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Method for the Numerical Solution of Linear Second-Order Differential Equations

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ABSTRACT

A method for the numerical solution of linear second-order differential equations is described. The method is an extension of the Numerov method, and has a truncation error of the same order, h^6. It reduces to the Numerov method if the term involving the first derivative is absent. The results obtained by applying the method to a particular example are given, and compared with results obtained with the fourth-order Runge-Kutta method.

1. INTRODUCTION

A popular method for the numerical solution of the Schrödinger equation

$$u''(x) = f(x)\,u(x) \tag{1}$$

is the well-known Numerov method, which has been thoroughly discussed by Blatt [1]. Our concern in this paper is the more general equation

$$u''(x) = a(x)\,u'(x) + b(x)\,u(x) + c(x), \tag{2}$$

and our aim is to develop an extension of the Numerov method that retains the main advantages of that method; in particular, the truncation error is of sixth-order in the steplength. The method is described in the following section, and discussed in relation to a particular example in the final section. It reduces to the Numerov method if $a(x)$ is identically zero.

The differential equation (2) occurs, of course, in many contexts. Our own interest arises from the method of polarized orbitals [2], [3] for the scattering of slow electrons by atoms, in which the combination of atom polarization and electron exchange introduces a term involving the first derivative into the effective Schrödinger equation [3]. An extension of the Numerov method to handle this situation has been described previously in [3] and used successfully there, but the method to be described in the following section is expected to have improved error propagation properties.

We remark that the first derivative in Eq. (2) may always be removed by an appropriate transformation [4], but the transformation is not always convenient.

2. The Numerical Method

We begin with the fundamental equation of the Numerov method [5]

$$u_1 - 2u_0 + u_{-1} = \frac{h^2}{12}(u_1'' + 10u_0'' + u_{-1}'') - \frac{h^6}{240}u_0^{(6)} + \cdots, \tag{3}$$

where u_j denotes $u(x_j)$, and h is the steplength,

$$h = x_j - x_{j-1}\,.$$

As in the Numerov method, the problem is to calculate u_1, assuming that u_0 and u_{-1} are known, and that terms of order h^6 in (3) can be neglected. If we suppose for the moment that $a(x)$ in (2) is identically zero, then the second derivatives on the right-hand side of (3) may be expressed in terms of u_1, u_0, and u_{-1} by means of the differential equation (2), and it is then trivial to solve for u_1 in terms of u_0 and u_{-1}. This constitutes the ordinary Numerov method.

In the general case, with $a(x)$ not identically zero, we can no longer eliminate the second derivatives in (3) exactly. Our approach is to develop useful approximations for u_1'' and u_0'', assuming that u_{-1}'' is known. The aim in a single step is then to obtain not only an approximate value for u_1, but also a value for u_0'', which will become the known second derivative in the next step.

The approximations to u_0'' and u_1'' are based on the differential equation (2); thus for u_0'' we have

$$u_0'' = a_0u_0' + b_0u_0 + c_0\,. \tag{4}$$

To eliminate u_0' we use the series expansion in powers of h (see Reference [6]),[1]

$$u_0' = \frac{1}{2h}(u_1 - u_{-1}) - \frac{h}{12}(u_1'' - u_{-1}'') + \frac{7}{360}h^4u_0^{(5)} + \cdots, \tag{5}$$

and obtain a useful approximation by omitting terms of order h^4. Similarly, for u_1'' we have

$$u_1'' = a_1u_1' + b_1u_1 + c_1\,, \tag{6}$$

[1] Reference [6] contains an error: within both square brackets the term 1 should be replaced by $\frac{1}{2}$.

but we cannot use the symmetrical expansion (5) to eliminate u_1', since u_2 is not known. We use instead [7]

$$u_1' = \frac{1}{2h}(9u_1 - 16u_0 + 7u_{-1}) - \frac{h}{3}(8u_0'' + u_{-1}'') - \frac{1}{45}h^4u_1^{(5)} + \cdots. \tag{7}$$

Equations (3), (5), and (7) may all be verified by Taylor series expansions.

It is convenient to introduce the notation

$$\begin{aligned} S(x) &= (h^2/12)\,u''(x), \\ A(x) &= (h/24)\,a(x), \\ B(x) &= (h^2/12)\,b(x), \\ C(x) &= (h^2/12)\,c(x). \end{aligned}$$

Then the fundamental equation (3) becomes

$$u_1 - 2u_0 + u_{-1} = S_1 + 10S_0 + S_{-1} - \frac{h^6}{240}u_0^{(6)} + \cdots, \tag{8}$$

and in it u_0, u_{-1}, and S_{-1} are assumed to be known. Equations (4) and (5) give an expression for S_0,

$$S_0 = A_0(u_1 - 2S_1 - u_{-1} + 2S_{-1}) + B_0u_0 + C_0 + \frac{7}{4320}h^6a_0u_0^{(5)} + \cdots, \tag{9}$$

while (6) and (7) give for S_1

$$\begin{aligned} S_1 = {} & A_1(9u_1 - 16u_0 + 7u_{-1} - 64S_0 - 8S_{-1}) + B_1u_1 + C_1 \\ & - \frac{h^6}{540}a_1u_1^{(5)} + \cdots. \end{aligned} \tag{10}$$

The practical formulas are obtained by omitting terms of order h^6 in (8), (9), and (10), to give a system of three linear equations in the three unknowns u_1, S_0, and S_1. We express the solution below in a form suitable for practical calculation. The first step in advancing the solution from x_0 to x_1 is to calculate the four auxiliary quantities

$$\alpha = 1/(1 - 20A_0), \tag{11}$$

$$\beta = \alpha(10 - 64A_1), \tag{12}$$

$$\gamma = A_0(4u_0 - 3u_{-1} + 4S_{-1}) + B_0u_0 + C_0, \tag{13}$$

$$\delta = (1 - 8A_1)(2u_0 - u_{-1} + S_{-1}) - A_1u_{-1} + C_1. \tag{14}$$

Then u_1 is given by

$$u_1 = \frac{\beta\gamma + \delta}{1 - 9A_1 - B_1 + \beta A_0}, \tag{15}$$

and S_0 is given by

$$S_0 = \alpha(\gamma - A_0 u_1). \tag{16}$$

The quantity S_1 need not be calculated, but S_0 is required in preparation for the next step. [If S_1 is required, for example for the midpoint interpolation below, it may be calculated directly from (10).] Equations (11)–(16) constitute the method. The initial values required for starting the solution may be provided by Taylor series expansion or other methods.

Midpoint interpolation, required for halving the steplength, may be achieved in the same way as in [1] by using again the fundamental equations of the method. Specifically, let us assume that u_{-1}, S_{-1}, u_1, and S_1 are known, and that u_0 is required. From Eqs. (8) and (9) we obtain

$$u_0 = \frac{u_1 + u_{-1} - S_1 - S_{-1} - 10A_0(u_1 - u_{-1} - 2S_1 + 2S_{-1}) - 10C_0}{2 + 10B_0},$$

with a truncation error of order h^6.

To conclude this section we point out the difference between the present method and that described in [3]. That method is similar in principle, but the first derivatives u_0' and u_1' are both approximated by the unsymmetrical expansion (7). In other words, the method of [3] is obtained if the equation for S_0, Eq. (9), is replaced by the analog of (10). The disadvantage of that method lies not in the truncation error, which is similar in (9) and (10), but in the dangerously large numerical coefficients in (10), which may lead to excessive error propagation. The present method appears more satisfactory, in that while the coefficients in the equation for S_1 are still large, those in the equation for S_0 are small. It should be noted that errors in S_1 are less important than those in S_0, since S_0 appears in the equation for u_1, Eq. (8), with the large coefficient 10.

3. Discussion and Example

The truncation errors in the method of the previous section arise from the omitted terms of order h^6 in Eqs. (8)–(10), thus it is immediately clear that the total truncation error in u_1 is itself of order h^6.[2] Since the method is based on the

[2] The divisions required in the solution of (8), (9), and (10) do not affect the order of the error, since the denominators are of the order of unity.

second difference equation (3), it follows that the cumulative error at a fixed value of x is of order h^4, just as in the Numerov method [8]. It has been pointed out elsewhere [8] that, in terms of the order of the cumulative error, the Numerov method for the solution of (1) has no clear superiority over other methods, and in particular that the fourth-order Runge-Kutta method [9] also has a cumulative error of order h^4. By extending the argument, the same conclusion may be established for the solution of (2): the extended Numerov method and the fourth-order Runge-Kutta method both have cumulative errors of order h^4. Any argument as to the relative accuracy of the methods must therefore be directed to the magnitude of the error, rather than to its order. To make a first assessment we therefore work out a particular example.

Our example is the differential equation

$$u'' + u' + u = 0, \tag{17}$$

subject to the initial conditions $u(0) = 0$, $u'(0) = \sqrt{3}/2$. The general solution of (17) is

$$u(x) = e^{-x/2}(C_1 \sin \frac{\sqrt{3}}{2} x + C_2 \cos \frac{\sqrt{3}}{2} x),$$

and the particular solution satisfying the initial conditions is

$$u(x) = e^{-x/2} \sin \frac{\sqrt{3}}{2} x.$$

The results are shown in Table I, with N denoting the method of Section 2, and RK

TABLE I

COMPUTED VALUES OF $u/e^{-x/2}$

		Errors multiplied by 10^8		
x	Exact	N ($h = 0.1$)	RK ($h = 0.1$)	RK ($h = 0.2$)
0	0	0	0	0
0.8	0.63870981	37	12	226
1.6	0.98290760	133	−23	−257
2.4	0.87388220	206	−127	−1946
3.2	0.36190571	164	−254	−4172
4.0	−0.31694716	−20	−311	−5356
4.8	−0.84965424	−278	−214	−3995

the fourth-order Runge-Kutta method for a second-order differential equation [9]. In the former case the results are shown for a steplength of 0.1, and in the latter case for the two steplengths 0.1 and 0.2. Exact starting values were used in every case.

From the results with $h = 0.1$ it is seen that, for this example, the two methods yield results of similar accuracy if the same steplength is used. We point out, however, that the Runge-Kutta method has the important limitation that values of the functions $a(x)$, $b(x)$, and $c(x)$ in (2) are required at the half-way points. In the frequently occuring situation that these functions require extensive calculation, or if they are available only in tabular form, a fairer comparison in between the N ($h = 0.1$) and RK ($h = 0.2$) results. On that basis the present method seems considerably the more accurate.

The method described in [3] was also applied to the example. The cumulative errors with that method were found to be approximately twice as large as those with the method of this paper.

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