RESEARCH ARTICLE | SEPTEMBER 01 1997

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Comput. Phys. 11, 514–515 (1997)
https://doi.org/10.1063/1.168593

Getting started with Numerov's method

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(Received 7 April 1997; accepted 28 May 1997)

Second-order ordinary differential equations of the Numerov type (no first derivative and the given function linear in the solution) are common in physics, but little discussion is devoted to the special first step that is needed before one can apply the general algorithm. We give an explicit algorithm to calculate the first point of the solution with an accuracy appropriate to that obtained with the general algorithm. © *1997 American Institute of Physics.* [S0894-1866(97)01605-2]

Numerov's method is an efficient algorithm for solving second-order differential equations of the form

$$\frac{d^2y}{dx^2}=U(x)+V(x)y. \tag{1}$$

Particular examples in physics of this type of equation are the one-dimensional time-independent Schrödinger equation,

$$\frac{d^2\psi}{dx^2}=\frac{2m}{\hbar}[V(x)-E]\psi, \tag{2}$$

and the equation of motion of an undamped forced harmonic oscillator,

$$m\frac{d^2y}{dx^2}=f_0\cos\omega x-ky. \tag{3}$$

In addition, Poisson's equation may reduce to this form when the charge distribution is sufficiently symmetrical.

The important features of Eq. (1) for the application of Numerov's method are that the first derivative is absent and the left-hand side (LHS) is linear in y. To obtain a finite-difference scheme, one uses the centered-difference equation,

$$y_{n+1}-2y_n+y_{n-1}\cong 2\left(\frac{h^2}{2}\frac{d^2y}{dx^2}+\frac{h^4}{4!}\frac{d^4y}{dx^4}+O(h^6)\right), \tag{4}$$

where $y_n=y(x_n)$ and we suppose that the x_n are uniformly spaced with a separation of h. If we denote the LHS of Eq. (1) by

$$F=U(x)+V(x)y, \tag{5}$$

then, by combining Eqs. (1) and (4), we have

$$y_{n+1}=2y_n-y_{n-1}+h^2F_n+\frac{h^4}{12}\left.\frac{d^2F}{dx^2}\right|_n+O(h^6). \tag{6}$$

However, we can replace the second derivative of F by a difference equation similar to Eq. (4), giving the final result for Numerov's algorithm,

$$y_{n+1}=\frac{2y_n-y_{n-1}+\frac{h^2}{12}(U_{n+1}+10F_n+F_{n-1})}{\left(1-\frac{V_{n+1}h^2}{12}\right)}+O(h^6). \tag{7}$$

It is in this step that we require the LHS of Eq. (1) to be linear in y.

The efficiency of Numerov's method lies in the fact that one obtains a local error of $O(h^6)$ with just one evaluation of U and V per step. This should be compared to the Runge–Kutta algorithm that needs six function evaluations per step to achieve a local error of $O(h^6)$.[1]

It is immediately obvious from Eq. (7) that we need two previous values of the solution in order to calculate a new one. Therefore, we must address the question of how to start the calculation. We suppose that we have, as initial conditions, the value of the solution y_0, which allows us to calculate F_0, and the gradient y_0'. In order to calculate y_2 with an accuracy $O(h^6)$ we need y_1 with this same accuracy. It is sufficient, however, to calculate y_1 with an accuracy $O(h^5)$ because the global error of the algorithm is $O(h^5)$ and we calculate y_1 just once.

The best that we can do to calculate y_1 from scratch, without doing any analytical differentiation, is to use the Taylor series expansion,

$$y_1=y_0+hy_0'+\frac{h^2}{2}F_0+\frac{h^3}{3!}F_0'+\frac{h^4}{4!}F_0''+O(h^5), \tag{8}$$

and truncate the series after replacing the first derivative with

$$F_0'=\frac{F_1-F_0}{h}+O(h), \tag{9}$$

giving

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  0894-1866/97/11(5)/514/2/$10.00

$$y_1 = \frac{y_0 + hy_0' + \frac{h^2}{6}(U_1 - 2F_0)}{\left(1 - \frac{V_1 h^2}{6}\right)} + O(h^4). \qquad (10)$$

Use of Eq. (10) as a first step could result in the loss of a factor of h in the global error of the solution.

It is clear from Eq. (8) that what is needed is some means of estimating the second derivative of F_0. The literature is not very helpful on this point, as there is often no discussion of this. One suggestion[2–4] is to calculate, analytically, the second derivative of F, which is not always practical. Another,[2,5] is to calculate y_1 according to Eq. (8), without including F_0' or F_0'', and then uses the standard Numerov algorithm to obtain a first estimate for y_2. This can then be used to estimate the value of F_0''. One then enters a cycle of iteration until the values of y_1 and y_2 stabilize. In fact, as we will show, such a cycle of iteration is not necessary. Finally, one can use a single step of a different self-starting algorithm to obtain y_1 and then switch over to Numerov's method.[6]

Let us suppose that we have somehow obtained a first estimate for y_2 that will allow us to estimate F_2. Using the values of F_0, F_1, and F_2 we can estimate F_0'' and hence, obtain y_1 with the required accuracy, that is to say, we seek to calculate y_1 in the form

$$y_1 = y_0 + hy_0' + h^2(aF_0 + bF_1 + cF_2). \qquad (11)$$

The constants a, b, and c have to be chosen such that Eqs. (8) and (11) agree, which we do by expanding F_1 and F_2 in the Taylor series about the origin. This gives

$$y_1 = y_0 + hy_0' + \frac{h^2}{24}(7F_0 + 6F_1 - F_2) + O(h^5). \qquad (12)$$

The standard Numerov step to calculate y_2 is

$$y_2 = \frac{2y_1 - y_0 + \frac{h^2}{12}(U_2 + 10F_1 + F_0)}{\left(1 - \frac{V_2 h^2}{12}\right)} + O(h^6). \qquad (13)$$

Equations (12) and (13) form a closed set of two linear algebraic equations for y_1 and y_2. We can write

$$\begin{aligned} a_{11}y_1 + a_{12}y_2 &= b_1, \\ a_{21}y_1 + a_{22}y_2 &= b_2, \end{aligned} \qquad (14)$$

with $a_{11} = 1 - V_1h^2/4$, $a_{12} = V_2h^2/24$, $a_{21} = -2 - 5V_1h^2/6$, $a_{22} = 1 - V_2h^2/12$, $b_1 = y_0 + hy_0' + h^2(7F_0 + 6U_1 - U_2)/24$, and $b_2 = -y_0 + h^2(F_0 + 10U_1 + U_2)/12$. The solution for y_1 is

$$y_1 = \frac{a_{22}b_1 - a_{12}b_2}{a_{11}a_{22} - a_{12}a_{21}} = \frac{y_0\left(1 - \frac{V_2h^2}{24}\right) + hy_0'\left(1 - \frac{V_2h^2}{12}\right) + \frac{h^2}{24}\big(7F_0 + 6U_1 - U_2\big) - \frac{h^4V_2}{36}\big(F_0 + 2U_1\big)}{1 - \frac{V_1h^2}{4} + \frac{V_1V_2h^4}{18}}, \qquad (15)$$

and y_2 can be calculated with Eq. (13). The importance of Eq. (15) is that it gives y_1 with the required accuracy $O(h^5)$ so that there is no need for either iteration or analytical derivatives.

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