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Parameter Estimation for the Gompertz Distribution Model Using Least-Squares Method in Conjunction with Simplex and Quasi-Newton Optimization Methods

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Abstract: We find Survival rate estimates using parametric (Gompertz probability distribution) model and nonparametric (Kaplan-Meier) model. For the Gompertz distribution model, when first partial derivatives were not available, the Simplex optimization Methods (Nelder and Mead and Hooke and Jeeves) were used and 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 least squares method was applied for both the cases (simplex optimization methods and Quasi-Newton optimization methods) to find the parameter estimates, optimal function values, variance-covariance matrix. The medical data sets of 21 Leukemiacancer patients with time span of 35 weeks were used.

Key words: Gompertz 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

INTRODUCTION

The simplex Methods (Nelder and Mead [1] and Hooke and Jeeves [2] do not require partial derivatives and the function values are compared to find the optimal value of the objective function. Whereas, the Quasi –Newton Methods (DFP [3], [4] and BFGS [5], [6], [7], [8] require first partial derivatives for the function. In this paper, we find the parameter estimates using simplex and Quasi-Newton methods. These optimization methods were applied using medical data sets of cancer patients [9].

For the applications of these optimization (simplex and Quasi-Newton) methods, we used the least-square method.

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 [4].

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, [10], [11] an effort hasbeen 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 [12], [13] consists of finding parameter estimates that minimizes 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;

$$r_i = y_i^{obs} - y_i^{est}, i = 1,2,\cdots,m \tag{1}$$

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

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

The objective function is the sum of the squares of the deviations between the observed values and the corresponding estimated values. The maximum absolute discrepancy between observed and estimated values is minimized using optimization methods.

We treated Kaplan-Meier estimates ($KM(t_i)$ [14] as the observed values (y_i^{obs}) of the objective functionand the survivor rate estimates ($S(t_i)$) of Gompertz [10] model as the estimated value (y_i^{est}) of the objective function$F$ [3]. We considered the objective function for the model of the form.

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

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 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 [15].
- We suppose that the survivor function of Gompertz distribution model [10] at time t_i is $S(t_i; a, b) = exp\left(\frac{b}{a}(1 - \exp(at)\right)$ 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 $S(t_i;\, a_0,b_0)$ of the Gompertz distribution modelat 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 (a^*, b^*) (optimal value of the parameters).

Gompertz distribution model using Least-Squares Methods and Applying Nelder and Mead and Hooke and Jeeves Search Methods: For a practical application of the least-squares estimation method, when assuming partial derivatives of the objective function F were not available, we considered the data of twenty-one leukemia patients. Nelder and Mead [16], [17], [18] and Hooke and Jeeves [19], [20] 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. The numerical results of Gompertz 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 [14] and other information have been presented in Table 1 and Table 2.

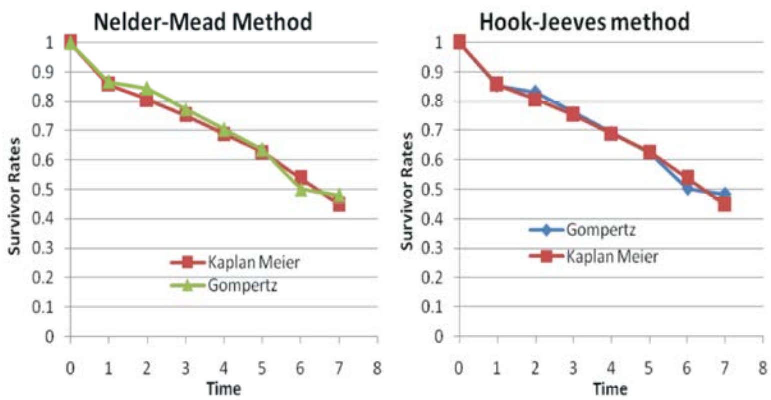
Numerical Results for Gompertz Probability Distribution Model using Least-Squares Methods and Applying Nelder and Mead(NM) and Hooke and Jeeves(HJ) Methods

Table 1: Comparison of Survival Rate estimates for Gompertz Distribution Model

		Nelder and Mead		Hooke and Jeeves Method	
Failure Time (Weeks)	Number of Failures	Gompertz Model	Kaplan Meier	Gompertz Model	Kaplan Meier
6	3	0.86616	0.85714	0.8544705	0.85714
7	1	0.84333	0.80722	0.8307175	0.80722
10	1	0.77433	0.75294	0.7605747	0.75294
13	1	0.70497	0.69019	0.6923736	0.69019
16	1	0.63587	0.62745	0.6264513	0.62745
22	1	0.50116	0.53815	0.5027187	0.53815
23	1	0.47947	0.44817	0.4832757	0.44817

Table 2: Parameter Estimates and Optimal Function Value for Gompertz Distribution Model

	Nelder and Mead Method	Hooke and Jeeves Method
Parameters Estimates	0.020989099	0.031560815
	0.037910900	0.045794945
Optimal Functional value	0.035096464	0.03664972



Gompertz 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 Gompertz distribution [13], [15] is:

$$S(t) = \exp\left(\frac{b}{a}\left(1-\exp(at)\right)\right) \tag{4}$$

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

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

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 using eq.(4.1.1) and eq.(4.1.2), we have

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

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

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 eqn.(5), eqn.(6) and eqn.(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 Gompertz distribution model and the results are presented in the Table 3.

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

Table 3:

Quasi Methods	Parameters Estimates	Optimal Functional value	Gradient at Optimal (a^*, b^*)	The Variance-Covariance at Optimal (a^*, b^*)
DFP Model	0.01886352	0.00305514	0.96230E-06	0.9623E-06
	0.02529382		0.64881E-05	0.64881E-05
BFGS Model	0.01886325	0.00305524	0.08262 -0.0186	0.08422 -0.01874
	0.02529981		-0.0186 0.00478	-0.01875 0.00480

CONCLUSION

The Survival rate estimates for the 21 Leukemia patients for the period of 35 week under observations were compared using parametricGompertz distribution model [13], [14] and non-parametric Kaplan Meier Model [1]. We found that the results (like the parameter estimates, optimal function values, variance-covariance matrices etc.) for the Gompertz distribution model were approximately samefor both the cases when the derivatives of an objective function were not available (using the Hooke and Jeeves and Nelder and Mead method) and when first partial derivatives of the objective function were available (using Quasi-Newton method (DFP and BFGS methods)). It was also found that the results using Nelder and Meads method were very close to the results of Quasi-Newton (DFP and BFGS) optimization methods.

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