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Review Article

A METHOD FOR COMPUTING INITIAL APPROXIMATIONS FOR A 3-PARAMETER EXPONENTIAL FUNCTION

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, Levenbreg-Marquardt e.t.c 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 MGFmethods, numerical studies are examined on the basis of two problems thats; 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 modfied method acheives 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.

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,

UNDER PEER REVIEW

Gauss-Newtons methods e.t.c. 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], 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 [4]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 [5,6] and the multiple goal function (MGF) [7],methodsfor 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. Formulation of the problem

2.1. General 3-parameterised exponential model

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

UNDER PEER REVIEW

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

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:

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

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 thatcould be used to estimate IGVs which guarantee convergence to the required solutionsand 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 [8].

UNDER PEER REVIEW

3. Methodology

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 method proposed by [7], is modified to a single goal function to estimate some of the required parameters.

3.1. The Multiple goal function (MGF) method

Under this section, we examine the MGF, this method provides solutions of transcendental problems via two stages of optimisation of the initial problem. Optimisation is achievedby formulating an objective function at each stage and subsequently solving the normal equationsfor the unknown set of parameters using ordinary least squares techniques. To improve on the accuracy ofestimatability 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.(3.1):

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

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:

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

UNDER PEER REVIEW

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.

FortheMGFmethod 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:

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

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 (MM)

The MGF method is based on the idea that the unknown parameters are estimatedfrom two formulated objective functions ofEqs. (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. 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:

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

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

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

It is then clear that:

UNDER PEER REVIEW

$$\beta(C - \lambda a) - f'(a) = \lambda, \tag{4.3}$$

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

$$f'(a) = \beta C - \lambda\beta a - \lambda. \tag{4.4}$$

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

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

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

implying;

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

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

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

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

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

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

$$\gamma = \frac{\lambda}{\beta}. \tag{4.9}$$

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. The

UNDER PEER REVIEW

methods were then applied to estimate the known theoretical models in each case.The measure of performance was the mean absolute percentage error (MAPE). This is a measure of accuracy commonly prefered because of its suitability in many practical and theoretical instances [9,10]. Table 2& 4summarise the performance of the three methods on the basis of the known models considered, and Tables 1& 2 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 ($\alpha, \beta \,\&\, \gamma$) in either problem.

parameter	**Exact values**	**Modified Method (MM)**	**Multiple goal function (MGF)**	**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 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.

MAPE for the Modified Method	**MAPE for the Multiple goal function**	**MAPE for the Levenberg-Marquardt**
3.36	7.33	12.87

Table 2: The mean absolute percentage errors of the Modified Method, the Multiple Goal Function and the Levenberg-Marquardt method on growth model.

parameter	**Exact values**	**Modified Method (MM)**	**Multiple goal function (MGF)**	**Levenberg-Marquardt Method (LM)**
α	10.2	10.19991	10.18640	10.06450
β	-1.1	-1.095585	-0.104719	-1.029130

UNDER PEER REVIEW

γ	15	15.00009	14.91630	14.89790

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.

MAPE for the Modified Method	MAPE for the Multiple goal function	MAPE for the Levenberg-Marquardt
0.13	30.39	2.82

Table 4: The mean absolute percentage errors of the Modified Method, the Multiple Goal Function and the Levenberg-Marquardt method on the decay model.

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& 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 methodrespectively 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 to a broader range of exponential models which fall in the class of 3-parameter problems.

COMPETING INTERESTS

The author has declared no competing interests

UNDER PEER REVIEW

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