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NUMEROV SOLUTION OF LINEAR SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS CONTAINING FIRST ORDER DERIVATIVE TERM

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ABSTRACT

A central activity in the numerical solution of differential equations is that of finding effective numerical methods to solve particular types of problems. One of such problems is the second order ordinary differential equations of the form $y'' = f(x, y)$. A very important algorithm towards the solution of this equation is the Numerov method. In this present work, the Numerov method is employed to solve linear second order ordinary differential equations involving a first derivative term. By a transformation of the equation, the first derivative term is eliminated by representing it with finite difference quotient at the grid points, resulting in an equation that makes it suitable for solution. Once this equation is solved, the approximate solution of the desired function $y(x)$ can be obtained at the grid points. Extensive numerical tests to illustrate the effectiveness and reliability of the method are presented. The numerical experiments were conducted using Maple 2019.0 software package.

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

INTRODUCTION

Solution of the linear second order ordinary differential equation that does not contain a first order term,

$$y''(x) = \boldsymbol{f}(x, y) = -g(x)y(x) + s(x) \qquad (1)$$

can be obtained using the well-known Numerov method, proposed by Boris Vasil'evich Numerov (Numerov, 1924).

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

If $\boldsymbol{f}$ is nonlinear in y, then the method (2) takes the form

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{12}(f_{n+2}+10f_{n+1}+f_n) + O(h^6) \quad (3)$$

The preclusion of second order equations containing a first derivative term:

$$y''(x) + f(x)y'(x) + g(x)y(x) + s(x) = 0 \qquad (4)$$

by the Numerov method makes it an unpopular choice in certain applications. To overcome this challenge, several researchers have proposed modifications and generalizations of the method in order to include equations of the type (4) and more general nonlinear equations. Among these include, Leroy and Wallace (1986), Van Daele *et al.* (1991) and Adeboye *et al.* (2018). Another way of achieving this is elimination of the first derivative using a simple transformation. For example, Salzman (2001) proposed this can be done by elimination of the first derivative in (4) using the transformation $y'' = h(x)z(x)$, and grouping terms by derivatives of z thus, $\frac{d^2z}{dx^2}h + \frac{dz}{dx}(2h' + fh) + z(x)(h'' + fh' + gh) + s(x) = 0$; from whence the first derivative term, $z'(x)$, can be eliminated by solving the equation $\frac{dh}{dx} = -\frac{1}{2}f(x)h(x)$. On dividing the equation through by the coefficient of $z''(x)$, what obtains is an equation of the form $\frac{d^2z}{dx^2} + A(x)z(x) + B(x) = 0$, whose solution can be obtained using the Numerov method. Also, Tselyaev (2004) proposed elimination of the first derivative by adopting the transformation $y(x) = w(x)\exp(-\frac{1}{2}\int f(x)\,dx)$.

MATERIALS AND METHODS

Derivation of the Method

Given the differential equation

$$y''(x) = -g(x)y(x) + s(x)$$

To derive the Numerov method to solve this equation, the operator $1 + \frac{h^2}{12}\frac{d^2}{dx^2}$ is applied to operate on the equation thus:

$$\left[1+\frac{h^2}{12}\frac{d^2}{dx^2}\right]\left(\frac{d^2y}{dx^2}\right) = [1+\frac{h^2}{12}\frac{d^2}{dx^2}](-g(x)y(x)+s(x))$$

$$\frac{h^2}{12}\frac{d^4y}{dx^4} + \frac{d^2y}{dx^2} = \frac{h^2}{12}\frac{d^2}{dx^2}[-g(x)y(x)+s(x)] - g(x)y(x) + s(x) \qquad (5)$$

Expanding the function $y(x)$ in Taylor series centred around $x + h$:

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \frac{h^3}{3!}y'''(x) + \frac{h^4}{4!}y^{iv}(x) + \frac{h^5}{5!}y^{v}(x) + \cdots \qquad (6)$$

And then expand $y(x)$ about $x - h$:

$$y(x-h) = y(x) - hy'(x) + \frac{h^2}{2!}y''(x) - \frac{h^3}{3!}y'''(x) + \frac{h^4}{4!}y^{iv}(x) - \frac{h^5}{5!}y^{v}(x) + \cdots \qquad (7)$$

Adding equations (6) and (7) gives

$$y(x+h) - 2y(x) + y(x-h) = h^2y''(x) + \frac{1}{12}h^4y^{iv}(x) + O(h^6)$$

$$y''(x) = \frac{y(x+h)-2y(x)+y(x-h)}{h^2} - \frac{h^2}{12}y^{iv}(x) + O(h^6) \qquad (8)$$

Substituting (8) into (5),

$$\frac{h^2}{12}\frac{d^4y}{dx^4}+\frac{y(x+h)-2y(x)+y(x-h)}{h^2}-\frac{h^2}{12}\frac{d^4y}{dx^4} = \frac{h^2}{12}\frac{d^2}{dx^2}[-g(x)y(x)+s(x)] - g(x)y(x)+s(x)$$

$$\frac{y(x+h)-2y(x)+y(x-h)}{h^2} = \frac{h^2}{12}\frac{d^2}{dx^2}[-g(x)y(x)+s(x)] - g(x)y(x)+s(x) \quad (9)$$

To approximate the second derivative of $-g(x)y(x)+s(x)$:

$$\frac{d^2}{dx^2}[-g(x)y(x)+s(x)] \approx \frac{[-g(x+h)y(x+h)+s(x+h)+2g(x)y(x)-2s(x) - g(x-h)y(x-h)+s(x-h)]}{h^2}$$

Substituting this equation into (6) and rearranging,

$$y(x+h)-2y(x)+y(x-h) = h^2[-g(x)y(x)+s(x)] + \frac{h^2}{12}[-g(x+h)y(x+h)+s(x+h) + 2g(x)y(x)-2s(x) - g(x-h)y(x-h)+s(x-h)] + O(h^6)$$

$$\left[1+\frac{h^2}{12}g(x+h)\right]y(x+h) = \left[1-\frac{5h^2}{12}g(x)\right]2y(x) - [1 + \frac{h^2}{12}g(x-h)]y(x-h) + \frac{h^2}{12}[s(x+h)+10s(x)+s(x-h)]$$

If this is phrased in terms of discrete indices, $x=nh$, and defining $y_n=y(x_n)$, $g_n=g(x_n)$, $s_n=s(x_n)$, $h=y_n=x_{n+1}-x_n$, it can be written more tidily as,

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

which is the Numerov method (2).

Proof of Convergence

Definition 1 The first and second characteristic polynomials of a $k-\text{step}$ linear multistep method are defined as

$$\rho(\xi)=\sum_{j=0}^{k}\alpha_j\xi^j=\alpha_k\xi^k+\alpha_{k-1}\xi^{k-1}+\alpha_{k-2}\xi^{k-2}+\cdots+\alpha_0 \quad (10)$$

and

$$\sigma(\xi)=\sum_{j=0}^{k}\beta_j\xi^j=\beta_k\xi^k+\beta_{k-1}\xi^{k-1}+\beta_{k-2}\xi^{k-2}+\cdots+\beta_0 \quad (11)$$

respectively.

Definition 2 A linear multistep method is said to be consistent if it is at least first-order.

Definition 3 A linear multistep method is said to be zero-stable if as $h\to 0$, the roots $\xi_j, j=1(2)k$ of the first characteristic polynomial $\rho(\xi)$ satisfy $|\xi_j|\le 1$, and for every $|\xi_j|=1$ the multiplicity must be simple.

Definition 4 A linear multistep method is convergent if and only if it is stable and consistent.

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 (7) and (8) 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 Numerov Method to Equations of the form $y''=f(x,y,y')$

Some linear second order ordinary differential equations involving a first derivative term are considered. Their exact solutions are obtained analytically and the absolute value difference between the exact and approximate solutions compared.

Problem 1 Consider the linear second order boundary value problem:

$$y''-2y'+y=2x, \qquad y(0)=4; y(1)=6, \quad h=0.1 \quad (12)$$

Let

$$y''_{n+1}=2y'_n-y_n+2x_n=f_n$$

$$y_{n+2}-2y_{n+1}+y_n=\frac{h^2}{6}(f_{n+2}+4f_{n+1}+f_n)$$

Thus, $f_n=2y'_n-y_n+2x_n$, $4f_{n+1}=4(2y'_{n+1}-y_{n+1}+2x_{n+1})=8y'_{n+1}-4y_{n+1}+8x_{n+1}$ and $f_{n+2}=2y'_{n+2}-y_{n+2}+2x_{n+2}$.

$$y_{n+2}-2y_{n+1}+y_n=\frac{h^2}{6}[2y'_{n+2}-y_{n+2}+2x_n+4h+8y'_{n+1}-4y_{n+1}+8x_n+8h+2y'_n-y_n+2x_n+12h]$$

$$y_{n+2}-2y_{n+1}+y_n=\frac{h^2}{6}[2y'_{n+2}+8y'_{n+1}+2y'_n-y_{n+2}-4y_{n+1}-y_n+12x_n+12h]$$

Now,

$2y'_n=\frac{2(y_{n+1}-y_n)}{h}=\frac{2y_{n+1}-2y_n}{h}$; $8y'_{n+1}=\frac{8(y_{n+2}-y_{n+1})}{h}=\frac{8y_{n+2}-8y_{n+1}}{h}$; $2y'_{n+2}=\frac{2(y_{n+2}-y_n)}{2h}=\frac{y_{n+2}-y_n}{h}$.

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{6}[\frac{y_{n+2} - y_n}{h} + \frac{8y_{n+2} - 8y_{n+1}}{h} + \frac{2y_{n+1} - 2y_n}{h} - \frac{(hy_{n+2} + 4hy_{n+1} + hy_n)}{h} + \frac{12hx_n + 12h^2}{h}]$$

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h}{6}[(9-h)y_{n+2} - (6+4h)y_{n+1} - (3+h)y_n + 12hx_n + 12h^2]$$

$$\left(1 - \frac{3h}{2} + \frac{h^2}{6}\right)y_{n+2} + \left(h - 2 + \frac{2h^2}{3}\right)y_{n+1} + \left(1 + \frac{h}{2} + \frac{h^2}{6}\right)y_n = 2h^2x_n + 2h^3$$

$$0.851666666y_{n+2} - 1.893333333y_{n+1} + 1.051666667y_n = 0.02x_n + 0.002$$

$$y_{n+2} = 2.223091978y_{n+1} - 1.234833661y_n + 0.023483365x_n + 0.0023483366 \quad (13)$$

Equation (13) is now the transformed Numerov method to be applied to the given problem (12). It is a two-step method requires two starting values, y_0 and y_1. Here, $y_0 = 4$ is obtained from the boundary condition, and $y_1 = 4.2$ is obtained from the exact solution $y(x)$, which is obtained analytically as $y(x) = 2x + 4$. The approximate solution is computed over the interval $0 \le x \le 1$ and the obtained results compared with the exact solutions are presented in Table I.

Problem 2 Consider the linear second order initial value problem:

$$y'' - y' - y = -4x, \qquad y(0) = 2; y'(0) = 2, \qquad h = 0.1 \quad (14)$$

Let

$$y''_{n+1} = y'_n + 2y_n - 4x_n = f_n$$

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{6}(f_{n+2} + 4f_{n+1} + f_n)$$

So, $f_n = y'_n + 2y_n - 4x_n$,$4f_{n+1} = 4(y'_{n+1} + 2y_{n+1} - 4x_{n+1}) = 4y'_{n+1} + 8y_{n+1} - 16x_{n+1}$ and $f_{n+2} = y'_{n+2} + 2y_{n+2} - 4x_{n+2}$.

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{6}[y'_{n+2} + 2y_{n+2} - 4x_{n+2} + 4y'_{n+1} + 8y_{n+1} - 16x_{n+1} + y'_n + 2y_n - 4x_n]$$

$$= \frac{h^2}{6}[y'_{n+2} + 2y_{n+2} - 4x_n - 8h + 4y'_{n+1} + 8y_{n+1} - 16x_n - 16h + y'_n + 2y_n - 4x_n]$$

Now,

$y'_{n+2} = \frac{y_{n+2} - y_{n+1}}{h}$; $4y'_{n+1} = \frac{4(y_{n+2} - y_n)}{2h} = \frac{2y_{n+2} - 2y_n}{h}$; $y'_n = \frac{y_{n+1} - y_n}{h}$;

It implies,

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{6}[\frac{y_{n+2} - y_{n+1}}{h} + \frac{2y_{n+2} - 2y_n}{h} + \frac{y_{n+1} - y_n}{h} + \frac{(2hy_{n+2} + 8hy_{n+1} + 2hy_n)}{h} - \frac{(24hx_n + 24h^2)}{h}]$$

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h}{6}[(3+2h)y_{n+2} + 8hy_{n+1} + (2h-3)y_n - 24hx_n - 24h^2]$$

$$\left[\left(1 - \frac{(3h + 2h^2)}{6}\right)\right]y_{n+2} - \left(2 + \frac{4h^2}{3}\right)y_{n+1} + [1 + [1 + \frac{(3h - 2h^2)}{6}]y_n = -4h^2x_n - 4h^3$$

That is,

$$y_{n+2} = 2.126760565y_{n+1} - 1.105633804y_n - 0.042253521x_n - 0.00422535212 \quad (15)$$

The starting values of (15) are $y_0 = 2$ and $y_1 = 2.231077594$. The exact solution is obtained as $y(x) = e^{2x} + 2e^{-x} + 2x - 1$. The results of Problem 2 are presented in Table II.

RESULTS AND DISCUSSION

Problems 1 and 2 involving linear second order ordinary differential equations are solved, analytically and numerically, and the computed results are compared. The results are presented in Tables I and II. In the tables, the values of x represent the integration points which are evenly spaced in steps of 0.1, the computed approximate values are represented by y_n, $y_E(x)$ is the exact solution and the absolute error is given by $|y_n - y_E(x)|$.

Table I Results of Problem 1

n	x	y_n	$y_E(x)$	$Error$ $\lvert y_n - y_E(x)\rvert$
0	0	4	4	0
1	0.1	4.2	4.2	0
2	0.2	4.400000001	4.4	1E-09
3	0.3	4.600000002	4.6	2E-09
4	0.4	4.799999999	4.8	1E-09
5	0.5	4.999999992	5	8E-09
6	0.6	5.199999979	5.2	2.1E-08
7	0.7	5.399999962	5.4	3.8E-08
8	0.8	5.599999942	5.6	5.8E-08
9	0.9	5.799999917	5.8	8.3E-08
10	1.0	5.999999885	6	1.15E-07

Table II Results of Problem 2

n	x	y_n	$y_E(x)$	$Error$ $\lvert y_n - y_E(x)\rvert$
0	0	2	2	0
1	0.1	2.231077594	2.231077594	0
2	0.2	2.529474884	2.529286204	0.00018868
3	0.3	2.904381922	2.903755241	0.000626681
4	0.4	3.367575943	3.366181020	0.001394923
5	0.5	3.933943474	3.931343147	0.002600327
6	0.6	4.622123285	4.617740195	0.00438309
7	0.7	5.455296528	5.448370575	0.006925953
8	0.8	6.462156315	6.451690352	0.010465963
9	0.9	7.678096151	7.662786783	0.015309368
10	1.0	9.146665472	9.124814981	0.021850491

Table I displays the results of solving the linear second order ordinary differential equation $y'' - 2y' + y = 2x$ with boundary conditions $y(0) = 4; y(1) = 6$ and exact solution

$y(x) = 2x + 4$. The displayed minimal errors translate to high level of accuracy of the method. Similarly, Table II shows the results of applying the Numerov method to solve the linear second order ordinary differential equation $y'' - y' - y = -4x$, with initial conditions $y(0) = 2; y'(0) = 2$. The displayed errors are of minimal consequence.

Conclusion

A reformulated version of the Numerov method is developed and applied to solve both initial and boundary value problems of linear second order ordinary differential equations involving first derivative terms. The mathematical software package Maple 2019.0, Maple Build ID 1384062 was employed to generate the results. The results of numerical examples established the method to be worthwhile.

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