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# FINITE DIFFERENCE METHOD FOR A SECOND-ORDER ORDINARY DIFFERENTIAL EQUATION WITH A BOUNDARY CONDITION OF THE THIRD KIND

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**Abstract** — We present a second-order finite difference method for obtaining a solution of a second order two-point boundary value problem subject to Sturm's boundary conditions. We use equidistant discretization points, and the discretization of the differential equation at an interior point is based on just two evaluations of the function. Numerical examples are considered and the convergence of the proposed method is proved computationally.

**2000 Mathematics Subject Classification:** 65L10.
**Keywords:** finite differences, boundary value problem, second-order discretization, energy equation of solid explosive.

## 1. Introduction

Consider the second-order nonlinear two-point boundary value problem

$$y'' = f(x, y, y'), \quad x \in [0, 1] \tag{1.1}$$

subject to Sturm's boundary conditions

$$y'(0) = \alpha, \tag{1.2}$$

$$\beta y(1) + y'(1) = \gamma, \tag{1.3}$$

where $\alpha, \beta$ and $\gamma$ are constants.

Some references [7, 8] contain a theorem that detail the conditions for the existence and uniqueness of solutions of high order boundary value problems. However, for simplicity we assume that

$$f \in C^{\infty}(I \times \mathbb{R} \times \mathbb{R}), \quad \text{both } \frac{\partial f}{\partial y}, \ \frac{\partial f}{\partial y'} \ \text{ exist, continuous and}$$

$$\frac{\partial f}{\partial y} > 0, \quad \left|\frac{\partial f}{\partial y'}\right| \leqslant W \ \text{ for some positive contant } \ W.$$

These conditions ensure the existence of a unique solution to reference boundary value problem [9].

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In the literature on numerical analysis, various methods for solving linear and non-linear boundary value problems when solutions cannot be obtained analytically, are available. One of the methods is the iterative method that involves the iterative process. Iterative methods such as the finite difference method [10–12], the shooting method [13, 14], the method of exact and truncated (of arbitrary order of accuracy defined by the user) difference schemes [15] and the integral equation method [13, 16, 17] have been developed for obtaining approximate solutions to the boundary value problems. Recently a finite difference scheme for second-order boundary value problems with a third boundary condition was reported in [18].

The aim of the present paper is to construct a second-order difference scheme for computing the derivative of the solution of (1.1) at equidistant discretizaion points in such a way that the discretization of the differential equation at each interior point is based on only two evaluations of $f$. However, to achieve this result, it was neccesary to discretize the differential equation for its solution, which is required as an intermediate result for the above problem. There are difficulties in obtaining a numerical solution for some classes of singular problems. We discuss the application of the proposed methods to one such singular problem. In section 2, we describe the finite difference method. In section 3, we obtain local truncation errors. In section 4, we consider numerical examples to illustrate the method. Our results show second order convergence for both the solution and the derivative of the solution.

## 2. Difference scheme

Let us now introduce the notation. In order to compute a numerical approximation of the solution $y(x)$ and its derivative $y'(x)$, we first divide the interval $[0,1]$ into $2N$ subintervals of length $h = 1/2N$. Let $i$ be a positive integer, at each point $x_i = (i-1)h$, $i = 1, 2, \dots, 2N+1$, we replace the differential equation (1.1) by difference equations at $x_{i-1/2} \in (0,1)$. Let us denote the value of the exact solution $y(x)$ at point $x_{i-1/2}$ by $y_{i-1/2}$ and continue in the same way for $y'(x)$. $y''(x)$, $f(x, y(x), y'(x))$ etc. The difference equations for $y_{i-1/2}$, $y'_{i-1/2}$ of problem (1.1) at point $x_{i-1/2}$ are defined [2] as

$$-y_{i-1/2} + y_{i+1/2} = hy'_{i-1} + \frac{h^2}{24}(23f_{i-1/2} + f_{i+1/2}) + s_i, \quad i = 1,$$

$$y_{i-3/2} - 2y_{i-1/2} + y_{i+1/2} = h^2 f_{i-1/2} + s_i, \quad 2 \leqslant i \leqslant N-1,$$

$$y_{i-5/2} - (\beta h + 4)y_{i-3/2} + 3(\beta h + 1)y_{i-1/2} = 2h(\beta y_i + y'_i)\times$$

$$\frac{-h^2}{24}[(3\beta h - 22)f_{i-3/2} + (15\beta h + 46)f_{i-1/2}] + s_i, \quad i = N, \tag{2.1}$$

and

$$3y'_{i-1/2} + y'_{i+1/2} = 4y'_{i-1} + 3hf_{i-1/2} + t_i, \quad i = 1,$$

$$-y'_{i-3/2} + y'_{i-1/2} = \frac{h}{2}(f_{i-3/2} + f_{i-1/2}) + t_i, \quad 2 \leqslant i \leqslant N, \tag{2.2}$$

where the terms $s_i$ and $t_i$ are

$$s_i = \begin{cases} \dfrac{h^4}{48}[y^{iv}(x_{i-1/2}+\gamma_i h) - y^{iv}(x_{i-1/2}+\theta_i h) - \\ 2y^{iv}(x_{i-1/2}+\delta_i h)], & i=1, \quad 0<\theta_i,\gamma_i,\delta_i<1, \\ \dfrac{h^4}{24}[-y^{iv}(x_{i-1/2}-\theta_i h) - y^{iv}(x_{i-1/2}+\delta_i h)], & 0<\theta_i,\delta_i<1, \quad 2\leqslant i\leqslant N-1, \\ \dfrac{h^4}{384}[-128y^{iv}(x_{i-1/2}-2h\delta_i) + \\ 8(\beta h+4)y^{iv}(x_{i-1/2}-h\gamma_i) + h\beta y^{iv}(x_{i-1/2}+\frac{h}{2}\theta_i) + \\ 8y^{iv}(x_{i-1/2}+\frac{h}{2}\alpha_i) - 8(3\beta h-22)y^{iv}(x_{i-1/2}-\varphi_i h)], & 0<\theta_i,\alpha_i,\gamma_i,\delta_i,\varphi_i<1, \quad i=N, \end{cases} \tag{2.3}$$

and

$$t_i = \begin{cases} \dfrac{-h^3}{12}[2y^{iv}(x_{i-1/2}+\alpha_i h) + y^{iv}(x_{i-1/2}-b_i h)], & 0<\alpha_i,b_i<1, \quad i=1, \\ \dfrac{h^3}{12}[-2y^{iv}(x_{i-1/2}-a_i h) + 3y^{iv}(x_{i-1/2}-b_i h)], & 0<a_i, \quad b_i<0, \quad 2\leqslant i\leqslant N. \end{cases} \tag{2.4}$$

Neglect the terms $s_i$ and $t_i$ in (2.1) and (2.2) respectively and solve the reduced system of equations for $y_{i-1/2}$, $y'_{i-1/2}$ by some advanced methods known in the literature (see [3–5]). Let $u_{i-1/2}, u'_{i-1/2}$ be an approximate value of $y_{i-1/2}$ and $y'_{i-1/2}$ for $i=1,2,\dots N$ respectively. We have values of $u_{1/2}$, $u_{3/2}, \dots$ and $u'_{1/2}$, $u'_{3/2}, \dots$ which will help us in computing approximate values $u_{i-1}, u'_{i-1}$ of $y_{i-1}, y'_{i-1}$, $i=1,2,3,\dots,N+1$ by the second-order interpolation

$$u_{i-1} = \begin{cases} u_{i-1/2} + \dfrac{h}{2}y'_{i-1}, & i=1, \\ \dfrac{1}{2}(u_{i-1/2}+u_{i-3/2}), & i=2,3,\dots N, \\ \dfrac{1}{2}(3u_{i-3/2}-u_{i-5/2}), & i=N+1, \end{cases} \tag{2.5}$$

and

$$u'_{i-1} = \begin{cases} \dfrac{1}{2}(u'_{i-1/2}+u'_{i-3/2}), & i=2,3,4,\dots,N, \\ \dfrac{1}{2}(3u'_{i-3/2}-u'_{i-5/2}), & i=N+1. \end{cases} \tag{2.6}$$

**2.1. Development of the difference method.** We use Taylor series and the undetermined coefficient method to introduce the difference equation in place of the differential equation (1.1).

Consider an expression of the form

$$a_0 y_{1/2} + a_1 y_{3/2} = hb_0 y'_0 + h^2(c_0 f_{1/2} + c_1 f_{3/2}). \tag{2.7}$$

Expand the terms (2.7) in a Taylor series about $y_{1/2}$ and replace $f_{1/2}$ by $y''_{1/2}$ etc. Now, comparing the coefficients of $h^p$ for $p=0,1,2,3$ on both sides and solving the thus obtained system of equations, we have

$$(a_0,a_1,b_0,c_0,c_1) = (-1,1,1,23/24,1/24). \tag{2.8}$$

Thus (2.7) can be rewritten as

$$-y_{1/2} + y_{3/2} = hy_0' + \frac{h^2}{24}(23f_{1/2} + f_{3/2}) + s_1 \tag{2.9}$$

and

$$s_1 = \frac{h^4}{48}[y^{iv}(x_{1/2} + \gamma_1 h) - y^{iv}(x_{1/2} + \theta_1 h) - 2y^{iv}(x_{1/2} + \delta_1 h)], \quad 0 < \gamma_1, \theta_1, \delta_1 < 1.$$

A similar procedure can be applied to obtain the other equations in (2.1) and (2.2).

**2.2. Application.** Consider the energy equation governing the temperature distribution in the explosion of a solid explosive, which can be written in terms of dimensionless variables [6] as

$$y'' + \frac{2}{x}y' + \alpha \exp\left(\frac{y}{1 + y/\beta}\right) = g(x) \tag{2.10}$$

subject to the boundary conditions

$$\frac{dy(0)}{dx} = 0, \quad N_{nu}y(1) + \frac{dy(1)}{dx} = 0, \tag{2.11}$$

where $N_{nu}$ is the Nusselt number and $\alpha, \beta$ are parameters. The force function $g(x)$ in the energy equation [1] vanishes identically for $0 \leqslant x \leqslant 1$. Problem (2.10) can not be solved either by the available methods in its present form or needs special attention due to the presence of the term $2y'/x$ at $x = 0$. The difference methods (2.1) and (2.2) do not require any special attention when used to solve (2.10) at the origine to get either the solution or the derivative of the solution.

Thus, we have obtained solutions to problem (2.10) at $x = 0$, without loosing the order and accuracy in computing $y$ and $y'$.

## 3. Local truncation error

Let $y^p(x)$ assume extreme values in $[0, 1]$ for $p = 0, 1, 2, \dots$, say

$$\max_{0 \leqslant x \leqslant 1} |y^p(x)| = M_p \quad \text{and} \quad \min_{0 \leqslant x \leqslant 1} |y^p(x)| = m_p.$$

Since $p = 4$, we have from (2.3)

$$\begin{cases} \dfrac{-h^4}{24} m_4 \leqslant |s_i| \leqslant \dfrac{h^4}{12} M_4, & i = 1, \\ \dfrac{-h^4}{12} m_4 \leqslant |s_i| \leqslant \dfrac{h^4}{12} M_4, & 2 \leqslant i \leqslant N-1, \\ \dfrac{h^4}{384}(88 - 15\beta h) m_4 \leqslant |s_i| \leqslant \dfrac{h^4}{384}(33\beta h - \delta) M_4, & i = N. \end{cases} \tag{3.1}$$

Let

$$s = \min_{1 \leqslant i \leqslant N-1} |s_i|, \quad M = \max\left(M_4, \frac{33\beta h - 8}{32} M_4\right), \quad m = \max\left[m_4, \frac{88 - 15\beta h}{16} m_4\right].$$

Thus,

$$\begin{cases} \dfrac{-mh^4}{24} \leqslant s \leqslant \dfrac{h^4}{12}M, \\ \dfrac{-mh^4}{12} \leqslant s \leqslant \dfrac{h^4}{12}M, \\ \dfrac{-mh^4}{24} \leqslant s \leqslant \dfrac{h^4}{12}M. \end{cases} \tag{3.2}$$

Thus, we conclude that the local truncation error associated with(2.3) is

$$\frac{-mh^4}{24} \leqslant s \leqslant \frac{h^4}{12}M. \tag{3.3}$$

So, using similar arguments and defining $t = \min_{2\leqslant i\leqslant N-1} |t_i|$, we can estimate the local truncation error associated with (2.4) as

$$\frac{-h^3}{12}m_4 \min\{3,-1\} \leqslant t \leqslant \frac{h^3}{12}M_4 \max\{3,5\}, \quad \frac{h^3}{12}m_4 \leqslant t \leqslant \frac{5}{12}h^3 M_4.$$

Thus, we conclude that the local truncation error associated with our method is $o(h^4)$. So, we have estimated the order of methods (2.1) and (2.2) as $O(h^2)$.

## 4. Numerical results

To illustrate the computational potency and order of the method, we have solved the following nonlinear two-point boundary value problems.

**Problem 1.** Consider the energy equation (2.10) with $N_{nu} = \alpha = 1.0$ and $\beta = 0.1$. Thus

$$y'' + \frac{2}{x}y' + \exp\left(\frac{y}{1+10y}\right) = g(x)$$

and the boundary conditions are $y'(0) = 0$ and $y(1) + y'(1) = 0$, with the exact solution

$$y(x) = \cosh\left(\frac{x}{\pi}\right) - \left[\cosh\left(\frac{1}{\pi}\right) + \frac{1}{\pi}\sinh\left(\frac{1}{\pi}\right)\right]\frac{x^2}{3}$$

and the maximum absolute errors for $y, y'$ are given in Table 4.1.

Table 4.1

| | $h$ | | | | | |
|---|---|---|---|---|---|---|
| | 8 | 16 | 32 | 64 | 128 | 256 |
| $y$ | .127746(-2) | .318537(-3) | .795582(-4) | .198826(-4) | .496979(-5) | .124234(-5) |
| $y'$ | .216884(-4) | .581626(-5) | .150379(-5) | .382184(-6) | .963266(-7) | .241793(-7) |

**Problem 2** (Reactor design). Consider the isothermal packed-bed reactor. The governing differential equation [1]

$$\frac{1}{N_{pe}}\frac{d^2y}{dx^2} + \frac{dy}{dx} - Ry^n = g(x)$$

is subject to the boundary conditions

$$y'(0) = 0, \quad y(1) + \frac{1}{N_{pe}} \frac{dy(1)}{dx} = 1.$$

Maximum absolute errors in both $y$ and $y'$ for different values of $N_{pe}$, order $n$ of reaction and the range of values of $R$ with the exact solution

$$y(x) = N_{pe} e^{(x^2 - x^3)} / (N_{pe} - 1.0)$$

are given in Table 4.2.

Table 4.2

| | h | | | | | |
|---|---|---|---|---|---|---|
| | 8 | 16 | 32 | 64 | 128 | 256 |
| | $N = 1,\ R = 1,\ N_{pe} = 2$ | | | | | |
| $y$ | .116733(-1) | .339170(-2) | .931260(-3) | .245032(-3) | .629093(-4) | .159420(-4) |
| $y'$ | .309695(-1) | .828688(-2) | .269651(-2) | .753022(-3) | .198104(-3) | .507542(-4) |
| | $N = 2,\ R = 1/8,\ N_{pe} = 2$ | | | | | |
| $y$ | .136306(-1) | .402905(-2) | .111447(-2) | .294187(-3) | .756419(-4) | .191822(-4) |
| $y'$ | .31777(-1) | .777896(-2) | .251621(-2) | .704275(-3) | .185440(-3) | .475274(-4) |
| | $N = 2,\ R = 1/8,\ N_{pe} = 4$ | | | | | |
| $y$ | .734833(-2) | .219308(-2) | .611578(-3) | .162298(-3) | .418562(-4) | .106314(-4) |
| $y'$ | .210407(-1) | .519106(-2) | .143203(-2) | .400509(-3) | .105374(-3) | .269939(-4) |
| | $N = 2,\ R = 1/8,\ N_{pe} = 6$ | | | | | |
| $y$ | .593756(-2) | .178032(-2) | .498000(-3) | .132456(-3) | .342071(-4) | .869510(-5) |
| $y'$ | .186833(-1) | .461761(-2) | .115384(-2) | .323188(-3) | .850697(-4) | .217963(-4) |
| | $N = 2,\ R = 1/8,\ N_{pe} = 8$ | | | | | |
| $y$ | .531787(-2) | .159943(-2) | .447948(-3) | .119274(-3) | .308258(-4) | .783901(-5) |
| $y'$ | .176005(-1) | .435189(-2) | .107760(-2) | .282273(-3) | .743814(-4) | .190671(-4) |
| | $N = 2,\ R = 1/8,\ N_{pe} = 10$ | | | | | |
| $y$ | .497198(-2) | .149877(-2) | .419886(-3) | .111857(-3) | .289213(-4) | .735668(-5) |
| $y'$ | .169661(-1) | .149515(-2) | .103960(-2) | .258824(-3) | .657145(-4) | .173174(-4) |
| | $N = 2,\ R = 1/4,\ N_{pe} = 2$ | | | | | |
| $y$ | .113589(-1) | .329487(-2) | .904056(-3) | .237801(-3) | .610442(-4) | .154682(-4) |
| $y'$ | .309633(-1) | .841952(-2) | .273273(-2) | .762334(-3) | .200454(-3) | .513440(-4) |
| | $N = 2,\ R = 1/4,\ N_{pe} = 4$ | | | | | |
| $y$ | .651908(-2) | .191194(-2) | .529367(-3) | .140049(-3) | .360677(-4) | .915501(-5) |
| $y'$ | .206409(-1) | .503522(-2) | .154020(-2) | .429007(-3) | .112672(-3) | .288398(-4) |
| | $N = 2,\ R = 1/4,\ N_{pe} = 6$ | | | | | |
| $y$ | .537483(-2) | .158355(-2) | .439815(-3) | .116623(-3) | .300763(-4) | .764010(-5) |
| $y'$ | .184036(-1) | .449815(-2) | .123746(-2) | .344810(-3) | .905508(-4) | .231751(-4) |
| | $N = 2,\ R = 1/4,\ N_{pe} = 8$ | | | | | |
| $y$ | .486327(-2) | .143738(-2) | .399720(-3) | .106105(-3) | .273842(-4) | .695928(-5) |
| $y'$ | .173753(-1) | .424901(-2) | .107646(-2) | .300433(-3) | .789409(-4) | .202083(-4) |
| | $N = 2,\ R = 1/4,\ N_{pe} = 10$ | | | | | |
| $y$ | .457485(-2) | .13552(-2) | .377094(-3) | .100146(-3) | .258569(-4) | .657288(-5) |
| $y'$ | .167698(-1) | .410117(-2) | .100876(-2) | .271769(-3) | .714711(-4) | .183031(-4) |

Table 4.2 (continuation)

| | $h$ | | | | | |
|---|---|---|---|---|---|---|
| | 8 | 16 | 32 | 64 | 128 | 256 |
| | $N=2,\ R=1/2,\ N_{pe}=2$ | | | | | |
| $y$ | .919069(-2) | .258613(-2) | .699456(-3) | .182760(-3) | .467660(-4) | .118319(-4) |
| $y'$ | .308069(-1) | .925305(-2) | .298050(-2) | .829390(-3) | .217865(-3) | .557779(-4) |
| | $N=2,\ R=1/2,\ N_{pe}=4$ | | | | | |
| $y$ | .560005(-2) | .159443(-2) | .435501(-3) | .114496(-3) | .293993(-4) | .745159(-5) |
| $y'$ | .205184(-1) | .527183(-2) | .169422(-2) | .469866(-3) | .123167(-3) | .314976(-4) |
| | $N=2,\ R=1/2,\ N_{pe}=6$ | | | | | |
| $y$ | .473275(-2) | .135286(-2) | .370646(-3) | .976598(-4) | .251097(-4) | .636904(-5) |
| $y'$ | .183562(-1) | .443447(-2) | .136721(-2) | .378588(-3) | .991375(-4) | .253379(-4) |
| | $N=2,\ R=1/2,\ N_{pe}=8$ | | | | | |
| $y$ | .453602(-2) | .124403(-2) | .341283(-3) | .900167(-4) | .231608(-4) | .587712(-5) |
| $y'$ | .173679(-1) | .419484(-2) | .119289(-2) | .330221(-3) | .864408(-4) | .220879(-4) |
| | $N=2,\ R=1/2,\ N_{pe}=10$ | | | | | |
| $y$ | .454204(-2) | .118265(-2) | .324630(-3) | .856654(-4) | .220498(-4) | .559660(-5) |
| $y'$ | .167844(-1) | .405163(-2) | .107853(-2) | .298694(-3) | .781901(-4) | .199791(-4) |
| | $N=2,\ R=1,\ N_{pe}=2$ | | | | | |
| $y$ | .776711(-2) | .210709(-2) | .558552(-3) | .144477(-3) | .367851(-4) | .928354(-5) |
| $y'$ | .318494(-1) | .100172(-1) | .321820(-2) | .894854(-3) | .234992(-3) | .601547(-4) |
| | $N=2,\ R=1,\ N_{pe}=4$ | | | | | |
| $y$ | .545391(-2) | .134998(-2) | .361027(-3) | .939126(-4) | .239864(-4) | .606359(-5) |
| $y'$ | .211240(-1) | .589791(-2) | .188051(-2) | .519916(-3) | .136091(-3) | .347784(-4) |
| | $N=2,\ R=1,\ N_{pe}=6$ | | | | | |
| $y$ | .513568(-2) | .117371(-2) | .314619(-3) | .819802(-4) | .209605(-4) | .530171(-5) |
| $y'$ | .189659(-1) | .485760(-2) | .154112(-2) | .424422(-3) | .110849(-3) | .282945(-4) |
| | $N=2,\ R=1,\ N_{pe}=8$ | | | | | |
| $y$ | .502377(-2) | .115884(-2) | .293788(-3) | .766129(-4) | .195984(-4) | .495869(-5) |
| $y'$ | .180001(-1) | .432812(-2) | .135903(-2) | .373265(-3) | .973344(-4) | .248241(-4) |
| | $N=2,\ R=1,\ N_{pe}=10$ | | | | | |
| $y$ | .497196(-2) | .116215(-2) | .285459(-3) | .735705(-4) | .188256(-4) | .476402(-5) |
| $y'$ | .174359(-1) | .418582(-2) | .123788(-2) | .339344(-3) | .883880(-4) | .225286(-4) |
| | $N=3,\ R=1,\ N_{pe}=2$ | | | | | |
| $y$ | .101653(-1) | .238735(-2) | .578009(-3) | .142366(-3) | .353180(-4) | .879551(-5) |
| $y'$ | .356874(-1) | .109506(-1) | .353468(-2) | .984407(-3) | .258660(-3) | .662296(-4) |
| | $N=4,\ R=1,\ N_{pe}=2$ | | | | | |
| $y$ | .115181(-1) | .281011(-2) | .694618(-3) | .172706(-3) | .430783(-4) | .107557(-4) |
| $y'$ | .384888(-1) | .113277(-1) | .369512(-2) | .103314(-2) | .271914(-3) | .696751(-4) |

## 5. Conclusion

The goal of this paper was to outline a procedure for deriving finite difference schemes for a second-order boundary value problem which has a singularity at some point in the problem domain. The same procedure can be used to derive the finite difference scheme for a problem with a discontinuous solution. The boundary conditions are incorporated in a very simple way in the process of deriving difference schemes. The effectiveness of the schemes and the convergence rate have been estimated and confirmed from the numerical results. Though the schemes are simple, they cannot be implemented because the resulting system of algebraic equations cannot be solved easily by the known methods. To implement the schemes, we need special attention and some global convergent methods.

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