A ONE-STEP METHOD FOR THE NUMERICAL SOLUTION
OF ORDINARY NON-LINEAR SECOND-ORDER DIFFERENTIAL
EQUATIONS BASED UPON LOBATTO FOUR-POINT
QUADRATURE FORMULA

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Abstract. This paper describes a one-step method based upon the Lobatto four-point quadrature formula for the numerical integration of differential equation: $y''(x) = f(x, y(x), y'(x)); y(x_0) = y_0, y'(x_0) = y'_0$. The method has a local truncation error $O(h^6)$ in $y(x)$ and $O(h^5)$ in $y'(x)$. In the case of linear second-order differential equation, a stability criterion has been developed. Theoretical and computational comparisons of the new method with existing method is discussed.

1. Introduction

The necessity of accurate numerical approximations to the solution of non-linear differential equations governing physical systems has always been an important problem with scientists and engineers. Hammer and Hollingsworth [5] have used Gaussian quadrature methods for solving ordinary differential equations. This method has been further developed by Morrison and Stoller [10], Korganoff [9], Kuntzmann [8], Henrici [6], Day [2, 3], Jain and Sharma [7], Sharma [13]. Day [1] used this method for the solution of non-linear second-order differential equations (first derivative absent) using Lobatto four-point quadrature formula.

The purpose of this paper is to investigate the use of Lobatto's four-point quadrature formula for solving the second-order non-linear differential equation: $y''(x) = f(x, y(x), y'(x)); y(x_0) = y_0, y'(x_0) = y'_0$. The method has local truncation error $O(h^6)$ in $y(x)$ and $O(h^5)$ in $y'(x)$. For n integration steps the present method requires $(5n + 1)$ evaluations of f as compared to the classical methods of Runge-Kutta, Runge-Kutta-Nyström's $4n$. A stability criterion has been developed for the linear second-order differential equation.

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2. Second-order differential equations

Consider the second-order differential equation:

(2.1) $y''(x) = f(x, y(x), y'(x)); \; y(x_0) = y_0, \; y'(x_0) = y_0'$

where x_0 is an initial-point.

Throughout our discussion we shall assume that the function $f(x, y(x), y'(x))$ occurring in (2.1) is sufficiently differentiable to ensure that the derivations we give are valid on any context in which they are used.

Integrating (2.1) from x_0 to $x_0 + h \, (h > 0)$, we obtain the system of integral equations:

(2.2) $y(x_0 + h) = y_0 + h y_0' + \displaystyle\int_{x_0}^{x_0 + h} [x_0 + h - \tau] f(\tau, y(\tau), y'(\tau)) d\tau$

(2.3) $y'(x_0 + h) = y_0' + \displaystyle\int_{x_0}^{x_0 + h} f(\tau, y(\tau), y'(\tau)) d\tau$

We shall approximate the above two integrals by the Lobatto four-point quadrature formula on the interval $[x_0, x_0 + h]$, see Hildebrand [4].

(2.4) $\displaystyle\int_{x_0}^{x_0 + h} F(x) dx = \frac{h}{2} \sum_{p=1}^{4} F(\tau_p) W_p + E_4$

where,

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

$$\tau_1 = x_0 \quad ,$$

$$\tau_2 = x_0 + rh, \quad r = (5 - \sqrt{5})/10, \cdot$$

$$\tau_3 = x_0 + sh, \quad s = (5 + \sqrt{5})/10,$$

$$\tau_4 = x_0 + h$$

and

$$E_4 = -\frac{4 h^7 F^{(6)}(\xi)}{3.2^7 . 15750}, \quad x_0 < \xi < x_0 + h.$$

We introduce the notations: $x_{r/2} = x_0 + rh/2$, $y_{r/2} = y(x_{r/2})$, $x_r = x_0 + rh$, $y_r = y(x_r) \cdots \cdots \cdots \cdots$. Then integral equations (2.3) and (2.4) can be replaced as:

(2.5)
$$y(x_0 + h) = y_0 + h y_0' + (h^2/12) [f(x_0, y_0, y_0') + 5\{r f(x_s, y_s, y_s')$$
$$+ s f(x_r, y_r, y_r')\}] + E$$

$$y'(x_0+h) = y_0' + (h/12)[f(x_0, y_0, y_0') + f(x_0 + h, y(x_0 + h), y'(x_0 + h))$$

(2.6)

$$+ 5\{f(x_r, y_r, y_r') + f(x_s, y_s, y_s')\}] + E'$$

wh ere E and E' are truncation errors of $0(h^6)$ and $0(h^5)$ respectively.

We note that we do not know y_r, y_s, y_r', y_s'; thus if such an algorithm is to be of computational value, we must obtain accurate approximate values for y_r, y_s, y_r' and y_s'. For this, we obtain the following Hermite expressions for y_r and y_r' (we shall denote $\sqrt{5}$ by p):

(2.7) $$y_r = y_0 + rhy_0' + \frac{(rh)^2}{6}[y'' + 2f(x_{r/2}, y_{r/2}, y_{r/2}')] + E_r$$

(2.8) $$y_r' = \frac{(25 - 19p)}{2h}y_0 + (3 - 2p)y_0' + \frac{h(5 - 3p)}{20}y_0'' + \frac{(15 + p)}{2h}y_r$$

$$+ \frac{(9p - 20)}{h}y_s + E_r'$$

where E_r and E_r' are truncation errors of $0(h^5)$ and $0(h^4)$ respectively. Similar expressions for y_s and y_s' can be obtained by changing r to s and p to $-p$ in equations (2.7) and (2.8) respectively.

The approximate values of $y_{r/2}'$ occurring in the equation (2.7) can be obtained by halving the values of r, s and h in (2.8) and the approximate values of $y_{r/2}$ can be obtained by Taylor's theorem in conjunction with (2.1). Substituting the values of $y_{r/2}$ and $y_{r/2}'$ in (2.7) we obtain the approximate values of y_r to the desired order of accuracy. Similar calculations yield the values of y_s, y_r' and y_s' Finally, these values are used in (2.5) to obtain the desired value of $y(x_0 + h)$. To calculate $y'(x_0 + h)$ we consider the expression:

$$y'(x_0 + h) = -\frac{33}{h}y_0 - 7y_0' - \frac{h}{2}y_0'' + \frac{25(1 + p)}{2h}y_r + \frac{25(1 - p)}{2h}y_s$$

(2.9)

$$+ \frac{8}{h}y(x_0 + h) + \frac{h^5}{150}f'''(x_0, y_0, y_0') + 0(h^6)$$

Substitution of the values of $f(x_r, y_r, y_r')$, $f(x_s, y_s, y_s')$ calculated above along with the newly calculated value of $f(x_0 + h, y(x_0 + h), y'(x_0 + h))$ into the equation (2.6) leads to the required value of $y'(x_0 + h)$.

Error Terms

Error terms for each of the expressions (as abbreviated above by E_r, E_r', E, E') have been calculated as follows:

$$E_r = h^5\left[-\frac{r^5}{720}f'''(x_0, y_0, y_0') + \frac{r^2}{2880}(26 - 10p)\tau_r + (4p + 8)\tau_s\right]$$

$$\times f''(x_0, y_0, y_0')f_y'(x_0, y_0, y_0') - \frac{r^5}{2880}f^{IV}(x_0, y_0, y_0')] + 0(h^6)$$

where

$$\tau_r = \frac{\xi_r - x_0}{h}, \qquad \tau_s = \frac{\xi_s - x_0}{h}$$

$$E_r' = h^4 \left[\frac{(3-p)}{2,400} f''(x_0, y_0, y_0') + \left\{ \frac{(15+p)}{2} R_1 + (9p - 20)R_2 \right\} \right] + 0(h^5)$$

$$E = \frac{5h^6}{12} \left[r \left\{ \frac{(44 + 25p)}{3600} f'''(x_0, y_0, y_0') + R_1 \right\} + s \left\{ \frac{(44 - 25p)}{3600} \right. \right.$$

$$\left. \left. f'''(x_0, y_0, y_0') + R_2 \right\} \right] \times f_{y'}(x_0, y_0, y_0') + 0(h^7)$$

and

$$E' = \frac{h^5}{12} \left[\frac{11}{90} f'''(x_0, y_0, y_0') + 5(R_1 + R_2) \right] f_{y'}(x_0, y_0, y_0') + 0(h^6)$$

where R_1 and R_2 are the coefficients of h^5 in E_r and E_s respectively.

3. Stability criterion

The stability of the present method will be discussed in a manner similar to that adopted by Jain and Sharma [7]. Consider the differential equation $y'' = \alpha y$; α is a real number. We shall discuss the three cases $\alpha = 0, -k^2, +k^2$ respectively. If we insert the values of $y_{n+r}, y_{n+s}, y_{n+r}', y_{n+s}'$ in y_{n+1} and y_{n+1}' in the algorithm, we obtain

$$(3.1) \quad \begin{bmatrix} y_{n+1} \\ y_{n+1}' \end{bmatrix} = \begin{bmatrix} 1 + \frac{h^2\alpha}{2} + \frac{h^4\alpha^2}{24} + \frac{h^6\alpha^3}{720} & h + \frac{h^3\alpha}{6} + \frac{h^5\alpha^2}{120} \\ h + \frac{h^3\alpha^2}{6} + \frac{h^5\alpha^3}{120} + \frac{h^7\alpha^4}{8640} & 1 + \frac{h^2\alpha}{2} + \frac{h^4\alpha^2}{24} + \frac{h^6\alpha^3}{1440} \end{bmatrix} \begin{bmatrix} y_n \\ y_n' \end{bmatrix}$$

For $\alpha = 0$, we have: $y_{n+1} = y_n + hy_n'$ and $y_{n+1}' = y_n'$. The solution of this system can be written as $y_n' = y_0'$ and $y_n = y_0 + nhy_0'$, which is an expected result.

We now consider the case $\alpha = -k^2$; the solution in this case is oscillating. We therefore consider the eigenvalues of the matrix in (3.1). We find that eigenvalues have unit modulus for $0 \leq h^2k^2 \leq 6.8$. The deviation of the modulus of the eigenvalues from unity is less than 0.01 for $6.8 < h^2k^2 \leq 9.5$. This shows that the method is stable for a sufficiently wide range of the values of h^2k^2. The same has also been observed in the case of sample examples computed for the method. The Runge-Kutta method as studied for the above problem $y'' = -k^2y$ is stable for $0 \leq h^2k^2 \leq 7.756$, and the range of stability for the Runge-Kutta-Nyström method for the same equation is $0 \leq h^2k^2 \leq 6.690$.

For the case $y'' = k^2 y$, of which the solutions are exponential in nature, we rely on the analysis given by Rutishauser [11, 12]. It is well known that the solution of the differential equation $y'' = k^2 y$, written in the matrix form is:

$$\text{(3.2)} \quad \begin{bmatrix} y(x) \\ y'(x) \end{bmatrix} = \exp\left[(x - x_0)M\right] \begin{bmatrix} y_0 \\ y_0' \end{bmatrix}, \text{ where } M = \begin{bmatrix} 0 & 1 \\ k^2 & 0 \end{bmatrix}$$

For the point $x = x_0 + nh$, this solution can be written in the form (with $\alpha = k^2$):

$$\text{(3.3)} \quad \begin{bmatrix} y(x) \\ y'(x) \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} y_0 \\ y_0' \end{bmatrix}$$

It may be observed that:

$$\underset{h \to 0}{\text{Lt}} \frac{1}{h^6} \left[\left\{ \exp(Mh) - \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \right\} \right] = \begin{bmatrix} 0 & 0 \\ 0 & +\frac{k^6}{1440} \end{bmatrix}$$

where

$$a_{11} = 1 + \frac{h^2 k^2}{2} + \frac{h^4 k^4}{24} + \frac{h^6 k^6}{720} + \cdots \cdots$$

$$a_{12} = h + \frac{h^3 k^2}{6} + \frac{h^5 k^4}{720} + \cdots \cdots$$

$$a_{21} = hk^2 + \frac{h^3 k^4}{6} + \frac{h^5 k^6}{120} + \frac{h^7 k^8}{8640} + \cdots \cdots$$

$$a_{22} = 1 + \frac{h^2 k^2}{2} + \frac{h^4 k^4}{24} + \frac{h^6 k^6}{1440} + \cdots \cdots$$

This indicates that the present method is of order five by definition of Rutishauser. In the case of a large number of integration intervals (large x, small h), the relative error of this method, for equation $y'' = k^2 y$ can be considered as follows:

The maximum eigen-value of the matrix in (3.1) for $\alpha = k^2$ is given by:

$$\lambda = (1/2)\left[(a_{11} + a_{22}) + \sqrt{[(a_{11} - a_{22})^2 + 4a_{12}a_{21}]} \right]$$

$$= 1 + hk + \frac{h^2 k^2}{2} + \frac{h^3 k^3}{6} + \frac{h^4 k^4}{24} + \frac{h^5 k^5}{720} - \frac{13 h^7 k^7}{2880}$$

and therefore the relative error F (in the sense of Rutishauser) of the method is:

$$F_\infty \simeq \frac{hk - \log \lambda}{h}$$

$$= \frac{\log(e^{hk}) - \log \lambda}{h}$$

$$= \frac{1}{h} \log\left[1 + \frac{(e^{hk} - \lambda)}{\lambda}\right]$$

$$\simeq \frac{19h^6 k^7}{4032} \text{ for large } x \text{ and small } h.$$

Rutishauser (1960) calculates the relative error for the Runge-Kutta-Nyström method for the equation $y'' = k^2 y$ and finds that $F_\infty \simeq (h^4 k^5 / 320)$; for the Runge-Kutta method he obtained $F_\infty \simeq h^4 k^5 / 120$.

4. Algorithm

To advance from x_n to $x_{n+1}(x_{n+1} = x_n + h)$ we note that $f(x_n, y_n, y'_n)$ has been computed in the previous step. The computation should proceed as follows:

Calculate,

$$y_{n+r/2} = y_n + \frac{rh}{2} y'_n + \frac{r^2 h^2}{8} y''_n$$

$$y_{n+s/2} = y_n + \frac{sh}{2} y'_n + \frac{s^2 h^2}{8} y''_n$$

$$y'_{n+r/2} = \frac{(25 - 19p)}{h} y_n + \frac{(3 - 2p)}{1} y'_n + \frac{(5 - 3p)h}{40} y''_n + \frac{(15 + p)}{h} y_{n+r/2}$$
$$+ \frac{2(9p - 20)}{h} y_{n+s/2}$$

$$y'_{n+s/2} = \frac{(25 + 19p)}{h} y_n + \frac{(3 + 2p)}{1} y'_n + \frac{(5 + 3p)h}{40} y''_n + \frac{(15 - p)}{h} y_{n+s/2}$$
$$- \frac{2(9p + 20)}{h} y_{n+r/2}$$

Then,

$$y_{n+r} = y_n + rh y'_n + \frac{(rh)^2}{6}[f(x_n, y_n, y'_n) + 2f(x_{n+r/2}, y_{n+r/2}, y'_{n+r/2})]$$

$$y_{n+s} = y_n + sh y'_n + \frac{(sh)^2}{6}[f(x_n, y_n, y'_n) + 2f(x_{n+s/2}, y_{n+s/2}, y'_{n+s/2})]$$

$$y'_{n+r} = \frac{(25 - 19p)}{2h} y_n + (3 - 2p)y'_n + \frac{(5 - 3p)h}{20} y''_n + \frac{(15 - p)}{2h} y_{n+r}$$
$$+ \frac{(9p - 20)}{h} y_{n+s}$$

$$y'_{n+s} = \frac{(25+19p)}{2h}y_n + (3+2p)y'_n + \frac{(5+3p)h}{20}y''_n + \frac{(15+p)}{2h}y_{n+s}$$
$$- \frac{(9p+20)}{h}y_{n+r}$$

Finally,

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{12}[f(x_n,y_n,y'_n) + 5\{sf(x_{n+r},y_{n+r},y'_{n+r}) + rf(x_{n+s},y_{n+s},y'_{n+s})\}]$$

Again calculate,

$$y'_{n+1} = -\frac{33}{h}y_n - 7y'_n - \frac{h}{2}y''_n + \frac{25(1+p)}{2h}y_{n+r} + \frac{25(1-p)}{2h}y_{n+s} + \frac{8}{h}y_{n+1}$$

Thus,

$$y'_{n+1} = y'_n + \frac{h}{12}[f(x_n,y_n,y'_n) + 5\{f(x_{n+r},y_{n+r},y'_{n+r}) + f(x_{n+s},y_{n+s},y'_{n+s})\}$$
$$+ f(x_{n+1},y_{n+1},y'_{n+1})]$$

5. Numerical results of the method

For the purpose of computational comparison of this method with other methods, we consider the following two examples. We have written programs for the ICL 1909 Computer in FORTRAN IV (in single precision) for the method under consideration and the results have been compared with the exact results and the results obtained by other methods.

Example One

The differential equation

$$\frac{d^2y}{dx^2} + (16\pi^2 e^{-2x} - 1/4)y = 0$$

with initial conditions:

$$y(0) = 1.0; \left(\frac{dy}{dx}\right)_{x=0} = 0.5$$

has the solution:

$$y(x) = e^{x/2}\cos(4\pi e^{-x}).$$

We computed approximate values of $y(x)$ at equally spaced points with $h = 0.02$ and obtained the approximate values listed in Table one.

TABLE ONE

x	Nyström	Runge-Kutta	New Method	Exact
2.0	−000.35227603	−000.35227603	−000.35205017	−000.35205060
4.0	007.19395636	007.19395636	007.19420981	007.19420412
6.0	020.07545103	020.07545103	020.07580847	020.07579367
8.0	054.59685889	054.59685888	054.59770481	054.59766497
10.0	148.41099023	148.41099021	148.41324328	148.41313528

Example Two

The Legendre differential equation:

$$(1 - x^2)\,\frac{d^2 y}{dx^2} - 2x\,\frac{dy}{dx} + 72y = 0$$

with initial conditions:

$$x = 0, \ y(0) = 0.2734375000, \ \left(\frac{dy}{dx}\right)_{x=0} = 0$$

has the solution:

$$y(x) = (6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35)/128.$$

We computed approximate values of $y(x)$ at equally spaced points with $h = 0.02$ and obtained the approximate values listed in Table two.

TABLE TWO

x	Nyström	Runge-Kutta	New Method	Exact
0.10	0.1803210877	0.1803217228	0.1803207210	0.1803207215
0.20	−0.0395736736	−0.0395615211	−0.0395647992	−0.0395548000
0.30	−0.2390734252	−0.2390709065	−0.2390745826	0.2390745910
0.40	−0.2669997410	−0.2669999266	−0.2669992858	−0.2669993000
0.50	−0.0736421547	−0.0736478032	−0.0736388781	−0.0736389159

6. Conclusion

We observe that the one-step Lobatto method developed here compares favourably with other methods. The relative error of this method is relatively much smaller than the classical Runge-Kutta and Nyström methods with only $(n + 1)$ additional functional evaluations for n steps.

Acknowledgement

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