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Multiderivative methods for linear second order boundary value problems

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Abstract

Second, fourth and sixth order methods are developed and analysed for the numerical solution of linear second order boundary value problems.

The methods are developed by replacing the exponential terms in a three—point recurrence relation by Padé approximants.

The methods are tested on a problem from the literature.

1. INTRODUCTION

Consider the general linear, variable coefficient, second-order boundary value problem given by

$$y''(x) = f(x)y(x) + g(x) , \quad \alpha_0 < x < \alpha_1 \tag{1}$$

$$y(\alpha_0) = A_0 , \quad y(\alpha_1) = A_1 , \tag{2}$$

where α_0 ,α_1 ,A_0 ,A_1 are finite real constants. It will be assumed that a unique solution, y(x) , to (1) and (2) exists for $x \in [\alpha_0 ,\alpha_1]$ (for a discussion of existence and uniqueness to (1) and (2) see Henrici [8], for instance). It will further be assumed that f(x), g(x) and y(x) are sufficiently often differentiable with respect to x for $x \in [\alpha_0 ,\alpha_1]$,

The literature on the numerical solution of (1) with (2) is large. Collocation methods are discussed by, among others, Russell and Shampine [13]; shooting methods are discussed by Henrici [8] and Roberts and Shipman [12], for instance; the problem is solved using variational techniques in Burden *et al* [5]; and commonly used finite difference methods are discussed by many authors, see, for instance, Lambert [11]. Ahlberg *et al* [1] investigated the possibility of using spline functions to obtain a smooth solution to (1) with (2); following this spline functions were also used by Ahlberg and Ito [2], Albasiney and Hoskins [3], Bickley [4] Fyfe [6], Khalifa and Eilbeck [10], and Usmani and Warsi [16], Albasiney and Hoskins [3] particularly emphasized the connection between a cubic spline solution and the solution obtained using the well-known Numerov method. The book by Jain [9] gives an introduction to many of the above methods of solution.

In the present paper, multiderivative methods, based on a three-point recurrence relation, are developed, analysed and tested on a problem from the literature.

2. A RECURRENCE RELATION

Suppose the independent variable x is incremented using a constant step size $h = (\alpha_1 - \alpha_0)/(N+1)$ where N is a positive integer. The solution will be computed at the points $x_r = \alpha_0 + rh$ $(r = 1,2,...,N)$ and the notation y_r will be used to denote the solution of a numerical method at x_r (it is obvious that $y_0 = A_0$ and $y_{N+1} = A_1$).

It is convenient to consider the model equation

$$y''(x) = a^2 y(x) \quad , \quad \alpha_0 < x < \alpha_1 \tag{3}$$

together with the boundary conditions (2). The general solution of (3) has the form

$$y(x) = c_1 e^{ax} + c_2 e^{-ax} \tag{4}$$

where c_1 and c_2 are arbitrary constants, and it is easy to verify that (4) satisfies the recurrence relation

$$-y(x-h) + (e^{ah} + e^{-ah})y(x) - y(x+h) = 0 \ . \tag{5}$$

It is this three-point relation which forms the basis for the family of multiderivative methods for the solution of (1) with (2).

Using this relation, each numerical method will determine the solution vector $\underline{Y} = (y_1, y_2, ..., y_N)^T$, T denoting transpose, implicitly. The family of multiderivative methods arising from (5) will be developed by using Padé approximants to the exponential terms e^{ah} and e^{-ah}.For some scalar θ, the (M,K) Padé approximant to e^{θ} takes the form

$$e^{\theta} = P_K(\theta)/Q_M(\theta) + 0(\theta^{M+K+1}) \ ,$$

where $P_K(\theta)$ and $Q_M(\theta)$ are polynomials in θ of degrees K and M respectively. Using any such approximant in (5), and clearing all denominators, leaves powers of a which are multiples of two. This indicates that the right hand side of (1) and its second, fourth, sixth, etc., derivatives will appear in the resulting multiderivative method, higher order Padé approximants requiring higher derivatives of this right hand side.

Clearly, the need to differentiate the right hand side of (1) implies that y'(x) becomes involved- This derivative is estimated to the required accuracy by using enough terms of the appropriate backward, central, or forward differentiation formula given, for example, in the text by Gerald and Wheatley [7].

The local truncation error associated with the numerical method based on the (M,K) Pade approximant at the point $x = x_r$, takes the form

$$t_r \equiv t(x_r) = C_{p+2} h^{p+2} y^{(p+2)}(x_r) + c_{p+4} h^{p+4} y^{(p+4)}(x_r) + \ldots \qquad (6)$$

where $p = 2[½(M+K)]$. In the usual notation, p is the order of the multiderivative method and the C_q $(q = p+2, p+4, ,..)$ are constants; the leading term C_{p+2} is the error constant of the method. For consistency, $p \geq 1$ and so the methods based on the use of the (0,1) or (1,0) Padé approximants in (5) are inconsistent. The error constants for eleven of the multiderivative methods arising from various values of M and K are given in Table 1.

Table 1 here

All the numerical methods to be examined in the paper have the form

$$-\delta^2 y_r + h^2 \sum_{m=-1}^{1} a_m y''_{r+m} + h^4 \sum_{m=-1}^{1} a^*_m y^{(iv)}_{r+m} + h^6 \sum_{m=-1}^{1} a^{**}_m y^{(vi)}_{r+m} = 0, \; r = 1,2,..., N \qquad (7)$$

where δ^2 is the central difference operator defined by

$$\delta^2 y_r = y_{r-1} - 2y_r + y_{r+1} \; , \qquad (8)$$

and the $a_m, a^*_m, a^{**}_m (m=-1,0,1)$ are parmeters dependent upon the padé approximant chosen for use in (5). Equation (7) incorporates members of the family of multiderivative methods of orders two, four and six; for higher order methods, further even powers of h must be added.

3. SECOND ORDER METHODS

There are five second order methods in the family of multiderivative methods. Three of them, in fact, could also be classified as linear multistep methods (each has $a_m^* = a_m^{**} = 0$ for m =-1,0,1); furthermore the method based on the (0,2) Padé approximant is the classical linear multistep method

$$-y_{r-1} + 2y_r - y_{r+1} + h^2 y''_r = 0 \tag{9}$$

for which $C_4 = -\frac{1}{2}$

Looking at the error constants of each of the five second order methods of the family (Table 1), it is seen that the numerical methods based on the (1,2) and (2,1) Padé approximants are the most accurate. The parameters $a_m, a_m^* = a_m^{**}$ of equation (7) for the method bases on the (1,2) Pade approximant are given by

$$(a_{-1}, a_0, a_1) = (1,7,1)/9\ , \quad a_m^* = a_m^{**} = 0.(m = -1,0,1) \tag{10}$$

while a quick calculation shows that $a_{-1}^* = a_1^* \neq 0$ for the methid bases on the (2,1) Padé approximant. This indicates that, for the latter method, the second derivative of the right hand side of (1) is required and it may be concluded consequently that the (1,2) method is the most accurate and economic of the second order methods of the family arising from the recurrence relation (5).

Every method discussed in the paper may be written in matrix form as

$$(A+Q)\underline{Y} = \underline{b} \tag{11}$$

in which $Q = [q_{i,j}]$ $(i,j = 1,2,..,N)$ and $\underline{b} = (b_1, b_2, \ldots, b_N)^T$ are different for each method, and A is the well-known tridiagonal matrix given by

$$A = \begin{bmatrix} 7 & -1 & & & 0 \\ -1 & 7 & -1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot & \cdot \\ & 0 & & 1 & 7 & -1 \\ & & & & -1 & 7 \end{bmatrix}. \tag{12}$$

In the case of the method based on the (1,2) Pade approximant defined by (7), (8) and (10), the matrix Q has the form

$$Q = h^2 BF \tag{13}$$

in Which

$$B = \frac{1}{9}\begin{bmatrix} 7 & 1 & & & 0 \\ 1 & 7 & 1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot & \cdot \\ & 0 & & 1 & 7 & 1 \\ & & & & 1 & 7 \end{bmatrix} \tag{14}$$

and $F = \mathrm{diag}(f_r)$, with $f_r = f(x_r)$. The vector $\underline{b}$ for this numerical method is given by

$$\begin{aligned} b_1 &= (1 - \tfrac{1}{9}h^2 f_0)A_0 - \tfrac{1}{9}h^2(g_0 + 7g_1 + g_2), \\ b_r &= -\tfrac{1}{9}h^2(g_{r-1} + 7g_r + g_{r+1}), \quad r = 2,3,\ldots, N-1, \\ b_N &= (1 - \tfrac{1}{9}n^2 f_{N+1})A_1 - \tfrac{1}{9}h^2(g_{N-1} + 7g_N + g_{N+1}), \end{aligned} \tag{15}$$

where $g_r = g(x_r)$, $r = 0,1,\ldots,N+1$.

The vector $\underline{y} = (y(x_1), y(x_2), \ldots, y(x_N))^T$ satisfies

$$(A + Q)\underline{y} = \underline{b} + \underline{t}, \tag{16}$$

where $\underline{t} = (t_1, t_2, \ldots, t_N)^T$ is the vector of local truncation errors associated with a particular method. Defining $\underline{z}$ by $\underline{z} = \underline{y} - \underline{Y}$ it follows that $\underline{z}$ satisfies

$$(A + Q)\,\underline{z} = \underline{t} \tag{17}$$

so that

$$\|\underline{z}\| \leq \|A^{-1}\| . \|\underline{t}\| / (1 - \|A^{-1}\| . \|Q\|)\,, \tag{18}$$

in which the norm is the maximum norm.

It is well known that $\|A^{-1}\| = (\alpha_1 - \alpha_0)^2/(8h^2)$ and from (6) it is seen that $\|\underline{t}\| = 0(h^{p+2})$ for every member of the family of methods yielded by (5). It then follows that

$$\|\underline{z}\| = 0(h^p) \tag{19}$$

provided

$$\|A^{-1}\| . \|Q\| < 1\,. \tag{20}$$

In the case of the method based on the (1,2) Padé approximant $\|B\| = 1$ (in (14)) and $\|\underline{t}\| = 0(h^4)$, and so it follows from (20) that this method is second order convergent provided

$$\max_r |f_r| < 8t/(\alpha_1 - \alpha_0)^2\ . \tag{21}$$

4. FOURTH ORDER METHODS

There are nine Padé approximants to the exponential function which lead to fourth order methods. The error constants of three of these methods are given in Table 1. It is an easy exercise to derive the error constants of the other six methods; having done so it will be seen that these six methods are no more accurate than the three displayed in Table 1.

It is evident that the use of the (2,3) Padé approximant in the recurrence relation (5) leads to the multiderivative method with smallest modulus error constant. The parameters a_m, a_m^*, a_m^{**} (m=-1,0,1) for this method are given by

$$(a_{-1}, a_0, a_1) = (3,44,3)/50, (a_{-1}^*, a_0^*, a_1^*) = (-3,34,-3)/1200,$$
$$a_m^{**} = 0 \qquad (m = -1,0,1). \tag{22}$$

Nothing that $a_m^{**} \neq 0 (m = -1,0,1)$, it follows that the second derivative of the right hand side of equation (1) is required in the implementation of this multiderivative method. As noted in §1 this implies that y' is involved in the method. This derivative may be approximated by the finite difference replacements

$$\begin{aligned} y'_{r-1} &= (2h)^{-1}(-3y_{r-1} + 4y_r - y_{r+1}) + 0(h^2), \\ y'_r &= (2h)^{-1}(-y_{r-1} + y_{r-1}) + 0(h^2), \\ y'_{r+1} &= (2h)^{-1}(y_{r-1} - 4y_r + 3y_{r+1}) + 0(h^2), \end{aligned} \tag{23}$$

(see, for instance, Gerald and Wheatley [7]); in (23) r = 1,2,...,N.

After making these replacements wherever appropriate, the multi-derivative method based on the (2,3) Padé approximant takes the form (11) where, now,

$$Q = h^2 C_1 F + h^3 C_2 + h^4 C_3 \tilde{F}. \tag{24}$$

In (24), $F = \text{diag}(f_r)$ as before, $\tilde{F} = \text{diag}(\tilde{f}_r) = \text{diag}(f_r + f''_r)$

$$C_1 = \frac{1}{50}\begin{bmatrix} 44 & 3 & & & & 0 \\ 3 & 44 & 3 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & 3 & 44 & 3 \\ & 0 & & & 3 & 44 \end{bmatrix}, \tag{25}$$

$$C_2 = \frac{1}{1200}\begin{bmatrix} \psi_1 & \eta_1 & & & & 0 \\ \varphi_2 & \psi_2 & \eta_2 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & \varphi_{N-1} & \psi_{N-1} & \eta_{N-1} \\ 0 & & & & \varphi_N & \psi_N \end{bmatrix} \tag{26}$$

with

$$\varphi_r = 9f'_{r-1} - 34'_{r+1} - 3f'_{r+1}, \psi_r - -12f'_{r-1} + 12f'_{r+1}, \eta_r = 3f'_{r-1} \rightarrow 34f'_f - 9f'_{r+1},$$

and

$$C_3 = \frac{1}{1200}\begin{bmatrix} 34 & -3 & & & & 0 \\ -3 & 34 & -3 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & -3 & 34 & -3 \\ 0 & & & & -3 & 34 \end{bmatrix} \tag{27}$$

The vector $\underline{b}$ in (11) is now defined by

$$b_1 = (1 - \frac{3h^2}{50} f_0 - \frac{h^3}{1200}\varphi_0 + \frac{h^4}{400}\tilde{f}_0)A_0 - \frac{h^2}{50}(3g_0 + 44g_1 + 3g_2) - \frac{h^4}{1200}(3\tilde{g}_0 + 34\tilde{g}_1 - 3\tilde{g}_2),$$

$$b_r = -\frac{h^2}{50}(3g_{r-1} + 44g_r + 3g_{r+1}) - \frac{h^4}{1200}(-3\tilde{g}_{r-1} + 34\tilde{g}_r - 3\tilde{g}_{r+1})\ r = 2,\ldots,\ N-1 \tag{28}$$

$$b_N = (1 - \frac{3h^2}{50} fN + 1 - \frac{h^3}{1200}\eta_{N+1} + \frac{h^4}{400}\tilde{f}_{N+1})A_1 - \frac{h^2}{50}(3g_{N-1} + 44g_N + 3g_{N+1})$$
$$- \frac{h^4}{1200}(-3\tilde{g}_{N-1} + 34\tilde{g}_N - 3\tilde{g}_{N+1}),$$

where

$$\tilde{g}_r = f_r g_r + g'_r (r = 0,1,\ldots\ldots, N+1).$$

It is clear that

$$\| C_1 \| \le 1, \| C_2 \| \le \frac{29}{300} \max_r | f'_r |, \| C_3 \| \le \frac{1}{30} \tag{29}$$

and a standard convergence analysis reveals, from (20), that the multi-derivative method based on the (2,3) Padé approximant is second order convergent provided

$$\left(\alpha_1 - \alpha_0\right)^2 \left[300 \max_r | f_r | + 29h \max_r | f_r' | + 10h^2 \max_r | f_r | \right] < 2400. \qquad (29)$$

5. SIXTH ORDER METHODS

A check of the local truncation errors of the sixth order multi-derivative method yielded by (5) shows that the (3,4) and (4,3) Padé approximants lead to the methods with the smallest moduli error constants .The (3,4) method ,hoeener ,requires ,a team in $h^8 y^{(viii}_{r+3}$ on right hand side of (7) whereas the (3,4) method needs only terms up to and including $h^6 y^{(iv)}_{r+m}$ and so is easier to implement

The parameters for the method based on the (3,4) Padé approximant are given by

$$(a_{-1}, a_0, a_1) = (2, 45, 2,) / 49 , \quad (a^*_{-1}, a^*_0, a^*_1) = (-3, 131, -3) /2940,$$

$$(a^{**}_{-1}, a^{**}_0, a^{**}_1) = (2, 31, 3) / 88200. \qquad (30)$$

Nothing that $a^*_m \neq 0(m = -1,0,1)$ in (300), it follows that the second Derivative of the right hand side of (1) is required in the application of the method. The a^*_m(m=-1,0,1) are multiplied by h^4 and so,to match the overall $0(h^8)$ local truncation error of the method, the first derivatives of y (which arise in the second derivations of the right baiid side of (1)) must be replaced by $0(h^4)$ approximants. Such approximants are

$$\begin{aligned}
y'_r &= h^{-1}\left(-\frac{25}{12}y_r + 4y_{r+1} - 3y_{r+2} + \frac{4}{3}y_{r+3} - \frac{1}{4}y_{r+4}\right) + 0(h^4) \\
y'_r &= h^{-1}\left(-\frac{1}{4}y_{r-1} - \frac{5}{6}y_r + \frac{3}{2}y_{r-1} - \frac{1}{2}y_{r+2} + \frac{1}{12}y_{r+3}\right) + 0(h^4), \\
y'_r &= h^{-1}\left(\frac{1}{12}y_{r-2} - \frac{2}{3}y_{r-1} + \frac{2}{3}y_{r+1} - \frac{1}{12}y_{r+2}\right) + 0(h^4), \qquad (31) \\
y'_r &= h^{-1}\left(-\frac{1}{12}y_{r-3} + \frac{1}{2}y_{r-2} - \frac{3}{2}y_{r-1} + \frac{5}{6}y_r + \frac{1}{4}y_{r+1}\right) + 0(h^4), \\
y'_r &= h^{-1}\left(\frac{1}{4}y_{r-4} - \frac{4}{3}y_{r-3} + 3y_{r-2} - 4y_{r-1} + \frac{25}{12}y_r\right) + 0(h^4).
\end{aligned}$$

Nothing also that $a_m^{**} \neq 0 (m=-1,0,1)$ implies futher that the fourth Derivative of the right hand side of (1) is required.This again, Involves y'(x)and as the parameters a_m^{**} are multiplied by h^6 the first derivative must, this time, be replaced by $O(h^2)$ approximates if the overall $O(h^8)$ local truncation error of the multiderivative method is to be maintained. Such approximants are given by (23).

After making these replacements, as appropriate, the multiderivative method based on the (3,4) Padé approximant takes the form (11) where, now,

$$Q = h^2 D_1 F + h^3 D_2 + h^4 D_3 \tilde{F} + h^5 D_4 + h^6 D_5 . \qquad (32)$$

In (32), $F = \text{diag}(f_r)$ and $\tilde{F} = \text{diag}(\tilde{f}_r) = \text{diag}(f_r^2 + f_r'')$ as in 4

$$D_1 = \frac{1}{49}\begin{bmatrix} 45 & 2 & & & 0 \\ 2 & 45 & 2 & & \\ & . & . & . & \\ & & . & . & . \\ & 0 & 2 & 45 & 2 \\ & & & 2 & 45 \end{bmatrix}; \qquad (33)$$

$$D_2 \frac{1}{2940}\begin{bmatrix} d^{(2)}_{11} & d^{(2)}_{12} & d^{(2)}_{13} & d^{(2)}_{14} & & 0 \\ d^{(2)}_{21} & d^{(2)}_{22} & d^{(2)}_{23} & d^{(2)}_{24} & & \\ d^{(2)}_{31} & d^{(2)}_{32} & d^{(2)}_{33} & d^{(2)}_{34} & d^{(2)}_{35} & \\ . & . & . & . & . & \\ . & . & . & . & . & \\ . & . & . & . & . & \\ d^{(2)}_{N-2,N-4} & d^{(2)}_{N-2,N-3} & d^{(2)}_{N-2,N-2} & d^{(2)}_{N-2,N-1} & d^{(2)}_{N-2,N} & \\ 0 & d^{(2)}_{N-1,N-3} & d^{(2)}_{N-1,N-2} & d^{(2)}_{N-1,N-1} & d^{(2)}_{N-1,N} & \\ & d^{(2)}_{N,N-3} & d^{(2)}_{N,N-2} & d^{(2)}_{N,N-1} & d^{(2)}_{N,N} & \end{bmatrix} \qquad (34)$$

in which $d^{(2)}_{11} = -24f'_0 - \frac{655}{3} f'_1 + 4f'_2, \quad d^{(2)}_{12} = 18f'_0 + 393f'_1,$

$$d^{(2)}_{13} = -8f'_0 - 131f'_1 - 4f'_2, , \quad d^{(2)}_{14} = \frac{3}{2} f'_0 + \frac{131}{6} f'_1 + \frac{1}{2} f^1_2,$$

$$d^{(2)}_{r,r-2} = \frac{3}{2} f'_{r-1} + \frac{131}{62} f'_r + \frac{1}{2} f'_{r+1}, \; d^{(2)}_{r,r-1} = 5f'_{r-1} - \frac{524}{3} f'_{r+1}, \; d^{(2)}_{r,r} = -9f'_{r-1} + 9f$$

$$d^{(2)}_{r,r+1} = 3f'_{r-1} + \frac{524}{3} f'_r - 5f'_{r+1},\ d^{(2)}_{r,r+2} = -\frac{1}{2} f'_{r-1} - \frac{131}{6} f'_r \frac{3}{2} f'_{r+1} (r = 2,3,....,N-1)$$

$$d^{(2)}_{N,N-3} = -\frac{1}{2} f'_{N-1} - \frac{131}{6} f'_N - \frac{3}{2} f'_{N+1},\ d^{(2)}_{N,N-2} = 4f'_{N-1} + 131f'_N + 8f'_{N+1},$$

$$d^{(2)}_{N,N-1} = -39f'_N - 18f'_{N+1},\ d^{(2)}_{N,N} = -4f'_{N-1} + \frac{655}{3} f'_N + 24f'_{N+1}; \tag{35}$$

$$D_3 = \frac{1}{2940}\begin{bmatrix} 131 & -3 & & & & 0 \\ -3 & 131 & -3 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & 0 & & -3 & 131 & -3 \\ & & & & -3 & 131 \end{bmatrix}; \tag{36}$$

$$D_4 = \frac{1}{88200}\begin{bmatrix} d^{(4)}_{11} & d^{(4)}_{12} & & & 0 \\ d^{(4)}_{21} & d^{(4)}_{22} & d^{(4)}_{23} & & \\ \cdot & \cdot & \cdot & & \\ & \cdot & \cdot & \cdot & \\ & & d^{(4)}_{N-1,N-2} & d^{(4)}_{N-1,N-1} & d^{(4)}_{N-1,N} \\ & & & d^{(4)}_{N,N-1} & d^{(4)}_{N,N} \end{bmatrix} \tag{37}$$

with

$$d^{(4)}_{r,r-1} = -6u_{r-1} - 31u_r + 2u_{r+1},\ d^{(4)}_{r,r} = 8u_{r-1} - 8u_{r+1}$$

$$d^{(4)}_{r,r+1} = -2u_{r-1} + 31u_r + 6u_{r+1}$$

where

$$U_r = 3f_r f'_r + 4f'''_r$$

for $r = 1,2,....N($ $d^{(4)}_{10}$ and $d^{(4)}_{N,N+1}$ are used in the vector $\underline{b}$ below); and

$$D = \frac{1}{88200}\begin{bmatrix} d_{11}^{(5)} & d_{12}^{(5)} & & & & 0 \\ d_{11}^{(5)} & d_{22}^{(5)} & d_{23}^{(5)} & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & & \cdot & \\ & & \cdot & \cdot & \cdot & \\ & & \cdot\ d_{N-1,N-2}^{(5)} & \cdot & d_{N-1,N-1}^{(5)}\ \cdot & d_{N-1,N}^{(5)} \\ & & & & \cdot & \\ 0 & & & & d_{N,N-1}^{(5)} & d_{N,N}^{(5)} \end{bmatrix}$$

with

$$d_{r,r\pm1}^{(5)} = 2v_{r\pm1},\ d_{r,r}^{(5)} = 31v_r$$

where

$$V_r = f_r^3 + f_r f_r'' + 4(f_r')^2 + 6f_r f_r'' + f_r^{(iv)}$$

for $r = 1,2,\ldots\ldots,\ N$ ($d_{10}^{(5)}$ and $d_{N,N+1}^{(5)}$ are used in $\underline{b}$).

The vector $\underline{b}$ for this sixth order method is defined by

$$b_1 = [1 - \frac{2h^2}{49} f_0 - \frac{25h^3}{5880} f_0' + \frac{131h^3}{5880} f_1' \frac{h^4}{5880} f_2' \frac{h^4}{980} \tilde{f}_0 + \frac{h^5}{14700} u_0$$

$$+ \frac{31h^5}{88200} u_1 - \frac{h^5}{44100} u_2 - \frac{h^6}{44100} V_0]A_0$$

$$- \frac{h^2}{49}(2g_0 + 45g_1 + 2g_2) - \frac{h^4}{2940}(-3\tilde{g}_0 + 131\tilde{g}_1 - 3\tilde{g}_2) - \frac{h^6}{88200}(2w_0 + 31w_1 + 2w_2),$$

$$b_2 = -\frac{h^2}{49}(2g_1 + 45g_2 + 2g_3) - \frac{h^3}{2940}\frac{3}{2} f_1' + \frac{131}{6} f_2' + \frac{1}{2} f_3' A_0$$

$$- \frac{h^4}{2940}(-3\tilde{g}_1 + 131\tilde{g}_2 - 3\tilde{g}_2) - \frac{h^6}{88200}(2w_1 + 31w_2 + 2w_3),$$

$$b_r = -\frac{h^2}{49}(2g_{r-1} + 45g_r + 2g_{r+1}) - \frac{h^4}{2940}(-3\tilde{g}_{r-1} + 131\tilde{g}_r - 3\tilde{g}_{r+1})$$

$$-\frac{h^5}{88200}(2w_{r-1} + 31w_r + 2w_{r+1}), \quad r = 3,\ldots\ldots, N-2,$$

$$b_{N-1} = -\frac{h^2}{49}(2g_{N-2} + 45g_{N-1} + 2g_N) - \frac{h^3}{2940}\left(-\frac{1}{2}f_{N-2}' - \frac{131}{6}f_{N-1}' - \frac{3}{2}f_N'\right)A_1$$

$$-\frac{h^4}{2940}(-3\tilde{g}_{N-2} + 131\tilde{g}_{N-1} - 3\tilde{g}_N) - \frac{h^6}{88200}(2w_{N-2} + 31w_{N-1} + 2W_N,$$

$$b_N = \left(1 - \frac{2h^2}{49} f_{N+1} - \frac{h^3}{5880} f'_{N-1} - \frac{131h^3}{5880} h^3 f'_{N+1} + \frac{25h^3}{5880} h^3 f'_{N+1} + \frac{h^4}{980} \tilde{f}_{N+1} + \frac{h^5}{44100} u_{N-1}\right.$$

$$\left. - \frac{31h^5}{88200} u_N - \frac{h^5}{14700} u_{N+1} - \frac{h^5}{44100} V_{N+1}\right) A_1$$

$$- \frac{h^2}{49}(2g_{N-1} + 45g_N + 2g_{N+1}) - \frac{h^4}{2940}(-3\tilde{g}_{N-1} + 131\tilde{g}_N - 3\tilde{g}_{N+1})$$

$$- \frac{h^6}{88200}(2w_{N-1} + 31w_N + 2W_{N+1}), \qquad (39)$$

where

$$w_r = f_r^2 g_r + f_r g''_r + 4f'_r g'_r + 6f''_r g_r + g_r^{(iv)}, \quad r = 0,1,\ldots\ldots, N+1.$$

The solution vector $\underline{Y}$ for this numerical method is obtained by solving a linear system of the form (11). Unfortunately, because of the matrix D given by (34) and (35), the coefficient matrix A+Q is no longer tridiagonal. In fact it is not even quindiagonal though a pre-elimination makes it so and any decomposition algorithm for a quin-diagonal linear system may then be used to obtain $\underline{Y}$ (see, for instance, Twizell [14]).

It may be shown that

$$\| D_1 \| \le 1, \; \| D_2 \| \le \frac{989}{3528} \max_r | f'_r | \; \| D_3 \| \le \frac{137}{2940}$$
$$\| D_4 \| \le \frac{47}{44100} \max_r | u_r |, \; \| D_5 \| \le \frac{1}{2520} \max_r | v_r | \qquad (41)$$

and a convergence analysis shows that the multiderivative method based on the (3,4) Pade approximant is sixth order convergent provided

$$(\alpha_1 - \alpha_0)^2 [88200 \max_r |f_r| + 24725h \max_r |f'_r| + 4110h^2 \max_r |f_r| \qquad (42)$$
$$+ 94h^3 \max_r |u_r| + 35h^4 \max_r |Vr| < 705600.$$

6. NUMERICAL EXPERIMENTS

The tnultiderivative methods developed in §§3,4,5 were tested on the following problem from the literature

Problem (Usmani [15])

$$y'' - \frac{2}{x} = \frac{1}{x}, \quad 2 < x < 3$$

with boundary conditions

$$y(2) = y(3) = 0 \ .$$

The analytical solution of the problem is

$$y(x) = (19x - 5x^2 - 36x^{-1})/38 \ .$$

Clearly $f(x) = -2/x$ and $g(x) = 1/x$ and the derivatives of these functions are easily obtained for use in the multiderivative methods, as appropriate.

The step size h was given the values $h = 2^{-m}$ (m=3,4,...,7) so that $N = 2^m - 1$ (m=3,4,...,7) respectively and the problem was solved using the methods based on the (1,2), (2,3) and (3,4) Padé approximants which, respectively, are second, fourth and sixth order convergent. For comparison purposes, numerical results were also obtained using the classical second order method (which is, in fact, "based on the use of the (0,2) Padé approximant in. (5); see also Henrici [8]), the fourth order Numerov method (Lambert [11]) and the fourth order method of Usmani and Warsi [16], and the sixth order method of Usmani [15].

The values of $||\underline{y} - \underline{Y}||$ for each numerical experiment, are contained in Tables 2, 3, 4, respectively, for the second, fourth and sixth order methods. It is noted from these tables that the methods developed in the present paper give superior results to the competing methods listed above. It is also noted that halving the step size h reduces $||\underline{y} - \underline{Y}||$ by a factor 2^{-p} approximately where p is the order of the method.

The results were obtained using a Honeywell 68 computer.

Tables 2, 3, 4 here

SUMMARY

Second, fourth and sixth order multiderivative methods have been developed for the numerical solution of the variable coefficient, linear, second order boundary value problem $y''(x) = f(x)y(x) + g(x)$, $\alpha_0 < x < \alpha_1$, with $y(\alpha_0) = A_0$ and $y(\alpha_1) = A_1$.

The methods were developed by replacing the exponential terms in a three—point recurrence relation by Padé approximants. The second order method with smallest error constant was also seen to fall into the general class of linear two—step methods for second order boundary value problems.

The computed solution vector was obtained by solving a linear system: in the cases of the second and fourth order methods this linear system was seen to have a tridiagonal coefficient matrix, while in the case of the sixth order method the coefficient matrix, after a pre-elimination, is seen to be quindiagonal.

The methods were tested on a problem from the literature.

Table 1. Error constants

order	Padé approximant	error constant
2	(1,1)	$c_4 = \frac{1}{6}$
	(0,2)	$c_4 = \frac{1}{12}$
	(1,2)	$c_4 = \frac{1}{36}$
	(2,1)	$c_4 = -\frac{1}{36}$
	(2,0)	$c_4 = -\frac{7}{12}$
4	(2,2)	$c_6 = \frac{1}{360}$
	(1,3)	$c_6 = \frac{7}{2880}$
	(2,3)	$c_6 = -\frac{1}{3600}$
	(3,2)	$c_6 = \frac{1}{3600}$
6	(3,3)	$C_8 = \frac{1}{50400}$
	(3,4)	$C_8 = \frac{1}{70560(}$

Table 2.Maximum error moduli for second order methods with $h = 2^{-m}$

m	Method (0,2) (classical)	Method (1,2)
3	0.41(-4)	0.14(-4)
4	0.10(-4)	0.35(-5)
5	0.26(-5)	0.80(-6)
6	0.65(-6)	0.22(-6)
7	0.16(-6)	0.54(-7)

Table 3. Maximum error moduli for fourth order methods with $h = 2^{-m}$

m	Method		
	Numerov	Usmani and Warsi [16]	(2,3)
3	0.17(-6)	0.31(-7)	0.12(-7)
4	0.11(-7)	0.29(-8)	0.74(-9)
5	0.69(-9)	0.22(-9)	0.46(-10)
6	0.43(-10)	0.14(-10)	0.29(-11)
7	0.27(-11)	0.89(-12)	0.18(-12)

Table 4. Maximum error moduli for sixth order methods with $h=2^{-m}$

m	Method	
	Usmani [15]	(3,4)
3	0.50(-7)	0.99(-11)
4	0.10(-8)	0.17(-12)
5	0.19(-10)	0.28(-14)
6	0.31(-12)	0.46(-16)
7	0.49(-14)	0.77(-18)

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