

ON NUMEROV METHOD FOR SOLVING FOURTH ORDER ORDINARY DIFFERENTIAL EQUATIONS

¹Ndanusa, A., ¹Adeboye, K. R., ²Mustapha, A. U., and ³Abdullahi, R.

¹Department of Mathematics, Federal University of Technology, Minna, Nigeria

²Department of Mathematics and Statistics, Federal Polytechnic, Offa, Nigeria

³Department of Mathematics and Statistics, Niger State Polytechnic, Zungeru, Nigeria

*Corresponding author's email: as.ndanusa@futminna.edu.ng

ABSTRACT

In this work, a fourth order ODE of the form $y^{iv} = f(x, y'')$ is transformed into a system of differential equations, that is suitable for solution by means of Numerov method. The obtained solutions are compared with the exact solutions, and are shown to be very effective in solving both initial and boundary value problems in ordinary differential equations.

Keywords: Numerov's method, Runge-Kutta method, Schrodinger equation, Second order, Initial value problems

INTRODUCTION

A most preferred method in industry and other applications for numerically solving ordinary differential equations (ODE) is the classical Runge-Kutta method (RK4). However, when the differential equation does not include a first order term, the Numerov method comes to mind, as it is more accurate than the RK4 by an order. More so, a great many general second order ODEs can be transformed into one without a first order term, the solution of which can be obtained via the Numerov method, which requires less computational complexity, thereby being easier to program. The Numerov's method, a fourth-order implicit linear multistep method (LMM), is a numerical method for solving second order ordinary differential equations wherein the first-order term is missing; that is,

$$y'' = f(x, y) \quad (1)$$

The method takes the form

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{12}(f_{n+2} + 10f_{n+1} + f_n) + O(h^6) \quad (2)$$

Suppose f is linear in y , then by letting $f(x, y) = -g(x)y(x) + s(x)$, the method (2) reduces to the explicit form

$$y_{n+2} \left(1 + \frac{h^2}{12} g_{n+2} \right) = 2y_{n+1} \left(1 - \frac{5h^2}{12} g_{n+1} \right) - y_n \left(1 + \frac{h^2}{12} g_n \right) + \frac{h^2}{12}(s_{n+2} + 10s_{n+1} + s_n) + O(h^6) \quad (3)$$

In terms of efficiency, the Numerov method is the most preferred method when compared to the Runge-Kutta method, in that with just one evaluation of g and s per step a local error of $O(h^6)$ is obtained, as against the Runge-Kutta method that requires six function evaluations per step to attain a local error of $O(h^6)$. More so, it is computationally easier for both the computer and the programmer. Accuracy wise, the Numerov method is an order more accurate than the fourth order Runge-Kutta method (Salzman, 2001).

The Numerov method is a popular algorithm that is widely used in physics and engineering. Particular examples of application of this method in numerical physics can be found in the solution of Schrodinger's one-dimensional time independent equation (Bennett, 2015).

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{h} [V(x) - E] \psi \quad (4)$$

This is a typical example of an equation of type (1). Another example is the equation of motion of an undamped forced harmonic oscillator,

$$m \frac{d^2 y}{dx^2} = f_0 \cos \omega x - ky \quad (5)$$

A comparison of the shooting and the matrix diagonalization forms of the finite difference method for the Schrodinger equation leads to an order doubling principle which produces an eigenvalue estimate of 8th order from the traditional Numerov method.

Several studies have made substantial contributions to the improvement or modification of Numerov method; for example, Killingbeck and Jolicard (1999) introduced an order doubling principle which produces an eigenvalue estimate of 8th order from the traditional Numerov method by comparing the shooting and the matrix diagonalization forms of the finite difference method for the Schrodinger equation. Vigo-Aguiar and Ramos (2005) developed a variable-step Numerov method for the numerical solution of the Schrodinger equation. This method needs fewer evaluations of the potential than the classical Numerov method of fixed stepsize. Dongjiao (2014) recast the generalized version of the Numerov method into the Generalized Matrix Numerov Method based on the algorithm of the existing Basic Matrix Numerov Method. The Generalized Matrix Numerov Method is capable of producing results to any desired accuracy. Adeboye *et al.* (2018) proposed a convergent iterative process modification of the Numerov method. The new algorithm is applicable to the solution of second order initial value problems, including those with periodic solutions. Tsitouras and Simos (2018) proposed a new family of effectively nine stages, ninth-order hybrid explicit Numerov-type methods for solving some special second order initial value problem. By having a reduced set of order conditions, they derived an optimal constant coefficients method along with a similar kind of method with reduced phase errors. Yasser and Nahool (2018) transformed the Numerov method into a representation of matrix form to solve Schrodinger equation. The validity of the new method (Matrix Numerov Method) was tested by applying it to calculate spectra of bottomonium. The obtained results were compared with the experimental observed masses and theoretically predicted results. The obtained results were found to be in good agreement with the experimental results. Afolayan *et al.* (2019) considered the classical four-stage family of explicit sixth-order Numerov-type method. Two kinds of interpolants were provided: (i) a three-step interpolation based on all available data at mesh points and (ii) a local interpolant (i.e. two steps) that is constructed after solving scaled equations of condition. Application of these interpolants in a set of tests produced global errors of the same magnitude with the underlying method. Simos and Tsitouras (2020) proposed a new low cost two-step hybrid Numerov-type method for solving inhomogeneous linear initial value problems with constant coefficients. By solving a special set of order conditions, it became possible to save one stage (function evaluation) per step for this type of problems when compared with the best existed methods. The present work employs the Numerov method to solve numerically the fourth order differential equation $y^{iv} = f(x, y'')$.

Definition 1 The first and second characteristic polynomials of a k – step linear multistep method are defined as

$$\rho(\xi) = \sum_{j=0}^k \alpha_j \xi^j = \alpha_k \xi^k + \alpha_{k-1} \xi^{k-1} + \alpha_{k-2} \xi^{k-2} + \dots + \alpha_0 \quad (6)$$

and

$$\sigma(\xi) = \sum_{j=0}^k \beta_j \xi^j = \beta_k \xi^k + \beta_{k-1} \xi^{k-1} + \beta_{k-2} \xi^{k-2} + \dots + \beta_0 \quad (7)$$

Respectively.

Definition 2 A linear multistep method is of order p if $c_0 = c_1 = \dots = c_p = 0$ and $c_{p+1} \neq 0$, where the term c_{p+1} is called the error constant, $T_{n+k} = c_{p+1}h^{p+1}y^{p+1}(x_n) + O(h^{p+2})$ is the truncation error at the point x_n .

Definition 3 A linear multistep method is said to be consistent if it is at least first-order.

Definition 4 A linear multistep method is said to be zero-stable if as $h \rightarrow 0$, the roots $\xi_j, j = 1(2)k$ of the first characteristic polynomial $\rho(\xi)$ satisfy $|\xi_j| \leq 1$, and for every $|\xi_j| = 1$ the multiplicity must be simple.

Definition 5 A linear multistep method is convergent if and only if it is stable and consistent.

MATERIALS AND METHODS

Derivation of the Method

Given the differential equation (1); in order to derive the Numerov method for solving this equation, we begin with the Taylor expansion of the function we want to solve, $y(x)$ at $x \pm h$, based on the idea of Mohamed (1979) thus,

$$y(x \pm h) = y(x) \pm hy'(x) + \int_x^{x \pm h} (x \pm h - t)y''(t) dt$$

where,

$$\begin{aligned} \Delta^2 y(x-h) &= y(x+h) - 2y(x) + y(x-h) \\ &= \int_x^{x+h} (x+h-t)f(t) dt + \int_x^{x-h} (x-h-s)f(s) ds \end{aligned}$$

and

$$\Delta^2 y(x-h) = h^2 \int_0^1 z\{f(x+h-zh) + f(x-h+zh)\} dz$$

when $+zh$ and $-zh$ are substituted for $x+h-t$ and $x-h-s$ respectively. Thus,

$$\Delta^2 y(x-h) = h^2 \int_0^1 z\{(1-\nabla)^z + (1-\nabla)^{2-z}\} f(x+h) dz$$

where the backward difference and the shift operators, ∇ and E , are defined respectively as $\nabla = 1 - E^{-1}$ and $E^p f(x) = f(x+ph)$.

The following expansions

$$(1-\nabla)^z = 1 - z\nabla + \frac{z(z-1)}{2}\nabla^2 - \frac{z(z-1)(z-2)}{6}\nabla^3 + \frac{z(z-1)(z-2)(z-3)}{24}\nabla^4 + \dots$$

$$\begin{aligned} (1-\nabla)^{2-z} &= 1 + (z-2)\nabla + \frac{(z-2)(z-1)}{2}\nabla^2 + \frac{(z-2)(z-1)z}{6}\nabla^3 \\ &\quad + \frac{(z-2)(z-1)z(z+1)}{24}\nabla^4 + \dots \end{aligned}$$

results in expression of $\Delta^2 y(x-h)$ as

$$\Delta^2 y(x-h) = h^2 \left[1 - \nabla + \frac{1}{12}\nabla^2 - \frac{1}{240}\nabla^4 + \dots \right] f(x+h).$$

By truncating the above expression after the second difference term and substituting x_n for x results in

$$y_{n+1} - 2y_n + y_{n-1} \cong \frac{h^2}{12}(f_{n+1} + 10f_n + f_{n-1}) - \frac{h^2}{240}\nabla^4 f_{n+1} \quad (8)$$

Equation (6) is now in form of the Numerov method (2) with the leading term of the local truncation error in the step from x_n to x_{n+1} expressed as

$$-\frac{h^2}{240} \nabla^4 f_{n+1} \cong -\frac{h^6}{240} y_{n+1}^{vi}$$

Thus, the global error is of order 4.

Absolute Stability of the Numerov Method

Following Lambert (1973), the locus of the boundary of the region of absolute stability is,

$$\bar{h}(\theta) = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}$$

where ρ and σ defined by (6) and (7) are explicitly expressed by $\rho(\xi) = \xi^2 - 2\xi + 1$ and $\sigma(\xi) = \frac{1}{12}(\xi^2 + 10\xi + 1)$ respectively. Consequently,

$$\bar{h}(\theta) = \frac{12(-18 + 16 \cos \theta + 2 \cos 2\theta)}{(102 + 40 \cos \theta + 2 \cos 2\theta)}$$

which makes the interval of the real axis to be the boundary of the region; and the extreme values (maximum and minimum) of the function $\bar{h}(\theta)$ are the end points of the interval. Consequently, the interval of absolute stability is computed as $[-6, 0]$.

From the foregoing sections, it is evident that the Numerov method is shown to be consistent and stable, hence its convergence.

Application of the Numerov Method to Solution of Fourth Order ODEs

Two fourth order ordinary differential equations will be considered. The exact solutions of the differential equations will be obtained analytically and the absolute value difference between the exact and approximate solutions compared.

Example 1 We consider the initial value problem:

$$y^{iv} - y'' = x, \quad y(0) = y'(0) = y''(0) = y'''(0) = 1, \quad h = 0.1 \quad (9)$$

Suppose $y'' = p$; then $y''' = p'$; $y^{iv} = p''$. Then by implication,

$$y'' = f(p, y) = p \quad (10)$$

$$p'' = f(x, p) = x + p \quad (11)$$

Equations (10) and (11) are second order ODEs wherein the first order terms are missing, thereby making them suitable for implementation by the Numerov method, respectively as follow.

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{12}(p_{n+2} + 10p_{n+1} + p_n) \quad (12)$$

$$p_{n+2} - 2p_{n+1} + p_n = \frac{h^2}{12}(x_{n+2} + p_{n+2} + 10x_{n+1} + 10p_{n+1} + x_n + p_n) \quad (13)$$

That is,

$$y_{n+2} = 2y_{n+1} - y_n + \frac{h^2}{12}(p_{n+2} + 10p_{n+1} + p_n) \quad (14)$$

$$p_{n+2} = 2p_{n+1} - p_n + \frac{h^2}{12}(p_{n+2} + 10p_{n+1} + p_n + 12x_{n+1}) \quad (15)$$

For application of the Numerov method (14), a two-step implicit method, the need arises to obtain two previous values of the solution, y_n and y_{n+1} , in order to calculate a new one, y_{n+2} . Now,

$$y_2 = 2y_1 - y_0 + \frac{h^2}{12}(p_2 + 10p_1 + p_0) \quad (16)$$

$$p_2 = 2p_1 - p_0 + \frac{h^2}{12}(p_2 + 10p_1 + p_0 + 12x_1) \quad (17)$$

From whence,

$$p_2 \left(1 - \frac{h^2}{12}\right) = \left(2 + \frac{5h^2}{6}\right)p_1 + \left(\frac{h^2}{12} - 1\right)p_0 + h^2 x_1$$

$$p_2 \left(1 - \frac{0.01}{12}\right) = \left(2 + \frac{0.05}{6}\right)p_1 - \left(1 - \frac{0.01}{12}\right)p_0 + 0.01x_1$$

$$p_2 = \frac{\left(2 + \frac{0.05}{6}\right)p_1 - \left(1 - \frac{0.01}{12}\right)p_0 + 0.01x_1}{\left(1 - \frac{0.01}{12}\right)}$$

$$p_2 = 2.010008339p_1 - p_0 + 0.01000834028x_1 \quad (18)$$

The exact solution of the DE (6) is obtained thus,

$$(D^4 - D^2)y = x, \quad D^2(D^2 - 1)y = x$$

Thus,

$$y_c = c_1 + c_2x + c_3e^x + c_4e^{-x}, \quad y_p = x^2(Ax + B) = Ax^3 + Bx^2$$

$$y(x) = c_1 + c_2x + c_3e^x + c_4e^{-x} + Ax^3 + Bx^2$$

$$y'(x) = c_2 + c_3e^x - c_4e^{-x} + 3Ax^2 + 2Bx, \quad y''(x) = c_3e^x + c_4e^{-x} + 6Ax + 2B$$

$$y'''(x) = c_3e^x - c_4e^{-x} + 6A, \quad y^{(4)}(x) = c_3e^x + c_4e^{-x}$$

Solving the above results in

$$y(x) = c_1 + c_2x + c_3e^x + c_4e^{-x} - \frac{x^3}{6}$$

$$y'(x) = c_2 + c_3e^x - c_4e^{-x} - \frac{x^2}{2}, \quad y''(x) = c_3e^x + c_4e^{-x} - x, \quad y'''(x) = c_3e^x - c_4e^{-x} - 1$$

Consequently,

$$y(0) = c_1 + c_3 + c_4 = 1, \quad y'(0) = c_2 + c_3 - c_4 = 1,$$

$$y''(0) = c_3 + c_4 = 1, \quad y'''(0) = c_3 - c_4 = 2$$

with the resultant values for the constants as,

$$c_1 = 0, \quad c_2 = -1, \quad c_3 = \frac{3}{2}, \quad c_4 = -\frac{1}{2}$$

And the exact solution is,

$$y(x) = -x + \frac{3}{2}e^x - \frac{1}{2}e^{-x} - \frac{x^3}{6} \quad (19)$$

Also,

$$y''(x) = \frac{3}{2}e^x - \frac{1}{2}e^{-x} - x \quad (20)$$

From the known boundary conditions, the following values are computed.

$$y_0 = 1, y(0.1) = 1.105171001 = y_1, y''(0) = 1 = p_0, y''(0.1) = 1.105337668 = p_1$$

The above are the starting values necessary to implement the first iteration step (16) and (18), where the following results are obtained

$$p_2 = 1.222738764 \text{ and } y_2 = 1.211175335$$

Subsequent iterations of (14) and (15) are performed and the computed solutions are compared with the exact solutions as shown in Table 1.

Example 2 We consider the boundary value problem:

$$y^{iv} - y'' = x, \quad y(0) = y'(0) = 0, y(1) = 11/6, y''(1) = 1, h = 0.1 \quad (21)$$

The exact solution of (21) is obtained analytically as

$$y(x) = 2e(e^{-x} + x - 1) - \frac{x^3}{6} \quad (22)$$

where,

$$y''(x) = 2ee^{-x} - x \quad (23)$$

Similar to problem 1, equations (14), (15) and (18) are employed to solve this problem with the following starting values:

$$y_0 = 0, y(0.1) = 0.0261322653 = y_1, y''(0) = 5.436563656 = p_0, y''(0.1) = 4.819206222 = p_1$$

RESULTS AND DISCUSSION

In order to verify numerically whether the proposed schemes are effective, the computations of the approximate numerical solutions of the two fourth order initial and boundary value problems of ordinary differential equations presented in Examples 1 and 2 are implemented using Maple 2019 software package and the results are presented in Tables 1 and 2. In the tables, n denotes the step number, x is the integration points, p_n represents the solutions of (15), $P_E(x)$ stands for exact solutions of (11), y_n is the approximate solution obtained from (14) and $y_E(x)$ is the exact solution of (9) or (21), as the case may be.

Table 1 Absolute errors for Problem 1

n	x	P_n	$P_E(x)$	y_n	$y_E(x)$	$Error$ $ y_n - y_E(x) $
0	0	1	1	1	1.0	0
1	0.1	1.105337668	1.105337668	1.105171001	1.105171001	0
2	0.2	1.222738764	1.222738760	1.221405432	1.221405427	5E-09
3	0.3	1.354379112	1.354379102	1.349879117	1.349879102	1.5E-08
4	0.4	1.502577047	1.502577024	1.491910391	1.491910357	3.4E-08
5	0.5	1.669816618	1.669816576	1.648983304	1.648983243	6.1E-08
6	0.6	1.858772450	1.858772382	1.822772480	1.822772382	9.8E-08
7	0.7	2.072336511	2.072336408	2.015169887	2.015169741	1.46E-07
8	0.8	2.313647056	2.313646910	2.228313781	2.228313577	2.04E-07
9	0.9	2.586120037	2.586119836	2.464620114	2.464619836	2.78E-07
10	1.0	2.893483290	2.893483021	2.726816723	2.726816354	3.69E-07

Table 2 Absolute errors for Problem 2

n	x	P_n	$P_E(x)$	y_n	$y_E(x)$	Error $ y_n - y_E(x) $
0	0	5.436563656	5.436563656	0	0	0
1	0.1	4.819206222	4.819206222	0.0261322653	0.0261322653	0
2	0.2	4.251081872	4.251081856	0.1004976204	0.1004975977	2.27E-08
3	0.3	3.727505458	3.727505414	0.2174109175	0.2174108550	6.25E-08
4	0.4	3.244237684	3.244237601	0.3716328597	0.3716327403	1.194E-07
5	0.5	2.797442677	2.797442541	0.5583275727	0.5583273797	1.93E-07
6	0.6	2.383649595	2.383649395	0.7730242137	0.7730239330	2.807E-07
7	0.7	1.999717890	1.999717615	1.0115822350	1.0115818510	3.84E-07
8	0.8	1.642805878	1.642805516	1.2701599510	1.2701594520	4.99E-07
9	0.9	1.310342296	1.310341836	1.5451860990	1.5451854700	6.29E-07
10	1.0	1.000000570	1.000000000	1.8333341050	1.8333333330	7.72E-07

Table 1 depicts the results of applying the Numerov method to the fourth order ODE, $y^{iv} - y'' = x$ with the initial conditions taken at $y(0) = y'(0) = y''(0) = y'''(0) = 1$ so that the solution is $y(x) = -x + 3e^x/2 - e^{-x}/2 - x^3/6$. All necessary starting values are taken as exact. The approximate results compare quite favourably with the exact solutions as exhibited by the negligible errors. In Table 2, the differential equation, $y^{iv} - y'' = x$ with boundary conditions taken at $y(0) = y'(0) = 0, y(1) = 11/6, y''(1) = 1$ is solved. Starting values for Numerov method is obtained from the exact solution. Similar to Table 1, the results are in close agreement with the exact solution.

CONCLUSION

The Numerov method, a two-step implicit linear multistep method for solving second order ordinary differential equations wherein the first order term is missing, has been employed to solve fourth order initial and boundary value problems in ordinary differential equations involving the second derivative. This has been achieved through a transformation of the original fourth order ordinary differential equation into a system of two coupled second order ordinary differential equations without a first derivative term, which is suitable for solution with the Numerov method. The solutions of the system of second order equations thus effectively provides the solutions of the original fourth order equations. The results of comparing the computed approximate solutions with the exact solutions exhibited very negligible errors, thus confirming clearly that the method is not only effective, but equally efficient.

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