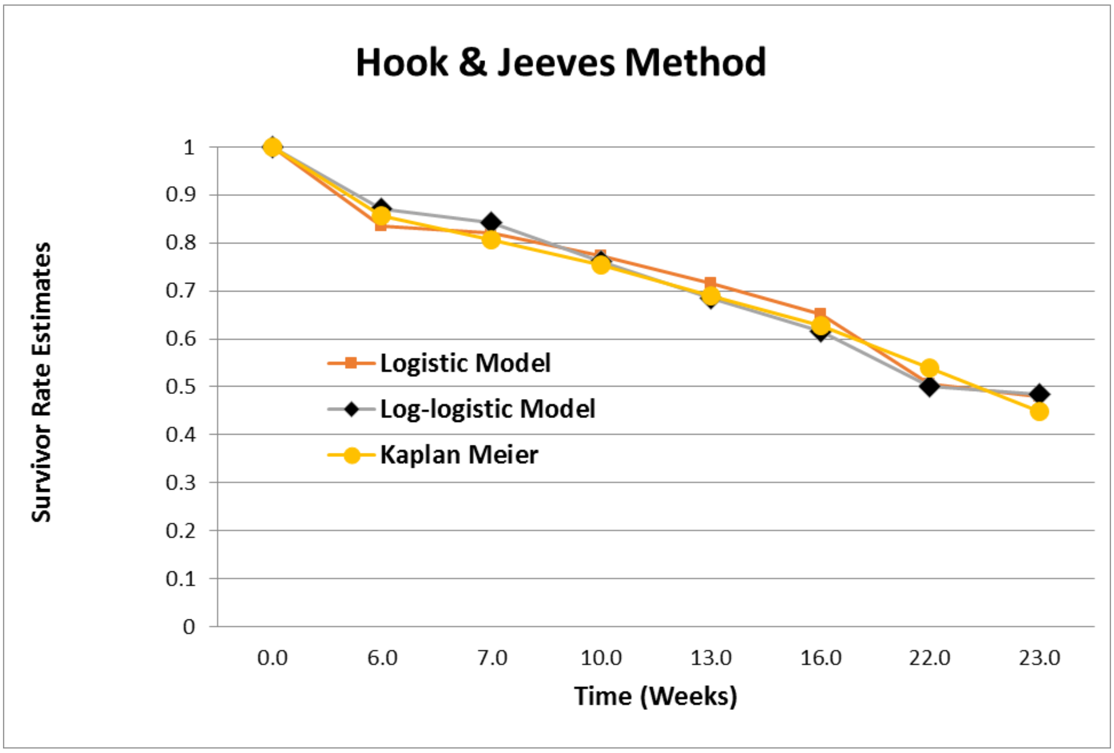
Table 1: Comparison of Survival Rate Estimates for Logistic and Log-logistic Models.

Failure Time (Weeks)	Number of Failures	Nelder and Meads			Hooke and Jeeves		
		Logistic Model	Log-logistic Model	Kaplan Meier	Logistic Model	Log-logistic Model	Kaplan Meier
6	3	0.848025	0.829281	0.85714	0.8350666	0.8710061	0.85714
7	1	0.834104	0.801072	0.80722	0.8208283	0.8434104	0.80722
10	1	0.786240	0.722941	0.75294	0.7724099	0.7614722	0.75294
13	1	0.729052	0.654735	0.69019	0.7154432	0.6848208	0.69019
16	1	0.663120	0.595636	0.62745	0.6506663	0.6157426	0.62745
22	1	0.513012	0.499975	0.53815	0.5054921	0.5011275	0.53815
23	1	0.486965	0.499975	0.44817	0.4805022	0.4848352	0.44817

Table 2: Parameter Estimates and Optimal Function Value for Logistic and Log-logistic Models.

	Logistic Probability Distribution		Log-logistic Probability Distribution	
	NM Model	HJ Model	NM Model	HJ Model
Parameters Estimates	2.3443738 0.10419653	2.2219694192 9.999999E-02	1.21655171465 4.545827735E-02	1.4664812999 4.531497E-02
Optimal Functional value	3.885607324E-02	3.2322992E-02	3.827960117E-02	3.66876847E-02


Nelder & Meads Method
Survivor Rate Estimates
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Log-logistic Model
Kaplan Meier
Logistic Model
0.0
6.0
7.0
10.0
13.0
16.0
22.0
23.0
Time (Weeks)


Hook & Jeeves Method
Survivor Rate Estimates
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Logistic Model
Log-logistic Model
Kaplan Meier
0.0
6.0
7.0
10.0
13.0
16.0
22.0
23.0
Time (Weeks)

Logistic and Log-logistic distribution models using Least-Squares Methods and Applying Quasi-Newton Methods (DFP and BFGS Methods)

Logistic Probability Distribution Model

We know that the survivor function for the two-parameter Logistic distribution model is $S(t) = 1/\left(1 + \exp(bt - a)\right)$ (4.1.1)

To find the parameter estimates for the Logistic distribution model using least-squares estimation procedures, we consider the function

$$F = \sum_{i=1}^{m} f_i (S(t_i) - KM(t_i))^2 \qquad (4.1.2)$$

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

We used the DFP and the BFGS optimization methods to find the parameter estimates.

To apply these optimization methods, we need to find the first partial derivatives of the objective function $F(a,b)$.

Thus, from eq.(4.1.2) we have

$$\frac{\partial F}{\partial a} = 2\sum_{i=1}^{m} f_i \left(S(t_i) - KM(t_i)\right) \frac{\partial S(t_i)}{\partial a} \qquad (4.1.3)$$

and

$$\frac{\partial F}{\partial b} = 2\sum_{i=1}^{m} f_i \left(S(t_i) - KM(t_i)\right) \frac{\partial S(t_i)}{\partial b}, \qquad (4.1..4)$$

where

$$\frac{\partial S(t)}{\partial a} = \exp(bt - a) \left(S(t)\right)^2$$

and

$$\frac{\partial S(t)}{\partial b} = -t \exp(bt - a) \left(S(t)\right)^2.$$

Using eq.(4.1.2), eq.(4.1.3) and eq.(4.1.4) in the DFP or the BFGS optimization method, we can find the estimated value of the parameters for which the least-squares function gives the minimum value.

Log-logistic Probability Distribution Model

We know that the survivor function for the two-parameter log-logistic distribution is

$$S(t) = 1/\left(1 + (bt)^a\right). \qquad (4.2.1)$$

To find the parameter estimates for the log-logistic distribution model using least-squares estimation procedure, we consider the function

$$F = \sum_{i=1}^{m} f_i (S(t_i) - KM(t_i))^2, \qquad (4.2.2)$$

where $KM(t)$ is the Kaplan-Meier estimate for the failure time t.
We used the DFP and the BFGS optimization methods to find the parameter estimates. To apply these optimization methods, we again evaluate the first partial derivatives of the objective function $F(a,b)$,

$$\frac{\partial F}{\partial a} = 2\sum_{i=1}^{m} f_i\left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial a} \qquad (4.2.3)$$

and

$$\frac{\partial F}{\partial b} = 2\sum_{i=1}^{m} f_i\left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial b}, \qquad (4.2.4)$$

where

$$\frac{\partial S(t)}{\partial a} = -(bt)^a \ln(bt)\left(S(t)\right)^2$$

and

$$\frac{\partial S(t)}{\partial b} = -\frac{a}{b}(bt)^a\left(S(t)\right)^2.$$

Using eq.(4.2.2), eq.(4.2.3) and eq.(4.2.4) in the DFP (Davidon-Fletcher-Powell) or the BFGS (Broyden-Fletcher-Goldfarb-Shanno) optimization methods, we can find the estimated value of the parameters for which the least-squares function gives the minimum value of discrepancies between the observed and the estimated value.

Numerical Results for Logistic and Log-logistic Probability Distribution Models using Least-Squares Methods and Applying Quasi Newton Methods

Table 3

Models	**Logistic Probability Distribution**		**Log-logistic Probability Distribution**	
Quasi Methods	**DFP Model**	**BFGS Model**	**DFP Model**	**BFGS Model**
Parameters Estimates	2.25454 0.10352	2.25455 0.10353	1.35276 0.04442	1.35276 0.04442
Optimal Functional value	0.4987337E-02	0.498733692E-02	0.375931868E-02	0.375931868E-02
Gradient at Optimal $\left(a^*,b^*\right)$	0.17883E-07 -0.55248E-07	0.20164E-05 0.21963E-04	-0.32462E-06 0.16922E-04	0.72079E-09 -0.94501E-07
The Variance-Covariance at Optimal $\left(a^*,b^*\right)$	9.4488 0.51724 0.5172 0.03349	9.55447 0.53117 0.53117 0.03537	6.54375 0.10152 0.10151 0.00321	6.61682 0.10536 0.10536 0.00323

Conclusion

The Survival rate estimates for the 21 Leukemia patients for the period of 35 week under observations were compared using parametric Logistic distribution model ([20]), Log-logistic distribution Model ([2]), and Non-parametric Kaplan Meier Model ([13]). We found that the results (like the survival rate estimates) for the Logistic and Log-logistic distribution models were approximately same for both the cases when the derivatives of an objective function were not available (Using the Hooke and Jeeves, and Nelder and Meads method) and when first partial derivatives of the objective function were available (using Quasi-Newton methods like DFP and BFGS methods). Using Quasi Newton optimization methods, we also found parameter estimates, optimal function, gradient at the optimal point and the variance-covariance matrices without evaluating the second derivatives of the objective function F.

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