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Numerov's method, which is commonly used in numerical integration of a class of second-order differential equations lacking the first derivative, is generalized to cover radial wave equations in cylindrical geometry. The proposed scheme is compared with the Runge–Kutta method and the conventional Numerov method by numerically integrating Bessel's differential equation.

INTRODUCTION

Numerov's algorithm is known as quite an efficient tool for solving differential equations of the form[1–7]

$$\frac{d^2\varphi}{dx^2}+K(x)\varphi=S(x). \tag{1.1}$$

In addition to the one-dimensional problem (1.1) itself, radial wave equations in spherical symmetry can also be cast into the above form by an appropriate change of the variable. Thus, the Numerov method has been frequently used in numerical integration of wave equations. The attractive efficiency of the Numerov integration arises from its high accuracy and low frequency of evaluating the functions $K(x)$ and $S(x)$.

In spite of this usefulness, the Numerov algorithm encounters a certain difficulty for radial differential equations in cylindrical symmetry,

$$\frac{d^2y}{dx^2}+\frac{1}{x}\frac{dy}{dx}+K(x)y=S(x). \tag{1.2}$$

It might appear, at first glance, that Eq. (1.2) could be reduced to Eq. (1.1) by substituting

$$\varphi(x)=x^{1/2}y(x), \tag{1.3}$$

and hence it could be solved by the Numerov method. This is mathematically correct. However, the right-hand side of Eq. (1.3) is singular at $x=0$, on the natural assumption that the physical solution $y(x)$ is regular. This singularity in φ gives rise to a difficulty, if Eq. (1.1) is to be solved numerically. Certainly, even apart from the Numerov algorithm, no numerical methods will be capable of giving an accurate solution, which behaves like Eq. (1.3) around the origin. Substitution (1.3) is useful only for x sufficiently separated from the origin. Then, one practical compromise would be to integrate Eq. (1.1) by the standard Numerov method for large x and solve Eq. (1.2) by some other method for small x, matching the result somewhere in between.

In this paper, we are going to explore a cylindrical–symmetry version of the Numerov method, which directly solves Eq. (1.2) without losing its remarkable efficiency. It avoids the problematic substitution (1.3) and allows direct integration of Eq. (1.2) from the origin with a single algorithm. We will also discuss some aspects of accuracy of the Numerov integration, which are common to the standard Numerov algorithm as well.

I. NUMEROV INTEGRATION IN CYLINDRICAL GEOMETRY

In this section, we are going to generalize the standard Numerov algorithm to solve the particular differential Eq. (1.2), which is less simple than Eq. (1.1) because of the factor $1/x$ multiplying the first derivative. For the sake of convenience below, we rewrite it as

$$xy''+y'=f, \tag{2.1}$$

or

$$\frac{d}{dx}(xy')=f, \tag{2.2}$$

where

$$f(x)=xS(x)-xK(x)y. \tag{2.3}$$

The essence of the Numerov method lies in repeated application of the difference formulas

$$\frac{y_{n+1}-2y_n+y_{n-1}}{h^2}=y_n''+\frac{h^2}{12}y_n''''+0(h^4), \tag{2.4}$$

$$\frac{y_{n+1}-y_{n-1}}{2h}=y_n'+\frac{h^2}{6}y_n'''+0(h^4), \tag{2.5}$$

which are both accurate to within third order in the step size h. Here, as usual, y_n denotes $y(x_n)$ at the mesh point $x_n=x_0+nh$. We will even use below the notation

$$x_{n\pm 1/2}=x_n\pm 1/2h$$

for midpoints.

To construct an approximation to the left-hand side of Eq. (2.1), we multiply Eq. (2.4) with x_n and add Eq. (2.5) to obtain

$$x_{n+1/2}y_{n+1}-2x_ny_n+x_{n-1/2}y_{n-1}$$
$$=h^2\frac{d}{dx}(xy')_n+\frac{h^4}{12}\frac{d^2}{dx^2}(xy'')_n+0(h^6), \tag{2.6}$$

which forms the basis of our analysis. The first term on the right-hand side can be simply replaced by $h^2 f_n$ on account of the differential Eq. (2.2). Thus, if one is satisfied with an error of $O(h^4)$, one has

$$x_{n+1/2}y_{n+1}-2x_n y_n+x_{n-1/2}y_{n-1}=h^2 f_n+0(h^4), \tag{2.7}$$

which leads to the integration formula

$$x_{n+1/2}y_{n+1}-x_n(2-h^2K_n)y_n+x_{n-1/2}y_{n-1}$$
$$=h^2x_nS_n+0(h^4), \tag{2.8}$$

for the differential Eq. (1.2).

To get higher accuracy, we retain the second term. Repeated use of Eq. (2.1) gives

$$\frac{d^2}{dx^2}(xy'')=f''-y'''=f''-\frac{f'}{x}+\frac{2y''}{x}. \tag{2.9}$$

Derivatives on the right-hand side can now be approximated by the differences (2.4) and (2.5) to within an $O(h^2)$ error, which does not affect the total error. As a result, we find

$$x_{n+1/2}y_{n+1}-2x_ny_n+x_{n-1/2}y_{n-1}$$
$$=\frac{h^2}{12}\left(\frac{x_{n-1/2}}{x_n}f_{n+1}+10f_n+\frac{x_{n+1/2}}{x_n}f_{n-1}\right)$$
$$+\frac{h^2}{6x_n}(y_{n+1}-2y_n+y_{n-1})+0(h^6), \tag{2.10}$$

as a recurrence relation to solve Eq. (2.1). It is interesting to note that the midpoint coordinates appear again on the right-hand side. Substitution of Eq. (2.3) yields

$$M_n^+y_{n+1}-2M_n^0y_n+M_n^-y_{n-1}$$
$$=\frac{h^2}{12}(x_{n-1/2}x_{n+1}S_{n+1}$$
$$+10x_n^2S_n+x_{n+1/2}x_{n-1}S_{n-1})+0(h^6), \tag{2.11}$$

where

$$M_n^+=x_{n+1/2}x_n+\frac{h^2}{12}x_{n-1/2}x_{n+1}K_{n+1}-\frac{h^2}{6},$$
$$M_n^0=x_n^2\left(1-\frac{5h^2}{12}K_n\right)-\frac{h^2}{6},$$
$$M_n^-=x_{n-1/2}x_n+\frac{h^2}{12}x_{n+1/2}x_{n-1}K_{n-1}-\frac{h^2}{6}.$$

In this way, we have established a generalized Numerov algorithm for the differential Eq. (1.2). This formula is somewhat more complicated than the standard one. However, it shares the advantage of high efficiency in that it requires evaluation of functions $K(x)$ and $S(x)$ only once at each step of integration.

Before implementing the above scheme in practice, it is advantageous to add a minor modification to it. Since the Numerov method relies on repeated use of difference formulas (2.4) and (2.5), it sometimes fails to attain the expected accuracy because of numerical cancellation, particularly for small step size h. In order to avoid such a loss in accuracy, rather than using the recurrence relation (2.11) as it stands, we compute the difference

Table I. Errors in the value of the Bessel function $J_0(1)$ obtained for the eight values of step size h. (a) Bessel's differential equation has been integrated from $x=0$ to $x=1$ using the recurrence relations (2.13). (b) For comparison, the same integration has been done with the fourth-order Runge–Kutta method.

h	(a)	(b)
0.2	-5.50×10^{-5}	2.46×10^{-6}
0.1	-5.87×10^{-6}	1.45×10^{-7}
0.05	-5.55×10^{-7}	8.47×10^{-9}
0.02	-2.20×10^{-8}	2.04×10^{-10}
0.01	-1.81×10^{-9}	1.25×10^{-11}
0.005	-1.44×10^{-10}	7.72×10^{-13}
0.002	-4.86×10^{-12}	1.97×10^{-14}
0.001	-3.71×10^{-13}	2.22×10^{-16}

$$z_{n+1}=y_{n+1}-y_n \tag{2.12}$$

at each step with use of the preceding difference z_n as well as y_n and y_{n-1}. Explicitly, instead of Eq. (2.11), we use

$$z_{n+1}=\frac{(x_{n-1/2}x_n-h^2/6)z_n-h^2/12D_n}{M_n^+} \tag{2.13}$$

to evaluate z_{n+1} and y_{n+1} at each step, where

$$D_n=(10x_n^2K_n+x_{n-1/2}x_{n+1}K_{n+1})y_n$$
$$+x_{n+1/2}x_{n-1}K_{n-1}y_{n-1}-x_{n-1/2}x_{n+1}S_{n+1}-10x_n^2S_n$$
$$-x_{n+1/2}x_{n-1}S_{n-1}. \tag{2.14}$$

This modification actually improves accuracy for small h, without introducing additional overhead and destroying high efficiency of the Numerov method. The above difference technique is very useful also for the conventional Numerov integration of the differential Eq. (1.1).

Finally, a comment is in order on the order of the Numerov integration. As Eq. (2.11) shows, local truncation error of the present scheme is $0(h^6)$, in common with the conventional Numerov scheme.[1] This local error occasionally misleads us as if it were a fifth-order method. As a matter of fact, it is of order 4,[1,6] as may be confirmed numerically. The apparent imbalance between the local and global errors is due to the fact that the Numerov scheme is essentially based on a three-point recurrence relation.

II. NUMERICAL EXAMPLE

To verify usefulness of the above result, we use the recurrence relation (2.12)–(2.14) to solve Eq. (1.2) simply for

$$K(x)=1,\quad S(x)=0 \tag{3.1}$$

with regular boundary condition at $x=0$. In this case, analytic solution is given by the Bessel function $J_0(x)$. The recurrence relation is started at $x=0$ using initial values $y_0=1$, $y_1=J_0(h)$ and is terminated at $x=1$ to obtain the numerical value of $J_0(1)$. Column (a) of Table I shows the error in the value of $J_0(1)$ obtained for the eight cases of the step size h. The code written in QUICKBASIC was run in double precision with machine epsilon $\epsilon_m\sim2\times10^{-16}$.

For the sake of comparison, the accuracy of the fourth-order Runge–Kutta method is shown in parallel. Since the Runge–Kutta method cannot be started from the origin in the present problem, the integration was started using $J_0(h)$ and its derivative $J_0'(h)$ at $x=h$.

Table II. Errors in the value of the Bessel function $J_0(1.75)$ when the integration is started from $x=0.75$. Columns (a) and (b) are the same as in Table I. Column (c) gives the errors when the conventional Numerov scheme is applied to Eq. (1.1) with the substitution (1.3).

h	(a)	(b)	(c)
0.2	-4.92×10^{-6}	1.80×10^{-6}	-2.08×10^{-5}
0.1	-3.37×10^{-7}	8.94×10^{-8}	-1.83×10^{-6}
0.05	-2.50×10^{-8}	4.62×10^{-9}	-1.36×10^{-7}
0.02	-6.72×10^{-10}	1.01×10^{-10}	-3.85×10^{-9}
0.01	-4.27×10^{-11}	5.96×10^{-12}	-2.48×10^{-10}
0.005	-2.69×10^{-12}	3.60×10^{-13}	-1.59×10^{-11}
0.002	-7.19×10^{-14}	7.94×10^{-15}	-4.20×10^{-13}
0.001	-2.79×10^{-14}	1.67×10^{-16}	-5.39×10^{-14}

The result shown in column (a) illustrates high accuracy characteristic of the Numerov algorithm. Unfortunately, however, its accuracy is lower than the Runge–Kutta method. For an impartial comparison of the two schemes, one has to take into account that the Runge–Kutta calculation involves more numerical computations than the Numerov one. It is therefore fair to compare the Numerov result for step size h with the Runge–Kutta one for step size $2h$. Even with this comparison, advantage of the Runge–Kutta method is apparent in Table I. In particular, the Numerov scheme becomes less competent for smaller h.

This seems to contradict the generally accepted superiority of the Numerov method. As a matter of fact, the above behavior of the present Numerov scheme may be understood as follows: In Eq. (2.9), we replaced the third derivative y''' with a combination of f' and y'' using the differential Eq. (2.1). Subsequently, the latter quantities were approximated by finite differences. For small argument x, cancellation takes place between f'/x and $2y''/x$, which explains why our version of the Numerov scheme is not fully satisfactory for small step size when the integration is started from the origin.

In this way, although our scheme can indeed solve Eq. (1.2) directly from the origin, it advantage is excelled by the Runge–Kutta method. If one could devise a better discretization formula for Eq. (2.9), the Numerov method would restore its intrinsic advantage.

The situation changes, if the range of integration stands away from the origin. Table II shows the result of integration when Bessel's equation is integrated from $x=0.75$ to $x=1.75$. In this case, the Numerov result gives lower accuracy than the Runge–Kutta one for the same step size. However, when the criterion of comparison is changed as mentioned above, the Numerov method shows a better performance. In this region of x, intrinsic usefulness of the Numerov method is prevailing, since numerical cancellation no more takes place in Eq. (2.9).

On the other hand, when x is sufficiently separated from the origin, one can as well use the conventional Numerov method using the transformation (1.3). Column (c) of Table II shows the result of such an integration. Here, substitution (1.3) was applied to Bessel's equation and the resulting differential equation of the form (1.1) was integrated by means of the standard Numerov method. In this numerical calculation, the difference technique mentioned toward the end of Sec. I was adopted. Comparison of columns (a) and (c) tells us that the conventional Numerov scheme is suffering from the square-root singularity at $x=0$, as mentioned in the Introduction. In order for the conventional Numerov method to give better accuracy, x has to be further away from the origin.

III. CONCLUSION

The Numerov method has been frequently used in solving second-order differential equations of the form (1.1) lacking the first derivative. In this paper, we generalized it to Eq. (1.2), which appears as wave equations in cylindrical symmetry. The proposed method can solve Eq. (1.2) directly from the origin with a single algorithm. Numerical comparison with the Runge–Kutta method has revealed that it is not yet very satisfactory for small step size when the integration is started from (or terminated at) the origin. However, when the range of integration is separated away from the origin, its performance is quite satisfactory. Thus, the present version of the Numerov method should be counted as one of useful methods when solving wave equations in cylindrical geometry.

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