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A Comparison of Survivor Rate Estimates for Some Probability Distribution Models Using Least-Squares Method in Conjunction with Simplex and Quasi-Newton Optimization Methods

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Abstract

In this paper, we find survival rate estimates, parameter estimates, variance covariance for some probability distribution models like, Exponential, Inverse Gaussian, Gompertz, Gumbels and Weibull distributions using least-squares estimation method. We found these estimates for the case when partial derivatives were not available and for the case when partial derivatives were available. The first case when partial derivatives were not available, we used the simplex optimization (Nelder and Meads ([6],[7]) and Hooke and Jeeves ([4],[5])) methods and the case when first partial derivatives were available we applied the Quasi – Newton optimization (Davidon-Fletcher-Powel (DFP) and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) methods. The medical data sets of 21 Leukemia cancer patients with time span of 35 weeks ([3]) were used.

Keywords: Exponential, Inverse Gaussian, Gompertz, Gumbel and Weibull distribution models, Nelder and Mead, Hooke and Jeeves, DFP and BFGS optimization methods, Parameter estimation, Least Square method, Kaplan-Meier estimates, Parameter estimates, Survival rate Estimates, Variance-Covariance Matrix.

1. 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 ([1],[2]).

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

$$F = \sum_{i=1}^{m} r_i^2 = \sum_{i=1}^{m} (y_i^{obs} - y_i^{est})^2 \tag{1.1}$$

Where $r_i = y_i^{obs} - y_i^{est}, i = 1,2,\cdots,m$, is a residual vector.

The objective function is the sum of the squares of the deviations between the observed values and the corresponding estimated values ([1],[2],[9]]). The maximum absolute discrepancy between observed and estimated values is minimized using optimization methods.

We treated Kaplan-Meier estimates ($KM(t_i)$) ([20], [3]) as the observed values (y_i^{obs}) of the objective function and the survivor rate estimates ($S(t_i)$) of some distribution models as the estimated value (y_i^{est}) of the objective function *F*. We considered the objective function for the models of the form

$$F(t,a,b) = \sum_{i=1}^{m} f_i (KM(t_i) - S(t_i,a,b))^2 \tag{1.2}$$

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

We find numerical value of the function at initial point (a_0, b_0) and is used in numerical optimization search methods to find the minimum point (a^*, b^*) (parameters estimates).

2. NUMERICAL RESULTS FOR DIFFERENT PROBABILITY DISTRIBUTION MODELS USING LEAST-SQUARES METHOD AND APPLYING NELDER AND MEADS AND HOOKE AND JEEVES OPTIMIZATION SEARCH METHODS

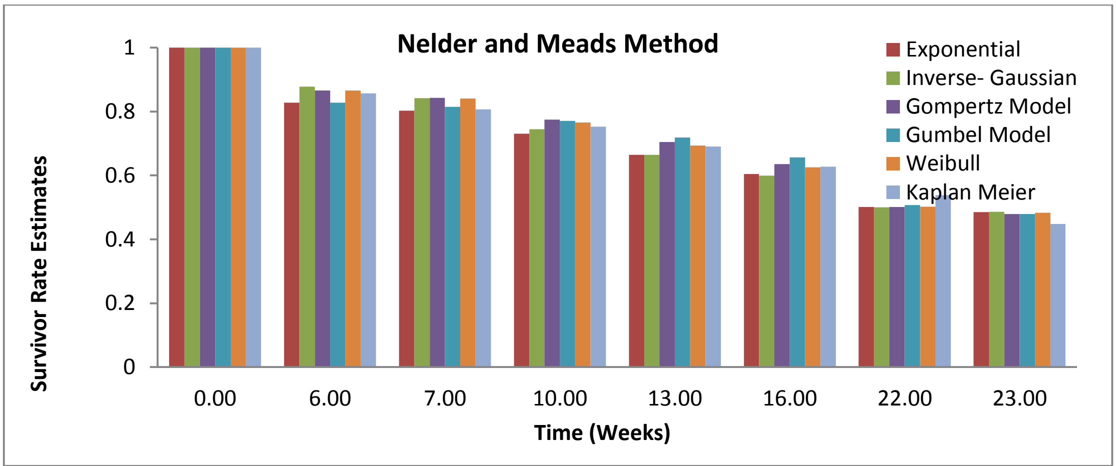
Table 1: Parameter Estimates and Optimal Function Value for the Exponential, Inverse Gaussian, Gompertz, Gumbel and Weibull Distribution Models using Nelder and Meads, and Hooke and Jeeves methods.

	Nelder and Meads Method				
	Exponential	**Inverse-Gaussian**	**Gompertz Model**	**Gumbel Model**	**Weibull**
Parameters Estimates	3.14283E-02	0.31317817 0.01823842	0.020989099 0.037910900	0.079469520 0.009399999	30.00336 1.203254
Optimal Functional value	3.71878E-03	0.03804917	0.035096464	0.030966696	0.003355

	Hooke and Jeeves Method				
	Exponential	Inverse-Gaussian	Gompertz Model	Gumbel Model	Weibull
Parameters Estimates	3.14389E-02	0.419982779 0.219999999	0.031560815 0.045794945	0.08008377 0.00934490	26.60585 1.496967
Optimal Functional value	3.70689E-03	0.04643498	0.03664972	0.03094435	0.066557

Table 2: Comparison of Survival Rate estimates for the Exponential, Inverse Gaussian, Gompertz, Gumbel and Weibull Distribution Models using Nelder and Meads, and Hooke and Jeeves methods.

Failure Time (Weeks)	**Number of Failures**	**Nelder and Meads Method**					
		Exponential	**Inverse-Gaussian**	**Gompertz Model**	**Gumbel Model**	**Weibull**	**Kaplan Meier**
0	1	1	1	1	1	1	1
6	3	0.828142	0.877412	0.86616	0.828057	0.86573	0.85714
7	1	0.802520	0.841704	0.84333	0.815132	0.84066	0.80722
10	1	0.7303127	0.744553	0.77433	0.771117	0.76598	0.75294
13	1	0.66460169	0.664633	0.70497	0.718565	0.69381	0.69019
16	1	0.60480320	0.599291	0.63587	0.656881	0.62543	0.62745
22	1	0.50086347	0.499796	0.50116	0.506870	0.50236	0.53815
23	1	0.4853670	0.486228	0.47947	0.478952	0.48371	0.44817



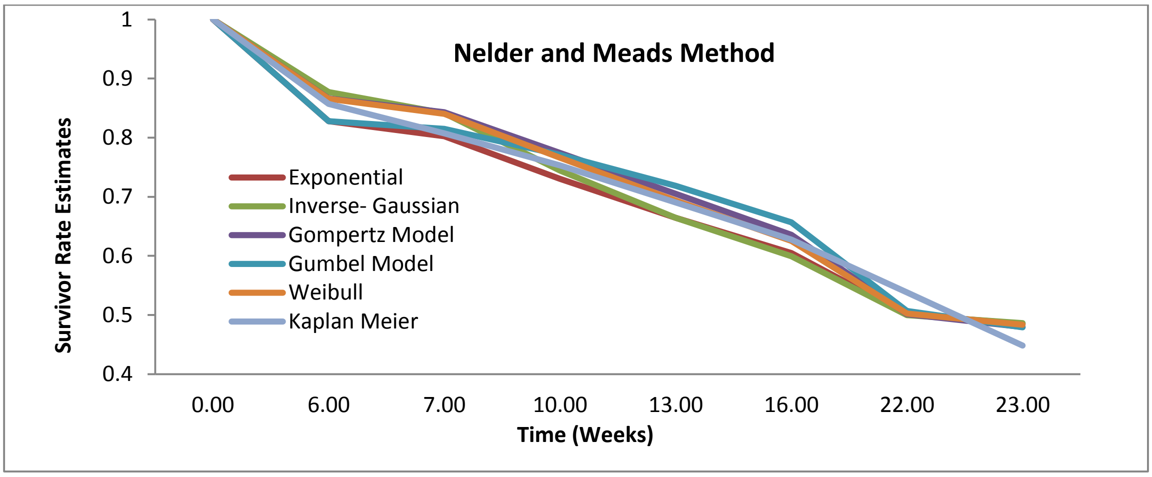
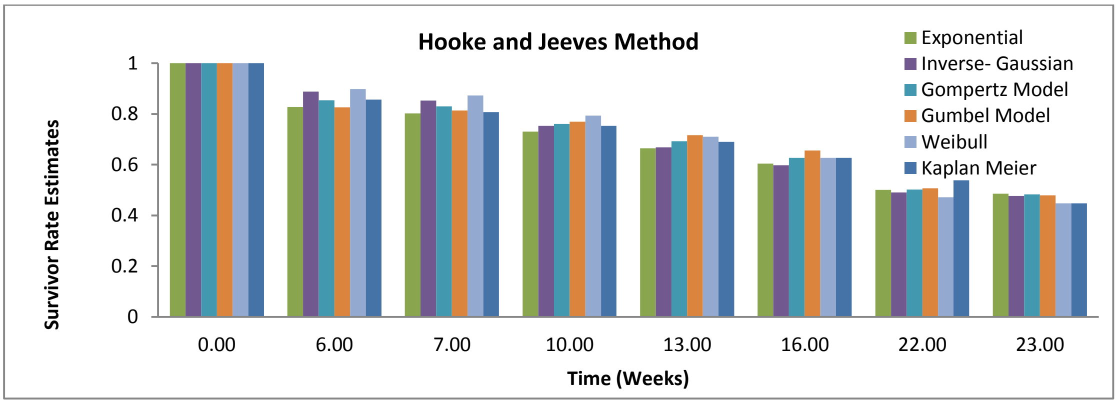
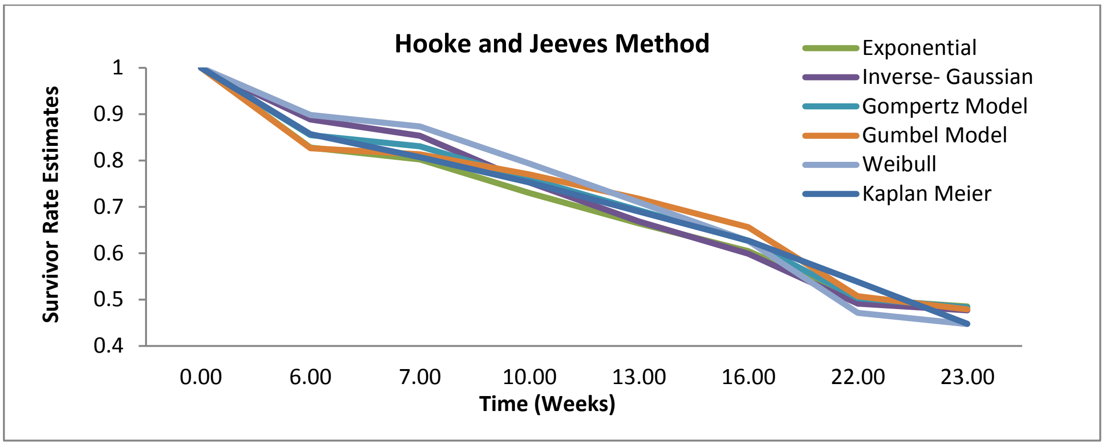


Table 3: Comparison of Survival Rate estimates Using Nelder and Meads, and Hooke and Jeeves Optimization methods

Failure Time (Weeks)	Number of Failures	Hooke and Jeeves Method					
		Exponential	**Inverse-Gaussian**	**Gompertz Model**	**Gumbel Model**	**Weibull**	**Kaplan Meier**
0	1	1	1	1	1	1	1
6	3	0.8280900	0.888879	0.8544705	0.826505	0.89801	0.85714
7	1	0.8024607	0.853157	0.8307175	0.813581	0.87327	0.80722
10	1	0.7302349	0.753023	0.7605747	0.769623	0.79365	0.75294
13	1	0.6645097	0.668558	0.6923736	0.717234	0.71014	0.69019
16	1	0.6047002	0.598642	0.6264513	0.655845	0.62683	0.62745
22	1	0.5007462	0.49138	0.5027187	0.506848	0.47125	0.53815
23	1	0.4852482	0.476720	0.4832757	0.479145	0.44748	0.44817





3. PROBABILITY DISTRIBUTION MODELS USING LEAST-SQUARES METHODS AND APPLYING QUASI-NEWTON METHODS (DFP AND BFGS METHODS)

For a practical application of the least-squares estimation method, when partial derivatives of the objective function F are available. We used Davidon-Fletcher-Reeves (DFP), ([13,14]) and Broyden-Fletcher and Shanno (BFGS), ([9.14,15]), methods to find the parameter estimates and survivor rate estimates for different probability distribution models.

3.1 Exponential Distribution Model

The exponential distribution ([22]) is a very commonly used distribution in reliability and life testing. The single-parameter exponential pdf is

$$f(t) = \lambda \exp(-\lambda t), t \geq 0, \lambda > 0 \tag{3.1}$$

The reliability (or survivor) function of the exponential distribution is

$$S(t) = 1 - F(t) = 1 - \int_0^t f(x)dx \tag{3.2}$$

$$\text{Or } S(t) = \exp(-\lambda t). \tag{3.3}$$

$$H(t) = \frac{f(t)}{S(t)} = \lambda \tag{3.4}$$

Where λ parameter is the constant failure rate (or hazard rate). To apply these optimization methods, we need to find the first partial derivatives of the objective function F of eq. (1.3).

$$\frac{\partial F}{\partial \lambda} = 2\sum_{i=1}^{m} f_i \left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial \lambda}, \text{ where } \frac{\partial S(t)}{\partial \lambda} = -tS(t). \tag{3.5}$$

3.2 Inverse Gaussian Distribution Model

The pdf for the Inverse Gaussian distribution, $f(t)=\frac{1}{\sqrt{2\pi\beta t^3}}\, d \exp\left(-\frac{(d-vt)^2}{2\beta t}\right)$,

or $f(t)=\sqrt{\frac{\kappa}{2\pi\rho t^3}}\exp\left[-\frac{\kappa}{2\rho t}\{(\rho t-1)^2\}\right]$, where $t>0$, $\kappa=\frac{d^2\rho}{\beta}$, $\rho=\frac{v}{d}$,

The survivor function for the inverse Gaussian distribution model ([16,17]) at time t_i is $S(t) = \Phi\left(-\sqrt{\frac{\kappa}{\rho t}}(\rho t-1)\right)-e^{2\kappa}\Phi\left(-\sqrt{\frac{\kappa}{\rho t}}(\rho t+1)\right)$, where Φ is the standard normal distribution function and $S(t_i,\alpha_0,\beta_0)$ is the survivor function ([17]) at the starting point (α_0,β_0).

3.3 Gompertz Distribution Model

The survivor function for the two-parameter Gompertz distribution ([13], [15]) is

$$S(t) = \exp\left(\frac{b}{a}\left(1-\exp(at)\right)\right). \tag{3.6}$$

To find the parameter estimates for the Gompertz distribution model using least-squares estimation procedures, we consider the objective function *F* as

$$F = \sum_{i=1}^{m} f_i\,(S(t_i)-KM(t_i))^2 \ , \tag{3.7}$$

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

For the DFP and BFGS optimization methods, we find the first partial derivatives of the objective function F, we have

$$\frac{\partial F}{\partial a} = 2\sum_{i=1}^{m} f_i\left(S(t_i)-KM(t_i)\right)\frac{\partial S(t_i)}{\partial a} \tag{3.8}$$

and
$$\frac{\partial F}{\partial b} = 2\sum_{i=1}^{m} f_i\left(S(t_i)-KM(t_i)\right)\frac{\partial S(t_i)}{\partial b}\ , \tag{3.9}$$

where
$$\frac{\partial S(t)}{\partial a} = -\frac{b}{a^2}\left(1+\exp(at)(at-1)\right)\, S(t)$$

and
$$\frac{\partial S(t)}{\partial b} = \frac{1}{a}\left(1 - \exp(at)\right)\, S(t).$$

Using eq.(3.7), eq.(3.8) and eq.(3.9) 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 Gompertz distribution model ([8,9,10]).

3.4 Gumbel Distribution Model

The survivor function for the two-parameter Gumbel distribution model ([18]) is

$$S(t) \;=\; \exp\left(-(\frac{b}{a})\exp(at)\right). \tag{3.10}$$

We construct the least-squares estimation function for the Gumbel distribution model

$$F \;=\; \sum_{i=1}^{m} f_i\,(S(t_i) - KM(t_i))^2 \tag{3.11}$$

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

To find the parameter estimates, we used the DFP and the BFGS optimization methods ([19]-[24]). These optimization methods require only first partial derivatives of the objective function F

$$\frac{\partial F}{\partial a} = \;2\sum_{i=1}^{m} f_i\big(S(t_i) - KM(t_i)\big)\frac{\partial S(t_i)}{\partial a} \tag{3.12}$$

and
$$\frac{\partial F}{\partial b} = \;2\sum_{i=1}^{m} f_i\big(S(t_i) - KM(t_i)\big)\frac{\partial S(t_i)}{\partial b}\;, \tag{3.13}$$

where
$$\frac{\partial S(t)}{\partial a} \;=\; \frac{b}{a^2}\exp(at)\big(1 - \exp(at)\big)\;S(t)$$

and
$$\frac{\partial S(t)}{\partial b} \;=\; -\frac{1}{a}\exp(at)\;S(t)\;.$$

Now using eq.(3.11), eq.(3.12) and eq.(3.13) 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 Gumbel distribution model ([10,11]).

3.5 Weibull Distribution Model

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

$$S(t) \;=\; \exp\left(-(\frac{t}{\alpha})^{\beta}\right), \tag{3.14}$$

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

$$F \;=\; \sum_{i=1}^{m} f_i\,(S(t_i) - KM(t_i))^2 \tag{3.15}$$

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, we have

$$\frac{\partial F}{\partial \alpha} = 2\sum_{i=1}^{m} f_i\left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial \alpha} \tag{3.16}$$

and

$$\frac{\partial F}{\partial \beta} = 2\sum_{i=1}^{m} f_i\left(S(t_i) - KM(t_i)\right)\frac{\partial S(t_i)}{\partial \beta}, \tag{3.17}$$

where

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

Using the objective function eq.(3.15), and the first partial derivatives eq.(3.16) and eq.(3.17) 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 ([24,25,26]).

The numerical results for the above said probability distribution models are presented in the table-4 and table-5.

Table 4: Parameter Estimates and Optimal Function Values, Gradient and the variance-covariance's for the Exponential, Inverse Gaussian, Gompertz, Gumbel and Weibull Distribution Models using DFP method.

	DFP Method				
	Exponential	**Inverse-Gaussian**	**Gompertz Model**	**Gumbel Model**	**Weibull**
Parameter Estimates $\left(a^*, b^*\right)$	2.96463E-2	0.18341065 0.01220035	0.018866 0.025292	0.08415445 0.00930334	30.75038 1.12722
Optimal Functional value	5.055E-03	0.565086E-02	0.003055	0.006062	0.00321109
Gradient at $\left(a^*, b^*\right)$	9.766E-08	-0.63533E-05 -0.46768E-04	0.962E-06 0.648E-05	0.9039E-09 0.8884E-08	-0.2713E-05 -0.2142E-04
Variance-Covariance at $\left(a^*, b^*\right)$	8.1389E-04	6.2405 0.3346 0.3346 0.0181	0.0826 -0.0186 -0.0186 .00478	0.022389 -0.0009 -0.0009 0.00012	1737. -73.95 -73.95 4.27

Table 5: Parameter Estimates and Optimal Function Values, Gradient and the variance-covariance's for the Exponential, Inverse Gaussian, Gompertz, Gumbel and Weibull Distribution Models using BFGS method.

	BFGS Method				
	Exponential	**Inverse-Gaussian**	**Gompertz Model**	**Gumbel Model**	**Weibull**
Parameter Estimates $\left(a^{*},b^{*}\right)$	2.964389E-2	0.18346625 0.01220656	0.01886325 0.02529981	0.08415415 0.00930323	30.75490 1.12708
Optimal Functional value	5.055E-03	0.56508E-02	0.00305524	0.00606156998	0.00321109491
Gradient at $\left(a^{*},b^{*}\right)$	-1.264E-05	-0.271E-06 0.595E-05	0.9623E-06 0.64881E-05	-0.12160E-07 -0.23565E-07	0.10014E-07 0.16052E-05
Variance-Covariance at $\left(a^{*},b^{*}\right)$	8.1396E-04	6.0991 0.3257 0.3257 0.0175	0.0842 -0.0187 -0.0187 0.0048	0.0211 -0.0009 -0.0009 0.00012	2253.58 -83.71 -83.71 4.46

5. CONCLUSION

The Survival rate estimates for the 21 Leukemia patients for the period of 35 week under observations were compared using parametric distribution models and non-parametric Kaplan Meier Model ([1]). We found that the results for the 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 method (DFP and BFGS methods)) and are also comparable with the non-parametric model. For the parametric models like (Exponential, Gompertz, Gumbel, Inverse and Weibull), we can find the parametric estimate, variance – covariance, optimal function values and some other useful information in different tables and graphical representations.

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