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A note on the construction of Numerov method through a quadratic continuous polynomial for the solution of general second order differential equation

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Abstract

This note presents a construction of Numerov method from a quadratic continuous polynomial solution (degree two continuous polynomial solutions). In contrast with* [1, 3, 5] *that was hitherto obtained from a degree four polynomial, the discrete Numerov method as a special case. This process lead to the block method applied to both initial and boundary value problem for the more general second order $y'' = f(x, y, y')$.

Keywords: Runge-Kutta Method (RKM), Block Method (BM), Numerov Method Continuous polynomial solution

1.0 Introduction

The study of numerical solution of initial and boundary value problem in the second order ordinary differential equations

$$y'' = f(x, y), \quad y(a) = y_o, \quad y'(a) = y'_o \tag{1.1}$$

$$y'' = f(x, y), \quad y(a) = \beta, \quad y(b) = \eta \tag{1.2}$$

and the more general form of second order ODE's $\quad y'' = f(x, y, y') \quad$ (1.3)

with two point boundary of the form

$$y(a) = y_o \ , \ y(b) = y_r$$

or with initial conditions, $y(a) = \eta$, $y'(a) = \psi$, where $a \le x \le b$, is considered. There are Runge-Kutta type of methods which solve (1.1) - (1.3) directly without reducing it to first order system. The present approach is found to be advantageous in many ways among this is that the continuous form can be used as interpolant for the computed numerical values for dense output for analytical work at no extra cost to provide interpolant. Besides this, the continuous form can also be a big advantage in error control for choosing a step size adjustment strategy for the proposed block method. Most importantly, obtaining y(x) = u(x) in the form (3.2) of section 3.0, involves a matrix inversion once. The continuous solution u(x) is evaluated at some meshes for simultaneous (Block) discrete method for the numerical solution in the parallel computing form. However, if the sequential computing is desired, the proposed two-step Numerov block method can be used to get the single linear multi-step method (LMM), evaluated at x_{n+k} , started. The approach is by continuous (LMM) of the form

$$\sum_{j=0}^{k} \alpha_j(x) f_{j+!} = h^2 \sum_{j=0}^{k} \beta_j(x) f_{j+1} \tag{1.4}$$

where k is the step number $\alpha_k(x) = 1, \alpha_o(x), \beta_o(x)$ are not both zeros, while $\alpha_j(x)$ and $\beta_j(x)$ are real continuous coefficients. The three-term recurrence formula

$$y_{r+2} - 2y_{r+1} + y_r = \frac{1}{12} h_r^2 (f_{r+2} + 10 f_{r+1} + f_r), \;\; r = 0,1... \tag{1.5}$$

called the Numerov method was earlier proposed for efficient solution of (1.1)-(1.2) on a discrete mesh point with constant step size h, in [1, 3, 5] whereas h_r can be variable step-size h in the form

$$x_{r+1} = x_r + h, \;\; r = 0,1,...,n-2, \;\; x_n = x_{n-1} + h_{r-1} \tag{1.6}$$

where $a = x_o, \;\; x_r < x_{r+1}, \;\; r = 1,...,n-1, \;\; x_n = b$.

The formula (1.5) is accurate and is of order four with an error constant $C_6 = \frac{-1}{240}$, its application to (1.1)-(1.2) results in a tridiagonal set of algebraic equations. For these two reasons the Numerov method is popular. However, its implementation requires the generation of $k-1$ initial starting values $y(x_n + j) = y_{n+j}, \; j = 1(1)k-1$ using a starting method which is most often Runge-Kutta method (RKM). The direct application of (1.4) to (1.1)-(1.2) has been found to be more advantageous in some application than the application of conventional LMM (1.4) to the reduced (1.1)-(1.2) in first order systems of initial value problem (IVP).

$$y' = g(x,y), \;\; y(a) = y_o \tag{1.7a}$$

$$g' = f(x,y), \;\; g(a) = y_{oo} \tag{1.7b}$$

Whereas its application to (1.3) as proposed in this paper, without recourse to any special integrator, the y' is replaced accurately as order four finite difference formula, the result is a symmetrical set of algebraic equations. Since, the idea behind the multi-step collocation is to let the collocation polynomial use information from the previous points in the integration. The method incorporates finite difference approximation for the first derivative into the integration from the start which thus allows the values of r in the block to be predetermined.

A parallel algorithm design to speed up the computation with (1.5) was proposed in Yusuph and Onumayi [5], and Onumayi et al [3]. Whether for parallel or sequential computations the issue of starting with Numerov method accurately has important consequence on the global error of the algorithms. For this reason Gonzalez and Thompson [6], obtained using Taylor series approach as a starting formula.

$$y_1 = y_0 + hy_0' + \frac{1}{24} h_0^2 (7 f_0 + 6 f_1 - f_2) \tag{1.8}$$

where (1.8) has a global error of $O(h_r^3)$. Yusuph and Onumanyi [5] sing multi-step collocation approach obtained the same formula (1.8). In this paper a report of quadratic polynomial that yields (1.5) at $x = x_{n+2}$, and a starting formula with error constant $C_5 = \frac{1}{45}$ (global error $O(h_r^3)$) is presented. Yusuph et al (2002) [5] and Gonzalez et al (1997) [6] reported similar schemes like (1.5) in magnitude using different concept, which made them differ.

2.0 Proposed multi-step collocation method for continuous approximation

Consider the construction of multi-step collocation methods for variable step-size h_r

and seek a method of the form,

$$y(x) \cong U(x) = \sum_{r=0}^{t-1} \phi_r(x) y_{n+r} + h^2 \sum_{r=0}^{m-1} \Psi_r(x) f_{n+r} \tag{2.1}$$

where $x \in [x_n, x_{n+k}]$ and introduce the following notations. The positive integer $k = 2$ denotes the step number of the method (2.1), M > 0 is the number of distinct collocation points used and t is the number of interpolation points used $2 \le t \le k$. Values of k and M are arbitrary except for collocation at the mesh points only.

Let $U(x_{n+r}) \approx y_{n+r} = y(x_{n+r}),\ r = 0,...,k-1$. Then a k-step multi-step collocation method with m collocation points is constructed using (2.1) which yeild a polynomial U(x) of degree $p = t + m - 1$ and such that it satisfies the conditions,

$$y(x_{n+r}) = y_{n+r},\ r \in [0,...,t-1] \tag{2.2}$$

$$U''(\overline{x}) = f_{n+r} \quad r = 0,...m-1$$

where f_{n+r} denote $f[\overline{x}_r, U(\overline{x}_r)]$, $\phi_r(x)$ *and* $\psi_r(x)$ are assumed polynomial basis func-tions.

$$\phi_r(x) = \sum_{i=0}^{t+m-1} \phi_{i+1,r} P_i(x),\ r \in (0,1..t-1) \tag{2.3}$$

and

$$h^2\psi_r(x) = \sum_{i=0}^{t+m-1} h^2\psi_{i+1,r} P_i(x),\ r = 0,1..m-1 \tag{2.4}$$

The collocation points are $x_r \in Q$, $Q = \{x_n, ...x_{n+k}\} \cup \{x_{n+k-1}, ...x_{n+k}\}$.

The constants $\phi_{i+1,r}$ *and* $h^2\psi_{i+1,r}$ are undetermined element of the following $(t+m)\times(t+m)$ dimensional matrix

$$C = \begin{pmatrix} \phi_{1,0} & \phi_{1,1} & \phi_{1,t-1} & h^2\psi_{1,0} & . & h^2\psi_{1,m-1} \\ \phi_{2,0} & \phi_{2,1} & \phi_{2,t-1} & h^2\psi_{2,0} & . & h^2\psi_{2,m-1} \\ . & . & . & . & . & . \\ \phi_{i+1,0} & \phi_{i+1,1} & \phi_{i+1,i-1} & h^2\psi_{i+1,0} & . & h^2\psi_{i+1,m-1} \\ . & . & . & . & . & . \\ \phi_{t+m,0} & \phi_{t+m,1} & \phi_{t+m,t-1} & h^2\psi_{t+m,0} & . & h^2\psi_{t+m,m-1} \end{pmatrix} \tag{2.5}$$

where $i = 0,1,...,t+m-1$, in (2.5). we define the following vectors

$$v = (y_n, y_{n+1},..., y_{n+t-1}, f_n, f_{n+1},..., f_{n+m-1})^T$$

$$p(x) = (p_0(x), p_1(x),..., p_{t+m-1}(x))^T$$

where $p(x)$ denotes an arbitrary function and T denote the 'transpose' of. The matrix M defined by

$$M = \begin{pmatrix} p_0(x_n) & . & . & p_{t+m-1}(x_n) \\ p_0(x_{n+1}) & . & . & p_{t+m-1}(x_{n+t}) \\ p_0(x_{n+t-1}) & . & . & p_{t+m-1}(x_{n+t-1}) \\ p_0''(\overline{x}_0) & . & . & p_{t+m-1}''(\overline{x}_0) \\ p_0''(\overline{x}_1) & . & . & p_{t+m-1}''(\overline{x}_1) \\ p_0''(\overline{x}_{m-1}) & . & . & p_{t+m-1}''(\overline{x}_{m-1}) \end{pmatrix} \qquad (2.6)$$

is assumed non-singular.

3.0 Numerov method from the quadratic polynomial solution

We consider the parameter specifications

$p_i(x) = x^i,\ i = 0,1,2,3,4.\ k = 2,\ t = 3\ \ m = 2,\ \{x_n, x_{n+1}, x_{n+2}\}$ as the interpolation points $\{x_n, x_{n+1}\}$ as the collocation points. $v = (y_n, y_{n+1}, y_{n+2}, f_n, f_{n+1})^T$

$$M = \begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & x_{n+1}^4 \\ 1 & x_{n+2} & x_{n+2}^2 & x_{n+2}^3 & x_{n+2}^4 \\ 0 & 0 & 2 & 6x_n & 12x_n^2 \\ 0 & 0 & 2 & 6x_{n+1} & 12x_{n+1}^2 \end{pmatrix} \qquad (3.1)$$

Hence,

$$\begin{aligned} U(x) = {} & \frac{\left[3(x-x_{n+1})^4 + 6h(x-x_{n+1})^3 - 9h^3(x-x_{n+1})\right]}{6h^4} y_n + \frac{\left[-3(x-x_{n+1})^4 - 6h(x-x_{n+1})^3 - 6h^3(x-x_{n+1})\right]}{3h^4} y_{n+1} \\ & + \frac{\left[3(x-x_{n+1})^4 + 6h(x-x_{n+1})^3 - 3h^3(x-x_{n+1})\right]}{6h^4} y_{n+2} + \frac{\left[-(x-x_{n+1})^3 + h^2(x-x_{n+1})\right]}{6h^2} f_n \\ & + \frac{\left[-3(x-x_{n+1})^4 - 5h(x-x_{n+1})^3 + 3h^2(x-x_{n+1})^2 + 5h^3(x-x_{n+1})\right]}{6h^2} f_{n+1} \end{aligned} \qquad (3.2)$$

Differentiating (3.2) twice, we obtain

$$\begin{aligned} U''(x) = {} & \frac{\left[36(x-x_{n+1})^2 + 36h(x-x_{n+1})\right]}{6h^4} y_n + \frac{\left[-36(x-x_{n+1})^2 - 36h(x-x_{n+1})\right]}{3h^4} y_{n+1} \\ & + \frac{\left[36(x-x_{n+1})^2 + 36h(x-x_{n+1})\right]}{6h^4} y_{n+2} + \frac{\left[-6(x-x_{n+1})\right]}{6h^2} f_n \\ & + \frac{\left[-36(x-x_{n+1})^2 - 30h(x-x_{n+1}) + 6h^2\right]}{6h^2} f_{n+1} \end{aligned} \qquad (3.3)$$

Equation (3.3) is the degree-two polynomial equation for the continuous approximation which when evaluated at $x = x_{n+2}$ yield the scheme

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{12}\{f_{n+2} + 10f_{n+1} + f_n\}, \quad C_6 = \frac{-1}{240},$$

popularly called the Numerov method.

If we also consider the first derivative function derived from the continuous method (3.2) we have

$$\frac{du(x)}{dx} = z(x), \quad \frac{du(a)}{dx} = z_0 \tag{3.4}$$

Thus we obtained from the second equation in (3.4) and (3.2)

$$z_0 = hy'(x_0) = -\frac{1}{2}y_0 + \frac{1}{2}y_2 - \frac{h^2}{3}\{f_0 + 2f_1\} \tag{3.5}$$

with global error $O(h^3 r)$, and an error constant $C_5 = -\frac{1}{45}$. To start the IVP on the sub-interval $[x_0, x_2]$, we combine (1.5) (Numerov method) when $r = n = 0$ together with (3.5), and then obtain

$$\left.\begin{aligned} y_2 - 2y_i + y_0 &= \frac{h^2}{12}(f_2 + 10f_1 + f_0) \\ hz_0 + \frac{1}{2}y_0 + \frac{1}{2}y_2 &= -\frac{h^2}{3}(f_0 + 2f_1) \end{aligned}\right\} \qquad 3.6)$$

where the form (3.6) has order three given by $[4, 3]^T$ and an error constant

$$\begin{pmatrix} \frac{-1}{240} = C_6 \\ \frac{-1}{45} = C_5 \end{pmatrix}$$

It is thus convergent and simultaneously provides values for y_1 *and* y_2 without looking for any other method to provide y_1. Hence this is an improvement over the use of (1.5) singly for IVP.

4.0 Application of Numerov method to $y'' = f(x,y,y')$

As an extension to application of Numerov method discussed extensively in [1, 3, 5] and in section3.0 of this paper. We shall now consider the more general form of second order ODEs (1.3). The solution to a two-point boundary valued program such as that given above by (1.2) and (1.3), involves seeking the solution at the points $x_i = x_0 + ih$, for $i = 1, 2, \ldots r-1$ and with $x_0 \equiv a,\ x_r \equiv b;\quad h = \frac{b-a}{r}$.

Let the approximate value of the require functions $y(x)$ and its derivative $y'(x)$ at point x_i be y_i' and y' respectively. Simply replace approximately the derivatives $y_i'(x),\ i = 0,1,\ldots n-2$ at each interior point in the proposed methods by the finite difference relations given below.

Central difference formula

$$6hy_i' = y_{i-1} - 8y_{i-1/2} + 8y_{i-1/2} - y_{i+1},\ O(h^4),\ C_5 = \frac{1}{288} \tag{4.1}$$

Backward Difference Formula

$$6hy_i' = 3y_{i-2} - 16y_{i-3/2} + 36y_{i-1} - 48y_{i-1/2} + 25y_i,\ O(h^4),\ C_5 = -\frac{1}{80} \tag{4.2}$$

Forward Difference Formula

$$6hy_i' = -25y_{i-2} + 48y_{i-1/2} - 36y_{i-1} + 16y_{i-3/2} - 3y_{i+2},\ O(h^4),\ C_5 = -\frac{1}{80} \tag{4.3}$$

(cf: Yahaya and Onumayi [7]). Thus, obtain a transformation of the form

$$y_{r+2} - 2y_{r+1} + y_r = \frac{h^2}{12}\{ f_{r+2} + 10 f_{r+1} + f_r \}$$

to the derivative form

$$y_{r+2} - 2y_{r+1} + y_r = \frac{h^2}{12}\{ y'_{r+2} + 10 y'_{r+1} + y'_r \}$$

while y'_{r+2}, y'_{r+1} *and* y'_r will be approximately replaced with either (4.1) or (4.2) or (4.3). the resulting systems also in block form. The direct solution of the resulting difference system of equation can be done using any of the methods developed specifically for solving system of such kind. Although, In Our Case, Microsoft Excel was used.

5.0 Numerical examples

To test the numerical efficiency of our schemes, presented here are some numerical results. First problem considered is a singular perturbation boundary value problem, while the second is an unperturbed initial value problem in the general equation form (1.3).

***Example* 1**

$$\varepsilon y'' = y'$$

$$y(0) = 0, \ \ y(1) = 1, \ \ with \ \ \varepsilon = 0.1, \ \ h = 0.1 \qquad (5.1)$$

$$y(x) = \frac{e^{-\frac{x}{\varepsilon}-1}}{e^{-\frac{1}{\varepsilon}-1}}$$

Table1: Numerical solution to problem (5.1) (theoretical and approximate solutions)

X	**Exact Solution** $y(x)$	**Numerov Block** $y_2(x)$	**Exact Error (** $y_2(x)$ - $y(x)$ **)**
0	0	0	0
0.1	0.6321492584	0.6197084753	1244 x10^{-5}
0.2	0.8647039743	0.8558765362	883 x10^{-5}
0.3	0.9502560732	0.9453610404	490 x10^{-5}
0.4	0.9817289315	0.9792544965	247 x10^{-5}
0.5	0.9933071491	0.9920991481	121 x10^{-5}
0.6	0.9975665373	0.9969665768	60 x10^{-5}
0.7	0.9991334786	0.9988110731	32x10^{-5}
0.8	0.9997099241	0.9995106981	20 x10^{-5}
0.9	0.9999219866	0.9997884563	13x10^{-5}
1.0	1.0	1.0	0

***Example* 2**

Also solve here the problem (IVP)

$$y'' + y' = 0$$

$$y(0) = 2, \ \ y'(0) = 1, \ \ h = 0.1 \qquad (5.2)$$

$$y(x) = 3 - e^{-x}$$

Table2: Numerical solution to problem (5.2) (theoretical and approximate solutions)

X	**Exact Solution** $y(x)$	**Numerov Block** $y_2(x)$	**Exact Error (** $y_2(x) - y(x)$**)**
0	2.0	2.0	2.0
0.1	2.095162582	2.0951643165	173.4×10^{-8}
0.2	2.181269247	2.1812726181	343.4×10^{-8}
0.3	2.259181797	2.2591867846	500.5×10^{-8}
0.4	2.329678854	2.3296864006	644.6×10^{-8}
0.5	2.39346934	2.3934771098	776.9×10^{-8}
0.6	2.451188364	2.4511973472	898.3×10^{-8}
0.7	2.503414696	2.5034247931	1009.7×10^{-8}
0.8	2.550671036	2.5506821542	1111.8×10^{-8}
0.9	2.59343034	2.5934424042	1206.2×10^{-8}
1.0	2.632120559	2.6321335595	1300×10^{-8}

6.0 Conclusion

A considerable literature exists for the conventional k-step linear multi-step methods (LMM) for the discrete solution of ordinary differential equations (ODEs) of the form (1.1)-(1.3). Interestingly, no known methods of LMM for (1.1) - (1.2) that can handle (1.3). This however, does not becloud their usefulness.

Method (3.6) as proposed in section (4.0) has substantial advantage as can be seen in numerical results. Table1and 2 is a successful application of Numerov method to the general form of second order ODEs. In the sense of backward differentiation formula BDF Numerov method have been converted to continuous solution form. This is indeed an improvement.

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