

Nelder--Mead Algorithm in Solving Ordinary Differential Equations Whose Solutions Possess Singularities

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ABSTRACT

This research considers Initial Value Problems (IVPs) in Ordinary Differential Equations (ODEs) whose solutions possess singularities. Here, we represent the theoretical solution by a rational function as it is more convenient representing a function close to a singularity by a rational function. The process of transforming the IVP to a constrained optimization problem and application of Nelder-Mead algorithm in obtaining approximate solution is presented in this work. Accuracy and efficiency of this scheme is demonstrated on two numerical examples. The proposed approach produced better results compared with existing methods discussed in literature.

Keywords: Ordinary Differential Equation; Initial Value Problems; Singularities; Optimization; Nelder-Mead Algorithm.

1 Introduction

The basic assumption in the construction of many numerical schemes for solving initial value problems in ordinary differential equations is that the theoretical solution is representable by a polynomial. In practice however, this assumption is not always true for problems whose solutions possess a singularity [9-11]. Results obtained by such methods around the point of singularity are usually poor [9, 11]. As they are based on local representation by polynomials, methods such as the Runge-Kutta type methods, Obrechhoff methods and general linear multistep methods usually produce poor solutions in the neighbourhood of singularity points [4, 5, 9, 10]. To overcome the limitation of these classical methods, it is convenient and more appropriate to use a rational functions in the local representation of the solutions of such problems whose solutions possess a singularity [4, 9, 10]. This is appropriate as rational functions are more suitable for representing a function around a singularity point. Methods based on local representation of the theoretical solution by rational function instead of polynomials gained popularity after the author in [10] published a pioneer work in which he constructed quadrature formulas based on rational interpolating functions. Rational interpolation methods constructed in [11] and [4] proved to be effective in the neighbourhood of the singularity and even beyond. The general rational function used in [10] was replaced with $F(x) = \frac{P_m(x)}{Q_n(x)}$ where $P_m(x)$ and $Q_n(x)$ are respectively polynomials of degree m and n in the work of author in [11]. Several efficient methods have been proposed using this approach [7, 14, 3, 21, 15]. The works of authors in [2, 14, 21, 3, 20, 16, 7] have been seen to establish that solutions

around singularity point are well approximated by this approach. The use of evolutionary algorithms in obtaining more accurate solutions of problems in ODEs is becoming now gaining wide popularity. Initial value problems are usually transformed to constrained optimization problems and solved using optimization techniques. Second-order initial value problems were solved in [6] and [13] respectively using classical genetic algorithm and combination of genetic algorithm with the Nelder–Mead method. Using a combination of collocation method and genetic algorithms approximate solutions of first-order initial value problem were obtained in [12]. Authors in [24] used the differential evolution algorithm to obtain solutions of stiff systems of first-order ODEs. In [19], continuous genetic algorithm in obtaining the solution of two-point boundary value problem $u'' = f(t, u); u(a) = \eta_1; u(b) = \eta_2$ with oscillatory behaviour and problems of the form $u'' + p(t)u' + q(t)y = r(t)$ were respectively presented in [23] and [1]. Authors in [17] also proposed the use of differential evolution algorithm in the minimization of the error that resulted from the curve fitting of the Nakagami distribution. Quantile approximation of the Erlang distribution using differential evolution algorithm was presented by authors in [18]. Neural network was introduced by authors in [8] to obtain approximate solution of second-order initial value problems. In this research, we transform a given initial value problem to a constrained optimization problem, represent the theoretical solution locally with a rational function and obtain the coefficients of the terms using Nelder–Mead algorithm.

2 Nelder–Mead Algorithm

The Nelder–Mead method is a direct search evolutionary algorithm. For a function of n variables, it maintains a set of $n+1$ points forming the vertices of a polytope in n -dimensional space. At each iteration, the points $x_1, x_2, \dots, x_{n+1}$ form a polytope and are ordered such that $f(x_1) \leq f(x_2) \leq \dots \leq f(x_{n+1})$. A new point is then generated to replace the worst point x_{n+1} .

Let c be the centroid of the polytope consisting of the best n points, $c = \frac{1}{n} \sum_{i=1}^n x_i$. A trial point x_t is generated by reflecting the worst point through the centroid $x_t = c + \alpha(c - x_{n+1})$, where $\alpha > 0$ is a parameter.

If the new point x_t is neither a new worst point nor a new best point, $f(x_1) \leq f(x_t) \leq f(x_n)$, x_t replaces x_{n+1} . If the new point x_t is better than the best point, $f(x_t) < f(x_1)$, the reflection is very successful and can be carried out further to $x_e = c + \beta(x_t - c)$, where $\beta > 1$ is a parameter to expand the polytope. If the expansion is successful, $f(x_e) < f(x_t)$, x_e replaces x_{n+1} ; otherwise the expansion failed, and x_t replaces x_{n+1} .

If the new point x_t is worse than the second worst point, $f(x_t) > f(x_n)$, the polytope is assumed to be too large and needs to be contracted. A new trial point is defined as

$$x_c = \begin{cases} c + \gamma(x_{n+1} - c), & \text{if } f(x_t) \geq f(x_{n+1}), \\ c + \gamma(x_t - c), & \text{if } f(x_t) < f(x_{n+1}), \end{cases}$$

where $0 < \gamma < 1$ is a parameter. If $f(x_c) < \min(f(x_{n+1}), f(x_t))$, the contraction is successful, and x_c replaces x_{n+1} . Otherwise a further contraction is carried out.

The process is assumed to have converged if the difference between the best function values in the new and old polytope, as well as the distance between the new best point and the old best point, are less than the tolerances.

3 Transformation of IVP to Constrained Optimization Problem

In this section, we present the process of transforming a given initial value problem into a constrained optimization problem. Here, the IVP

$$y' = f(x, y(x)), \quad x \in [x_0, X], \quad y(x_0) = \eta \quad (1)$$

whose solution possesses singularity is considered. We represent the solution of (1) with a rational function of the form

$$y(x) = \frac{\sum_{j=0}^m \alpha_j x^j}{\sum_{k=0}^n \beta_k x^k} \quad (2)$$

where $m, n \in \mathbb{N}$, α_j , $j = 0, 1, 2, \dots, m$ and β_k , $k = 0, 1, 2, \dots, n$ are real constants whose values are to be determined. Substituting the derivative of (2) into (1) gives

$$\frac{\sum_{j=0}^m j \alpha_j x^{j-1}}{\sum_{k=0}^n \beta_k x^k} - \frac{\left(\sum_{j=0}^m \alpha_j x^j\right) \sum_{k=0}^n k \beta_k x^{k-1}}{\left(\sum_{k=0}^n \beta_k x^k\right)^2} \approx f(x, y(x)). \quad (3)$$

Using the associated initial condition in (1), we have,

$$y(x_0) = \frac{\sum_{j=0}^m \alpha_j x_0^j}{\sum_{k=0}^n \beta_k x_0^k} \Big|_{x=x_0} = \frac{\sum_{j=0}^m \alpha_j x_0^j}{\sum_{k=0}^n \beta_k x_0^k} \approx \eta \quad (4)$$

From (3), the associated error expression $\mathcal{E}_i(x)$ at each node point x_i is obtained as

$$\mathcal{E}_i(x) = \left[\frac{\sum_{j=0}^m j \alpha_j x^{j-1}}{\sum_{k=0}^n \beta_k x^k} - \frac{\left(\sum_{j=0}^m \alpha_j x^j\right) \sum_{k=0}^n k \beta_k x^{k-1}}{\left(\sum_{k=0}^n \beta_k x^k\right)^2} - f(x, y(x)) \right]_{x=x_i} \quad (5)$$

Now we need to find values of α_j , $j = 1, 2, \dots, m$ and β_k , $k = 1, 2, \dots, n$, that minimizes the expression

$$\sum_{i=1}^{\frac{X-x_0}{h}} \mathcal{E}_i^2(x) \quad (6)$$

where h is the steplength. Using (6) and (4), the problem of finding approximate solution of (1) is now formulated as an optimization problem in the following manner:

$$\begin{aligned} \text{Minimize:} \quad & \sum_{i=1}^{\frac{X-x_0}{h}} \mathcal{E}_i^2(x) \\ \text{Subject to:} \quad & \frac{\sum_{j=0}^m \alpha_j x_0^j}{\sum_{k=0}^n \beta_k x_0^k} \approx \eta \end{aligned} \quad (7)$$

Equation (7) is solved using the Nelder–Mead algorithm. Suitable values of α_j , $j = 1, 2, \dots, m$ and β_k , $k = 1, 2, \dots, n$ which satisfies (7) were obtained using this direct search method. We shall refer to this scheme as *NMfPWS*.

4 Numerical Examples

In this section, two test problems whose solutions possess singularities were considered. For the first problem, we choose m and n in (2) as $m = n = 3$, while for the second problem m and n in (2) are

chosen as $m = n = 1$, The proposed procedure is implemented on both problem and the results obtained are compared with those discussed in the literature.

4.1 Problem 1

The first problem considered is the nonlinear initial value problem

$$y' = 1 + y^2; \quad y(0) = 1 \quad (8)$$

whose theoretical solution is

$$y(x) = \tan\left(x + \frac{\pi}{4}\right). \quad (9)$$

The solution has a singularity at $x = \frac{\pi}{4}$. Using a steplength of $h = 0.1$, the problem is solved over the interval $[0,1]$ via our proposed procedure. For this problem, we obtained the coefficients of terms in (2) as:

$$\left. \begin{aligned} \alpha_0 &= \frac{2785482491434062695770540221201}{630486482276998536369112597942} \\ \alpha_1 &= \frac{1320434717272988202293820675290}{337904383805767870125028984877} \\ \alpha_2 &= -\frac{5162317951269091912597231872014}{2327111400613658131750203021971} \\ \alpha_3 &= -\frac{983857310702903552486215956805}{11261679403442702832725815125073} \\ \beta_0 &= \frac{1822625174192420766830041152002}{412546314011998613116741532327} \\ \beta_1 &= -\frac{2648097607138421264981459694410}{537352675807977628683896115609} \\ \beta_2 &= -\frac{648051610158734064150656874760}{539757763925714451283984505127} \\ \beta_3 &= \frac{353574351435058017955816383447}{887075848309392118760737513321} \end{aligned} \right\} \quad (10)$$

Figure 1 shows the comparison of the natural logarithm of the absolute errors in the results obtained via our procedure with those presented in [16]. A comparison of the natural logarithm of the maximum absolute error obtained by the proposed procedure with classical third-order methods in [21, 7, 15, 14, 10] is also presented in Figure 2.

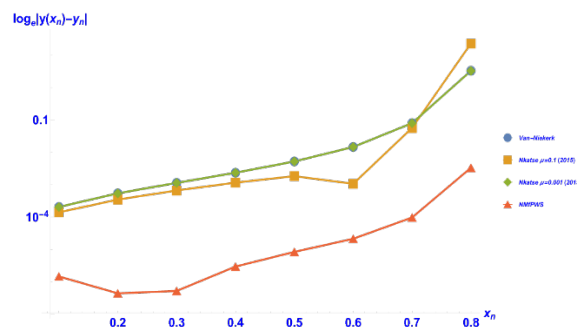


Figure 1: Logarithm of absolute errors for the solutions of Problem 1 with step-size $h = 0.01$

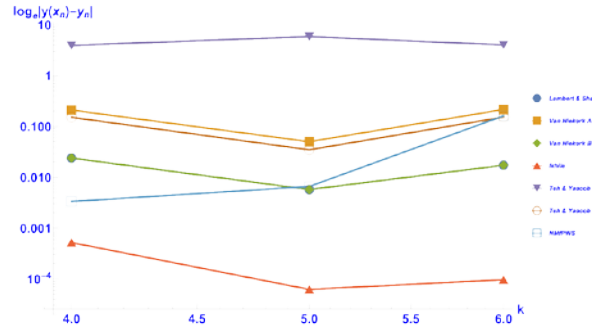


Figure 2: Log plot of maximum absolute errors for Problem 1 as a function of the step-size $h = \frac{0.8}{2^k}$, $k = 4(1)6$

Figure 1 and Figure 2 show that our approach competes favourably well with existing classical methods discussed in literature.

4.2 Problem 2

The second problem considered here is

$$y' = y^2; \quad y(0) = 1. \quad (11)$$

with theoretical solution

$$y(x) = \frac{1}{1-x}. \quad (12)$$

The solution has a singularity at $x = 1$. Again, a steplength of $h = 0.1$ was used and the coefficients in (2) were obtained as:

$$\left. \begin{aligned} \alpha_0 &= -\frac{1387246790756464659121721772995}{377924833815994505354035993832} \\ \alpha_1 &= \frac{10193302623204123}{72672365962345246451825456331944171737586882} \\ \beta_0 &= -\frac{2400774543186824719451368528447}{654038146859791336706809324384} \\ \beta_1 &= \frac{2962830580361835871831852161090}{807157934816779733393408378969} \end{aligned} \right\} \quad (13)$$

The logarithm of absolute errors for the solutions obtained are compared with other methods discussed in [20] as given in Figure 3.

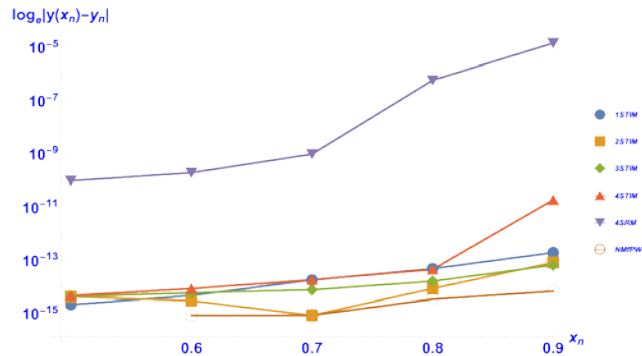


Figure 3: Logarithm of absolute errors for the solutions of (11) with step-size $h = 0.01$

Again, as expected, our technique approximated the solution more accurately.

5 Conclusion

The procedure for transforming a given initial value problem to a constrained optimization problem and determining the values of the parameters in the objective function using the Nelder–Mead algorithm has been presented. Based on some test problems, we show that the proposed technique can be used to in obtaining better solution. Comparison of the results obtained via our technique compared with those discussed in the literature shows the degree of accuracy of our technique.

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