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A Method for Computing Initial Approximations for a 3-parameter Exponential Function

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Authors' contributions

This work was carried out in collaboration between all authors. Author CRK formulated the problem, validated the algorithm and wrote the manuscript. Author MYS formulated the problem and revised the manuscript. Author PHK programmed and validated the algorithm. All authors read and approved the final manuscript.

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ABSTRACT

This paper proposes a modified method (MM) for computing initial guess values (IGVs) of a single exponential class of transcendental least square problems. The proposed method is an improvement of the already published multiple goal function (MGF) method. Current approaches like the Gauss-Newton, Maximum likelihood, Levenberg-Marquardt etc. methods for computing parameters of transcendental least squares models use iteration routines that require IGVs to start the iteration process. According to reviewed literature, there is no known documented methodological procedure for computing the IGVs. It is more of an art than a science to provide a "good" guess that will guarantee convergence and reduce computation time.
To evaluate the accuracy of the MM method against the existing Levenberg-Marquardt (LM) and the MGF methods, numerical studies are examined on the basis of two problems that's; the growth and decay processes. The mean absolute percentage error (MAPE) is used as the measure of accuracy among the methods. Results show that the modified method achieves higher accuracy than the LM and MGF methods and is computationally attractive. However, the LM method will always converge to the required solution given "good" initial values.

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The MM method can be used to compute estimates for IGVs, for a wider range of existing methods of solution that use iterative techniques to converge to the required solutions.

Keywords: Initial approximations; transcendental least squares; iteration routines; exponential problems; mean absolute percentage error.

MSC: 11D61, 11D72, 11J99.

1. INTRODUCTION

Nonlinear problems are regularly encountered in both engineering and physical science fields. These problems are reformulated into mathematical nonlinear equations which are solved using existing optimization methods like the Expectation-Maximum (EM) algorithm, Gauss-Newtons methods etc. which employ iteration routines in order to converge to the optimal solution. When practical and theorectical nonlinear problems are formulated, the final step is always finding the solutions of the subsequent simultaneaous nonlinear equations [1]. The equations can not be solved explicitly for exact solutions. However, a sufficiently “good” initial estimate can be provided so that any iterative technique that may be applied will converge to the required optimal solution.It is acknowledged that the word “good” is in itself vague, but theproposed modified method (MM) will provide solutions for initial guess values (IGVs) that will always guarantee convergence to the required optimal solution. Most of the current methods of solution are very sensitive to initailization and this serves as a bench mark for our study to develop systematic and algorithmic procedures for estimating IGVs.

Exponential equations are a class of nonlinear problems that are mainly solved by linearisation through algorithmic procedures. Traditional methods for solving nonlinear problems transform the nonlinear function into a linear one using the approximation of the well-known Taylor expansion [2].

To solve nonlinear least square problems in the applied sciences and mathematics, numerical iteration methods are usually applied such as the Newton method [3,4], Gauss-Newton method [2] which transform the integral equations into linear systems of algebraic equations which can be solved by direct or iterative methods. The iterative methods require provision of IGVs to compute the optimal solutions.Other methods in current use are; derivative free methods, direct optimization and the Levenberg-Marquardt (LM) which is more preferred because of it robustness [5,6,] as it always finds a solution even if it starts far from the required minimum. In this paper amethod to the problem of finding IGVs, is presented. The algorithm is described in (modification of the multiple goal function) section and its performance is compared with that of Levenberg-Marquardt [7,8] and the multiple goal function (MGF) [7], methods for a given class of exponential problems. First an analytical nature of the approach is discussed and numerical studies to evaluate the performance of the MM method against the conventional LMand MGF methods is examined.

2. PROBLEM FORMULATION OF A 3-PARAMETERISED EXPONENTIAL MODEL

We consider a generalised three parameter single exponential model of the form:

$$f(x) = \alpha e^{\beta x} + \gamma, \tag{2.1}$$

where α , β and γ are the unknown parameters, whose initial guess values must be provided.

The goal function for the determination of unknown parameters α , β and γ :

$$G(\alpha,\beta,\gamma) = \frac{1}{2}\sum_{i=1}^{N}\left\{\alpha e^{\beta x_i} + \gamma - f(x_i)\right\}^2 \to \min. \tag{2.2}$$

Partially differentiating Eq.(2.1)with respect to α , β and γ leads to the following system of equations that are transcendental with respect to the unknown parameters:

$$\frac{\partial G}{\partial \alpha} = \alpha\sum_{i=1}^{N} e^{2\beta x_i} + \gamma\sum_{i=1}^{N} e^{\beta x_i} - \sum_{i=1}^{N} f(x_i)e^{\beta x_i} = 0. \tag{2.3}$$

$$\frac{\partial G}{\partial \gamma} = \alpha\beta\sum_{i=1}^{N} e^{\beta x_i} + \gamma N - \sum_{i=1}^{N} f(x_i) = 0 \tag{2.4}$$

$$\frac{\partial G}{\partial \beta} = \alpha\sum_{i=1}^{N} x_i e^{2\beta x_i} + \gamma\sum_{i=1}^{N} x_i e^{\beta x_i} - \sum_{i=1}^{N} x_i f(x_i)e^{\beta x_i} = 0. \tag{2.5}$$

The system of Eqs. (2.3–2.5) can not be solved explicitly to give closed form solutions because, each side of the equations contains unknowns in every term. However, their methods of solution are well known like the Newton methods, secant methods, likelihood methods etc, but all these methods demand the use of iterative procedures which require IGVs to start the iteration process.

In this paper a method that could be used to estimate IGVs which guarantee convergence to the required solutions and lead to a shorter computation time is formulated.According to the reviewed literature, there exists no known algorithms and systematic approaches for computing the IGVs. The method of trial and error is oftenly employed and in some cases the underlying problem is estimated as a linear model and identified using the ordinary least squares techniques ignoring the nonlinearities in the model. The computed parameters are then used as IGVs [9,10,11].

3. OVERVIEW OF THE MULTIPLE GOAL FUNCTION METHOD

The main idea is to transform the original transcendental problem into a new problem which is linear with respect to new unknown parameters. Differential methods are applied in order to linearise the problem and the problem solved using ordinary least squares techniques via integral methods. The multiple goal function (MGF) method proposed by [7], is modified to a single goal function to estimate some of the required parameters.

We firstly examine the MGF method which provides solutions of transcendental problems via two stages of optimisation of the initial problem. Optimisation is achieved by formulating an objective function at each stage and subsequently solving the normal equations for the unknown set of parameters using ordinary least squares techniques. To improve on the accuracy of estimatability of this method (MGF), a new method is proposed that applies optimisation of an objective function at one stage to obtain some of the unknown parameters and continues to solve for the rest of the unknown parameters using simple algebraic formulations of the initial problem. The solutions are then applied as IGVs to start the iteration process to a range of existing optimisation methods that use iteration procedures to estimate the required solution.

Considering the first and second derivatives of Eq.(2.1):

$$f'(x) = \eta e^{\beta x}, \text{ with } \eta = \alpha\beta, \tag{3.1}$$

taking the second derivative and making approprate substitutions, we have;

$$f''(x) = \beta f'(x). \tag{3.2}$$

Integrating Eq.(3.2) over the region $[a;x]$ yields:

$$f'(x) - \beta f(x) - f'(a) + \beta f(a) = 0. \tag{3.3}$$

Letting $\lambda = \beta f(a) - f'(a)$ in Eq.(3.3), we obtain:

$$f'(x) - \beta f(x) + \lambda = 0. \tag{3.4}$$

Integrating Eq.(3.4), over the region $[a;x]$ again yields:

$$f(x) = \beta I(x) - \lambda x + f(a) + \lambda a \text{ with } I(x) = \int_a^x f(\xi)d\xi. \tag{3.5}$$

When a dataset $(x_i, f(x_i))$ for $i = 1,...,n$ is available, it is possible to obtain a system of linear equations represented by Eq. (3.6);

$$Y = \beta X_1 - \lambda X_2 + C, \tag{3.6}$$

where $Y = f(x_i), X_1 = I(x_i), X_2 = x_i$ and $C = f(a) + \lambda a$; parameters β, λ and C are estimated by solving the system of equations represented by Eq. (3.6) using ordinary least squares methods.

For the MG Fmethod estimates $\hat{\lambda}$ and $\hat{C}$ are considered as nuisance parameters and subsequently ignored, only $\hat{\beta}$ is considered for further analyses. After estimating $\hat{\beta}$ from Eq. (3.6), the original problem can be reformulated as a system of linear regression equations:

$f(x_i) = \alpha X_3 + C_1$ for $X_3 = e^{\hat{\beta}x_i}$ and $C = \gamma.$ (3.7)

The unknwon parameters α and C_1 are as well estimated using the ordinary least squares methods.

4. MODIFICATION OF THE MULTIPLE GOAL FUNCTION ALGORITHM (MMGF)

The MGF method is based on the idea that the unknown parameters are estimated from two formulated objective functions of Eqs. (3.6 & 3.7) from which normal equations that have closed form solutions are formed.

One major disadvantage of the MGF method is that numerical differentiation procedures are done several times which leads to greater loss of information or data at these subsequent stages [12]. This eventual loss of data compromises the accuracy of the MGF method. Thecopious differentiation procedures may be minimised as follows.

Consider Eq. (3.6), rewritten as:

$$f(x) - \beta I(x) + \lambda x - C = 0. \quad (4.1)$$

Estimation of the parameters β, λ and C was done in Eq. (3.6) using ordinary least squares methods. Now considering that:

$$f(a) + \lambda a = C, \text{ for } \lambda = \beta f(a) - f'(a) \quad (4.2)$$

It is then clear that:

$$\beta\left(C - \lambda a\right) - f'(a) = \lambda\,, \quad (4.3)$$

solving for $f'(a)$ from Eq. (4.3), we obtain:

$$f'(a) = \beta C - \lambda\beta a - \lambda. \quad (4.4)$$

Therefore, $f'(a)$ and $f(a)$ are now known.

Taking the first derivative of the original problem in Eq. (2.1), we have:

$$f'(x)\big|_{x=a} = \frac{d\left[\alpha e^{\beta x} + \gamma\right]}{dx} = \alpha\beta e^{\beta a}, \quad (4.5)$$

implying;

$$f'(a) = \alpha\beta e^{\beta a}. \quad (4.6)$$

Equating Eq. (4.4) and Eq. (4.6), and solving for α we obtain:

$$\alpha = (C - \lambda a - \frac{\lambda}{\beta})e^{-\beta a}. \quad (4.7)$$

For $x = a$ in Eq. (2.1) and equating the result with Eq. (4.2) yields:

$$\gamma = C - \lambda a - \alpha e^{\beta a}. \quad (4.8)$$

Substituting for α in Eq. (4.8) from Eq. (4.7), and simplifying, we obtain:

$$\gamma = \frac{\lambda}{\beta}. \quad (4.9)$$

Hence the unknown parameters (α, β and γ) in Eq. (2.1) are identified from Eqs. (4.7, 3.6, & 4.9) respectively. The estimated parameters could then be used as initial guess values to a wider range of the single exponential class of problems.

5. PERFORMANCE OF THE ALGORITHMS

The criterion used to evaluate the performance of the methods (i.e LM, MGF and MM) was that; two datasets were generated which simulated the growth and decay processes [13]. The methods were then applied to estimate the known theoretical models in each case. The measure of performance was the mean absolute percentage error (MAPE). It's a measure of accuracy of a technique or routine used to construct estimated or predicted values in statistical data, usually timeseries forecats for trend analysis [14,15]. This is a measure of accuracy commonly prefered because of its suitability in many practical and theoretical instances [16,17]. Tables 2 and 4 summarise the performance of the three methods on the basis of the known models considered, and Tables 1 and 3 show the estimated parameters from the respective methods. The main focus on the performance of the three methods was on how well each of them estimated the already known (exact) model parameters (α, β & γ) in either problem.

Table 1. Comparison of the parameter estimates using the modified, the multiple goal function and the Levenberg-Marquardt methods with the exact values for the growth model

Parameter	Exact values	Modified method	Multiple goal function	Levenberg-marquardt method (LM)
α	0.2	0.219092	0.177825	0.156527
β	1.1	1.095585	1.114730	1.135970
γ	15	14.98090	16.43410	17.03950

Table 2. The mean absolute percentage errors of the modified method, the multiple goal function and the Levenberg-Marquardt method on growth model

MAPE for the modified method	MAPE for multiple goal function	MAPE for levenberg-marquardt
3.36	7.33	12.87

Table 3. Comparison of the parameter estimates using the modified, the multiple goal function and the Levenberg-Marquardt methods with the exact values for the decay model

Parameter	Exact values	Modified method	Multiple goalfunction	Levenberg-marquardt method (LM)
α	10.2	10.19991	10.18640	10.06450
β	-1.1	-1.095585	-0.104719	-1.029130
γ	15	15.00009	14.91630	14.89790

Table 4. The mean absolute percentage errors of the modified method, the multiple goal function and the Levenberg-Marquardt method on the decay model

MAPE for the modified method	MAPE for multiple goal function	MAPE for levenberg-marquardt
0.13	30.39	2.82

6. DISCUSSION AND CONCLUSION

From a comparision of the current MM method and results obtained on the same problems (growth and dacay models) by the existing and general methods (i.e MGF and LM), it is clear that the MM method has a comparative advantage over the other methods see Tables 2 and 4. The MM method has an accuracy of about 2 and 4 times that of the MGF and the commonly applied and more robust LM method respectively on estimating the growth model. We also examined the performance of the MM method on the decay model, and it was found that its performance was far more appealing on identification of the decay model than the growth model parameters. It exhibited an accuracy of about 234 and 22 times that of the MGF and LM methods respectively. The authors have compared the MM method with their earlier work using the MGF and the existing LM methods and found that the MM performs better in estimating solutions (IGVs) than other methods. It is thus recommended that results from the modified method be used as initial guess values when estimating optimal solutions for exponential models that fall in the class of 3-parameter problems.

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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