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A variable-step Numerov method for the numerical solution of the Schrödinger equation

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Numerov's method is one of the most widely used algorithms for solving second-order ordinary differential equations of the form $y'' = f(x, y)$. The one-dimensional time-independent Schrödinger equation is a particular example of this type of equation. In this article we present a variable-step Numerov method for the numerical solution of the Schrödinger equation.

KEY WORDS: Numerov method, Schrödinger equation, variable stepsize

1. Introduction

Recently the goal of providing efficient numerical methods for solving particular types of problems has been a central activity within the full scope of solving differential equations numerically.

One of such problem is the so-called *special second-order* differential equation, which has the form

$$y''(x) = f(x, y(x)), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{1}$$

where the right-hand side does not include the derivative of y.

These problems arise in a wide variety of physical situations and a good sign of their importance is the fact that many of them have their own proper name: Airy's equation, Duffing's equation, Hill's equation, Mathieu's equation, and even the Bessel's equation may be reduced to the form in (1).

Different authors have dealt with the problem in (1) [1–6] providing different approaches to solving it, but the pioneer work was probably due to Störmer,

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who developed his method in connection with numerical calculations concerning the aurora borealis.

The k-step Störmer method may be derived similarly to the Adams method, by twice integrating the differential equation in (1), and then replacing f by the interpolating polynomial passing through the points

$$(x_{n-(k-1)}, y_{n-(k-1)}), \ldots, (x_n, y_n),$$

where the x_i are equally spaced.

However, to obtain more accurate formulas, it is possible used the interpolation polynomial passing through the additional point (x_{n+1}, y_{n+1}). In this case, we obtain the implicit Störmer method (also known in certain contexts as the Cowell method or the Numerov method).

The methods just mentioned are of multistep-type, suitable for solving the problem in (1) with more or less accuracy, and they have in common a fixed stepsize. Nevertheless, to be efficient, as some authors have remarked [7,8], an integrator based on a particular formula must be suitable for a variable stepsize formulation.

We have obtained a generalization of the Numerov method in its variable stepsize version [9]; this is presented in section 2. Section 3 provides a technique for changing the steplength, and finally, in section 4 we apply the new method for solving the Schrödinger equation numerically.

The one-dimensional time-independent or radial Schrödinger equation has the form in (1) with $f = \left[l(l+1)/x^2 + V(x) - E\right] y(x)$, where the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$; l is a given integer related to the *angular momentum*; $V(x)$ is a given function that denotes the potential, and E is a real number denoting the energy [10]. Thus, the final equation reads

$$y''(x) = \left[\frac{l(l+1)}{x^2} + V(x) - E\right] y(x). \tag{2}$$

The boundary conditions are: $y(0) = 0$, plus a second boundary condition, for large values of x, which is determined by physical considerations.

Many techniques have appeared in the literature for solving this problem [6, 11–20], but the common feature among the multistep methods used is the constant stepsize.

We shall test the performance of the variable two-step Numerov method by considering the numerical integration of the Schrödinger equation in the case where $V(x)$ is the so-called Woods–Saxon potential (see [10, p. 298]):

$$V(x) = \frac{u_0}{1+t} - \frac{u_0 t}{a(1+t)^2}, \tag{3}$$

where $t = \exp[(x - x_0)/a]$, $u_0 = -50$, $x_0 = 7$ and $a = 0.6$.

2. The Numerov method of variable stepsize

The variable k-step Cowell method is an implicit multistep code of order $k+1$ that is suitable for the numerical integration of problems of the type in (1) and can be expressed in the form (see [9])

$$y_{n+1} - \left(1 + \frac{h_{n+1}}{h_n}\right) y_n + \frac{h_{n+1}}{h_n} y_{n-1} = h_{n+1}(h_{n+1} + h_n) \sum_{j=0}^{k} \gamma_j^* f[\overline{x}_{n+1}, \ldots, \overline{x}_{n+1-j}], \tag{4}$$

where h_n and h_{n+1} are two of the stepsizes; namely,

$$h_n = \overline{x}_n - \overline{x}_{n-1}, \qquad h_{n+1} = \overline{x}_{n+1} - \overline{x}_n,$$

with $\overline{x}_{n-(k-1)}, \ldots, \overline{x}_{n+1}$ the grid points that are unevenly spaced, and the terms $f[\overline{x}_n, \ldots, \overline{x}_{n-j}]$ the Newton-divided differences, as are usually defined. Finally, γ_j^* are some coefficients that depend on the stepsizes in the grid points (in [9] there is a detailed description on how to obtain these coefficients).

If we introduce the notations

$$\frac{h_{n+1}}{h_n} = c_1, \quad \frac{h_n}{h_{n-1}} = c_2, \quad \frac{h_{n-1}}{h_{n-2}} = c_3, \quad \ldots \tag{5}$$

for the stepsize ratios, the above formula may be expressed as

$$y_{n+1} = (1 + c_1)\, y_n - c_1 y_{n-1} + h_{n+1}(h_{n+1} + h_n) \sum_{j=0}^{k} \gamma_j^* f[\overline{x}_{n+1}, \ldots, \overline{x}_{n+1-j}]. \tag{6}$$

For $k = 2$ and constant stepsize, that is $c_1 = 1$, we obtain from (6) the well-known *Numerov formula* [21,22]:

$$y_{n+1} - 2y_n + y_{n-1} = \frac{1}{12} h^2 (f_{n+1} + 10 f_n + f_{n-1}), \tag{7}$$

which is the most popular particularization of algorithm (6).

The counterpart formulation for the Numerov method in the case of variable stepsize may be obtained from (6) for $k = 2$, and reads

$$\begin{aligned} y_{n+1} = (1 + c_1)\, y_n - c_1 y_{n-1} + \frac{1}{12} h_n^2 \big[&(-1 + c_1 + c_1^2) f_{n+1} \\ &+ (1 + 4c_1 + 4c_1^2 + c_1^3)\, f_n + (c_1 + c_1^2 - c_1^3) f_{n-1}\big]. \end{aligned} \tag{8}$$

Analogously, it is possible to extend the variable-step Numerov formula for values of $k > 2$.

3. Strategy for stepsize selection

When using a variable multistep code, one needs a strategy for deciding how to change the steplength (and the order if this is the case). We adopt similar strategies to those used in [23] or [24] for Adam's multistep methods.

The reader is referred back to the considerations about stepsize selection in [9], but now, for the implicit formula (8), we take the local error estimate as given by

$$\mathrm{LE}(\overline{x}_n, h_{n+1}) = h_{n+1}(h_{n+1} + h_n)\gamma_3^* \, f[\overline{x}_{n+1}, \overline{x}_n, \overline{x}_{n-1}, \overline{x}_{n-2}]. \tag{9}$$

Our goal is to obtain a suitable value for h_{n+1} so that a norm of the local error in advancing the numerical solution from $\overline{x}_n$ to $\overline{x}_{n+1}$ will be approximately equal to a given tolerance. Indeed, given a requested tolerance, TOL, the optimal projected stepsize h_{n+1}^* (that is, the maximum steplength we could have taken to produce an error estimate equal to a given tolerance) should be obtained by solving an equation of the form

$$\rho \, \mathrm{TOL} = \left\| \mathrm{LE}(\overline{x}_n, h_{n+1}^*) \right\|, \tag{10}$$

where ρ is a safety factor (<1) whose purpose is to avoid failed steps. Since we do not know the value y_{n+1}, in general this equation is impossible to solve.

Even if we consider the implicit method as a corrector of a predictor–corrector pair, and we approximate the value $y_{n+1} \simeq y_{n+1}^{(p)}$, (that is, for the value obtained with the predictor), taking $\overline{x}_{n+1} = \overline{x}_n + h_{n+1}^*$, the equation resulting from (10) may be very complicated. Therefore, it is necessary to make some simplifying assumptions.

It is natural in this situation to take one-step back, and approximate

$$f[\overline{x}_{n+1}, \overline{x}_n, \overline{x}_{n-1}, \overline{x}_{n-2}] \quad \text{by} \quad f[\overline{x}_n, \overline{x}_{n-1}, \overline{x}_{n-2}, \overline{x}_{n-3}]$$

in order to reduce the problem. The price to be paid for this, apart from accuracy, is that at the starting procedure we must calculate the values of the solution at 3 points instead of 2. With these considerations, the stepsize estimator for the step from $\overline{x}_n$ to $\overline{x}_{n+1}$ is the solution of the equation

$$\rho \, \mathrm{TOL} = \left\| h_{n+1}^*(h_{n+1}^* + h_n) \, \gamma_3^*(h_{n+1}^*) \, f[\overline{x}_n, \overline{x}_{n-1}, \overline{x}_{n-2}, \overline{x}_{n-3}] \right\|,$$

where $\gamma_3^*(h_{n+1}^*)$ means that in the polynomial in h_{n+1} of degree 3, γ_3^*, we have replaced h_{n+1} by h_{n+1}^*. Calculating γ_3^* directly, we obtain

$$\gamma_3^*(h_{n+1}) = \tfrac{1}{60}\left(2h_n^3 + 3h_n^2 \, h_{n+1} - 3h_n \, h_{n+1}^2 - 2h_{n+1}^3\right),$$

and the final equation

$$h_{n+1}^*(h_{n+1}^* + h_n) \, \gamma_3^*(h_{n+1}^*) = \frac{\rho \, \mathrm{TOL}}{\| f[\overline{x}_n, \overline{x}_{n-1}, \overline{x}_{n-2}, \overline{x}_{n-3}] \|}$$

by Descartes' Theorem proves to have a unique positive root. This root, which must be calculated numerically, will be our choice for the new step.

4. Numerical illustrations

In this section we present some numerical results to illustrate the performance of the method. We consider the numerical integration of the Schrödinger equation (2) with $l = 0$ for the potential in (3). In the case of negative eigenenergies (that is, $E \in [-50, 0]$) we have the so-called *bound-states problem*, and in case of positive eigenenergies (that is, $E \in [1, 1000]$) we have the so-called *resonance problem*.

4.1. Bound-states problem

We have applied the variable-step Numerov method to the problem of computing the eigenvalues for equation (2) in the domain $[0, 10]$.

In fact, the problem is a Sturm–Liouville eigenvalue problem, and we are interested in the numerical computation of the eigenvalues E_i in the energy interval $[-50, 0]$ for which a solution of equation (2), satisfying the boundary conditions, exists. The boundary value problem is split up into two initial value problems. We follow the strategy in [10], taking initial conditions $y(0) = 0$, and arbitrary $y'(0) \neq 0$. Using a trial eigenvalue, the given differential equation is integrated, and by means of an iterative process the corrections to the eigenvalue are performed.

In all cases we have established $\rho = 1$. Given a small h, from the conditions $y(0) = 0$, $y(h) = h$, we have taken the starting values computed using the Numerov scheme of fixed stepsize h.

In table 1 we present the absolute errors for the energy values $E_n, n = 0, 4, 9, 13$, for the potential (3). The exact values for comparative purposes were taken from [10],

$$E_0 = -49.457788728, \qquad E_9 = -22.588602258,$$

$$E_4 = -41.232607772, \qquad E_{13} = -3.908232481.$$

4.2. Resonance problem

In the case of positive energies, $E = k^2 > 0$, the potential $V(x)$ dies away faster than the term $l(l+1)/x^2$, and the Schrödinger equation effectively reduces to

$$y''(x) = \left[\frac{l(l+1)}{x^2} - k^2\right] y(x) \tag{11}$$

for x greater than some value X.

Table 1
Bound-states problem. Data for different values of starting step, h, and tolerance, TOL.

Eigenvalue	Absolute error
$h = 0.05$, TOL $= 10^{-10}$	
E_0	5.5×10^{-8}
E_4	2.3×10^{-6}
E_9	2.3×10^{-5}
E_{13}	4.1×10^{-5}
$h = 0.05$, TOL $= 10^{-12}$	
E_0	1.0×10^{-9}
E_4	1.1×10^{-7}
E_9	1.6×10^{-6}
E_{13}	5.8×10^{-6}
$h = 0.05$, TOL $= 10^{-14}$	
E_0	0
E_4	6.0×10^{-9}
E_9	7.9×10^{-8}
E_{13}	2.1×10^{-7}
$h = 0.002$, TOL $= 10^{-16}$	
E_0	0
E_4	0
E_9	3.0×10^{-9}
E_{13}	1.7×10^{-8}

The above equation has two linearly independent solutions; namely, $S(x) = kx j_l(kx)$ and $C(x) = kx\, n_l(kx)$, where $j_l(kx), n_l(kx)$ are the *spherical Bessel* and *Neumann functions* respectively. Thus, the solution of equation (2) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\sim A\, k\, x\, j_l(kx) - B\, k\, x\, n_l(kx) \\ &\sim D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)], \end{aligned}$$

where δ_l is the *phase shift*, which may be calculated from the formula

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)}$$

for x_1 and x_2 two distinct points in the asymptotic region (we take x_1 as the right-hand end point of the interval of integration, and $x_2 = x_1 - h_n$, h_n being the last stepsize).

Before starting the multistep method we have to know y_0 and y_1. From the initial condition, we have $y_0 = 0$. For values of x close to the origin, the solution behaves like $y(x) \simeq c\, x^{l+1}$, where c is an independent constant [13]. In view of

Table 2
Resonance problem. Data for different values of starting step, h.

Initial step	Steps	Absolute error
$h = 0.01$	1505	1.0×10^{-2}
$h = 0.005$	2894	7.5×10^{-4}
	3015	6.3×10^{-4}
$h = 0.001$	4022	2.5×10^{-4}
	7778	2.0×10^{-5}
	13, 978	1.3×10^{-6}
$h = 0.0005$	3530	3.9×10^{-4}
	8556	1.2×10^{-5}
	17, 053	6.6×10^{-7}
	28, 866	1.7×10^{-10}

this, we take $y_1 = h^{l+1}$. The two other starting values, necessary for the stepsize strategy, are computed using the Numerov method with fixed stepsize h. From this point, the variable stepsize Numerov method is applied.

The resonance problem consists of finding the phase shift $\delta(E) = \delta_l$ for a given $E \in [1, 1000]$, or finding those $E \in [1, 1000]$ at which δ_l equals $\pi/2$.

We consider the first procedure, using the technique fully described in [25], and compare the calculated phase shift to the analytic value of $\pi/2$, integrating in the domain $[0, 15]$. The boundary conditions for this problem are

$$y(0) = 0, \quad y(x) \sim \cos(\sqrt{E}\, x) \text{ for large } x.$$

The results for the known highest eigenvalue $E_3 = 989.7019195$ are presented in table 2, where Steps refers to the total number of steps in the integration process and Absolute error refers to the absolute error of the calculated phase shift.

5. Conclusions

We have developed a variable-stepsize Numerov method that may afford high accuracy. As expected, for the Schrödinger equation this method needs fewer evaluations of the potential than the classical Numerov method of fixed stepsize.

Nevertheless, it should be noted that these methods are of general purpose; that is, we do not know a priori the behavior of the solution. When the solution of the initial value problem is, for example, of oscillatory or Bessel nature, particular methods such as those trigonometrically-fitted or Bessel-fitted would be appropriate for such problems. For more details see [6, 17–20].

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