is compared with $E_n(x)$, $E_{n-1}(x)$, and $E_n(x) + e_n^*(x)$. Even at $x^2 = 1$ the improved approximation has only about one per cent error compared to forty per cent for $E_n(x)$.

ACCURACY OF ASYMPTOTIC APPROXIMATIONS

x^2	$-i \operatorname{erf}(x)$	$E_n(x) + e_n^*(x)$	$E_n(x)$	$E_{n-1}(x)$
1.00	1.461	1.449	2.039	1.359
1.25	1.826	1.816	2.185	1.561
1.50	2.250	2.280	3.049	1.830
1.75	2.748	2.750	3.329	2.440
2.00	3.343	3.339	3.755	2.796
2.50	4.935	4.951	5.548	3.865
3.00	7.313	7.310	7.650	6.042
3.50	10.917	10.926	11.430	8.761
4.00	16.450	16.451	16.745	13.419

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A One-Step Method for the Numerical Solution of Second Order Linear Ordinary Differential Equations

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In this paper we shall give a one-step method for the numerical solution of second order linear ordinary differential equations based on Hermitian interpolation and the Lobatto four-point quadrature formula. One-step methods based on quadrature were introduced into the literature by Hammer and Hollingsworth [3]; for subsequent work see Morrison and Stoller [7], and Henrici [5].

Throughout our discussion we shall assume that the functions $N(x), f(x), g(x)$ of the differential equation $y'' = N(x)y' + f(x)y + g(x)$ are sufficiently differentiable to ensure that the derivations we give are valid in any context in which they are used.

In order to simplify somewhat the discussion of the method under consideration we shall first treat the differential equation $y'' = f(x)y + g(x)$, $y(x_0) = y_0$, $y'(x_0) = y_0'$. The necessary modifications for the general second order differential equation $y'' = N(x)y' + f(x)y + g(x)$ will be given later.

After integrating the above differential equation from x_0 to $x_1 = x_0 + h$ $(h > 0)$, we obtain the system of integral equations:

$$(1) \quad y'(x_0 + h) = y'(x_0) + \int_{x_0}^{x_0+h} [f(\tau)y(\tau) + g(\tau)]\, d\tau,$$

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$$(2) \qquad y(x_0 + h) = y(x_0) + hy'(x_0) + \int_{x_0}^{x_0+h} [f(\tau)y(\tau) + g(\tau)](x_0 + h - \tau)\, d\tau.$$

We shall approximate the above integrals by the Lobatto four-point quadrature formulae on the interval $[x_0, x_0 + h]$, cf. [6],

$$(3) \qquad \int_{x_0}^{x_0+h} F(x)\, dx = \frac{h}{2} \sum_{k=1}^{4} W_k F(\tau_k) + R_4 .$$

Here $W_1 = W_4 = \frac{1}{6}$, $W_2 = W_3 = \frac{5}{6}$.

$$\tau_1 = x_0, \quad \tau_2 = x_0 + (5 - \sqrt{5})h/10, \quad \tau_3 = x_0 + (5 + \sqrt{5})h/10,$$

$$\tau_4 = x_0 + h, \quad R_4 = \frac{-4h^7 F^{\mathrm{VI}}(\xi)}{3 \cdot 2^7 \cdot 15750},$$

where $x_0 < \xi < x_0 + h$.

In order to shorten the succeeding calculations we denote $(5 - \sqrt{5})/10$ by r, $(5 + \sqrt{5})/10$ by s.

We have, approximating the integrals of (1) and (2) by the above quadrature formula,

$$(4) \qquad y'(x_0 + h) = y'(x_0) + \frac{h}{2} \sum_{k=1}^{4} W_k[f(\tau_k)y(\tau_k) + g(\tau_k)] + T_0,$$

$$(5) \qquad \begin{aligned} y(x_0 + h) &= y(x_0) + hy'(x_0) \\ &\quad + \frac{h}{2} \sum_{k=1}^{4} W_k(x_0 + h - \tau_k)[f(\tau_k)y(\tau_k) + g(\tau_k)] + \bar{T}_0 . \end{aligned}$$

(T_0 and $\bar{T}_0$ will be discussed in detail later.)

We must know $y(\tau_2)$, $y(\tau_3)$ in order to apply the above formulae as a numerical method. We do this as follows. In addition to $y(x_0)$, $y'(x_0)$, $y''(x_0)$, we suppose we know $y(x_0 + h)$, $y'(x_0 + h)$, $y''(x_0 + h)$; we fit this data to a Hermite interpolating polynomial, cf. [6]:

$$(6) \qquad \begin{aligned} y(x_0 + th) &= y(x_0)[1 - t^3 + 3t^3(t - 1) - 6t^3(t - 1)^2] \\ &\quad + y'(x_0)[t - t^3 + 2t^3(t - 1) - 3t^3(t - 1)^2]h \\ &\quad + y''(x_0)[t^2 - 2t^3 + t^4 - t^3(t - 1)^2]h^2/2 \\ &\quad + y(x_1)[t^3 - 3t^3(t - 1) + 6t^3(t - 1)^2] \\ &\quad + y'(x_1)\, [t^3(t - 1) - 3t^3(t - 1)^2]h \\ &\quad + y''(x_1)[t^3(t - 1)^2]h^2/2 + y^{\mathrm{VI}}(\xi_1)\, t^3(t - 1)^3 h^6/720, \end{aligned}$$

where $x_0 < \xi_1 < x_0 + h$, $0 \leqq t \leqq 1$.

Using the differential equation and the abbreviated form for $y(x_0 + th)$,

$$(7) \qquad \begin{aligned} y(x_0 + th) &= A(t)y(x_0) + B(t)y'(x_0)h + C(t)y''(x_0)h^2/2 \\ &\quad + D(t)y(x_1) + E(t)y'(x_1)h + F(t)y''(x_1)h^2/2 + H(t), \end{aligned}$$

we obtain

$$
\begin{aligned}
y(x_0 + th) &= y(x_0)[A(t) + f(x_0)C(t)h^2/2] \\
&\quad + y'(x_0)B(t)h + y(x_1)[D(t) + F(t)f(x_1)h^2/2] \\
&\quad + y'(x_1)E(t)h + [g(x_0)C(t) + g(x_1)F(t)]h^2/2 + H(t).
\end{aligned} \tag{8}
$$

Letting

$$
\begin{aligned}
\alpha(t, h) &= A(t) + f(x_0)C(t)h^2/2, \\
\gamma(t, h) &= D(t) + F(t)f(x_1)h^2/2,
\end{aligned}
$$

and $A(r) = A_r$, $B(r) = B_r$, etc., $f(x_0) = f_0$, $f(x_0 + rh) = f_r$, etc., we have, substituting Eq. (8) into Eqs. (4) and (5) for the values of $y(\tau_2)$, $y(\tau_3)$, two linear equations to be solved for $y(x_0 + h)$, $y'(x_0 + h)$. They reduce to

$$
\begin{pmatrix} y(x_0 + h) \\ y'(x_0 + h) \end{pmatrix} = \bar{A}_0 \bar{B}_0 \begin{pmatrix} y(x_0) \\ y'(x_0) \end{pmatrix} + \bar{A}_0 G_0 + \bar{A}_0 T_0^*, \tag{9}
$$

where $\bar{A}_0 = \tilde{C}/\det(\tilde{C})$, in which

$$
\tilde{C} = \begin{bmatrix} 1 - \frac{5h^2}{12}(f_r E_r + f_s E_s) & \frac{5h^3}{12}(sf_r E_r + rf_s E_s) \\ \frac{5h}{12}[f_r \gamma_r + f_s \gamma_s] + \frac{hf_1}{12} & 1 - \frac{5h^2}{12}(sf_r \gamma_r + rf_s \gamma_s) \end{bmatrix}. \tag{10}
$$

It is easily seen that $\det(\tilde{C}) \neq 0$ if h is sufficiently small. $\bar{B}_0$ denotes the matrix

$$
\bar{B}_0 = \begin{bmatrix} 1 + \frac{h^2}{12} f_0 + \frac{5h^2}{12}(sf_r \alpha_r + rf_s \alpha_s) & h + \frac{5h^3}{12}(sf_r B_r + rf_s B_s) \\ \frac{h}{12} f_0 + \frac{5h}{12}(f_r \alpha_r + f_s \alpha_s) & 1 + \frac{5h^2}{12}(f_r B_r + f_s B_s) \end{bmatrix}, \tag{11}
$$

G_0 denotes the column vector

$$
G_0 = \begin{pmatrix} \frac{h^2}{12} g_0 + \frac{5h^2}{12}[sg_r + rg_s] + \frac{5h^4}{24}[g_0(sC_r f_r + rC_s f_s) + g_1(sF_r f_r + rF_s f_s)] \\ \frac{h}{12}[g_0 + g_1] + \frac{5h}{12}[g_r + g_s] + \frac{5h^3}{24}[g_0(C_r f_r + C_s f_s) + g_1(F_r f_r + F_s f_s)] \end{pmatrix}. \tag{12}
$$

In order to obtain an upper bound for the truncation error vector we consider the quantities $H(t)$, T_0, $\bar{T}_0$.

By the definition of $H(t)$ given above,

$$
H(r) = -h^6 r^3 s^3 y^{\mathrm{VI}}(\xi_r)/720 = -h^6 y^{\mathrm{VI}}(\xi_r)/90{,}000.
$$

$H(s) = -h^6 y^{\mathrm{VI}}(\xi_s)/90{,}000$ where ξ_r and ξ_s are in the open interval $(x_0, x_0 + h)$.

T_0 and $\bar{T}_0$ are given by the following formulae:

$$
T_0 = -[f(x)y(x) + g(x)]_{\xi_3}^{\mathrm{VI}} h^7/(96 \cdot 15750), \tag{13}
$$

$$
\bar{T}_0 = -[(x_0 + h - \tau)(f(x)y(x) + g(x))]_{\xi_4}^{\mathrm{VI}} h^7/(96 \cdot 15750), \tag{14}
$$

where ξ_3 and ξ_4 are in the open interval $(x_0, x_0 + h)$.

Thus we obtain for T_0^* the following:

$$T_0^* = \begin{Bmatrix} \frac{5h^2}{12}[sf_r H_r + rf_s H_s] + \bar{T}_0 \\ \\ \frac{5h}{12}[f_r H_r + f_s H_s] + T_0 \end{Bmatrix}. \tag{15}$$

Thus the approximate solution at x_1 given by

$$\begin{pmatrix} y_1 \\ y_1' \end{pmatrix} = \bar{A}_0 B_0 \begin{pmatrix} y_0 \\ y_0' \end{pmatrix} + \bar{A}_0 G_0 \tag{16}$$

has local truncation error $O(h^7)$.

We shall consider three computational examples. We have written programs for the CDC 1604 computer, FORTRAN (single-precision), for the following methods: Runge-Kutta, Numerov [4] and Gautschi (Stromer interpolation of trigonometric order two) [2]. We have used the same estimate of the period $T = \pi/5$ as Gautschi's article [2].

Example 1. A Mathieu differential equation $y'' + 100(1 - .1 \cos(2x))y = 0$, with the initial conditions taken as $x = 0$, $y(0) = 1$, $y'(0) = 0$. After starting Numerov's and Gautschi's methods by the Runge-Kutta method we obtain the values shown in Table 1.

Example 2. Bessel differential equation $y'' + (100 + \frac{1}{4}x^2)y = 0$. We take the initial conditions at $x = 1$, such that the solution is $\sqrt{x}\, J_0(10x)$. We have h as 0.02 again. We have taken the initial values from [1] to 10D. For Numerov's and Gautschi's method we have taken the other starting values from the table also (Table 2).

Example 3. Our last example is the differential equation $y'' = (1 + x^2)y$. The initial conditions in this example were chosen at $x = 0$ so that the solution is $e^{x^2/2}$. We again take $h = 0.02$ and obtain the results of Table 3, after taking all the necessary starting values as exact.

The general second order equation $y'' = N(x)y' + f(x)y + g(x)$ can be treated by the above techniques, if one treats the $N(x)y'$ term by integration by parts. One may also use a well-known transformation [6] to eliminate the y' term from the above differential equation. The procedure one should use depends primarily on whether or not $N(x)$ is explicitly integrable.

It is well known that two-point boundary value problems of the form $y'' = f(x)y + g(x)$, $y(a) = A$, $y(b) = B$, $-\infty < a < b < \infty$, $f(x) > 0$ can be solved by initial value techniques either by the method of superposition or by the numerical construction of the Green's function of the above differential equation. We have made calculations on problems of the above type with the one-step method under consideration and have found the results to be quite satisfactory.

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TABLE 1
Mathieu Differential Equation

X	Lobatto	Runge-Kutta	Numerov	Gautschi	Exact (7D)
.5	.069208517	.069156017	.069220716	.0692114316	.0692085
1.0	−.908417862	−.908438043	−.908410736	−.908415864	−.9084179
1.5	−.693960833	−.693810059	−.693995071	−.693958722	−.6939608
2.0	.230958975	.230894461	.230964653	.230964653	.2309590
2.5	.976369849	.976344156	.976362821	.976369948	.9763699
3.0	.205766632	.205359297	.205865854	.205761493	.2057667
3.5	−.961679414	−.961718360	−.961651417	−.961679510	−.9616794
4.0	−.426531682	−.426046799	−.426645356	−.426531047	−.4265317
4.5	.602236752	.602611939	.602128771	.602238461	.6022367
5.0	.941737244	.941526628	.941766210	.941734467	.9417373

TABLE 2
Bessel Differential Equation

X	Lobatto	Runge-Kutta	Numerov	Gautschi	Exact (7D)
2	.236208546	.236214981	.236205562	.236208655	.2362085
3	−.149593736	−.149640613	−.149580121	−.149594204	−.1495937
4	.014733783	.014832263	.014708498	.014734630	.0147338
5	.124800157	.124673672	.124829485	.124799188	.1248002
6	−.224059244	−.223958092	−.224078623	−.224058612	−.2240592
7	.251104887	.251090902	.251099928	.251105055	.2511049
8	−.197260634	−.197374820	−.197223810	.079892131	−.1972606
9	.079890053	.080127641	.079826058	.079892131	.0798900
10	.063200835	.062899111	.063274262	.063198428	.0632007

TABLE 3
Differential Equation $y'' = (1 + x^2)y$

X	Lobatto	Runge-Kutta	Numerov	Exact (10D) Machine
1.0	1.648721269	1.648721264	1.648721287	1.648721271
2.0	7.389056087	7.389055819	7.389056409	7.389056099
3.0	90.01713107	90.01710938	90.01714644	90.01713130
4.0	2980.957976	2980.954707	2980.959682	2980.957987
5.0	268337.2853	268336.2736	268337.7249	268337.2864

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