A one-step method for the numerical integration of the differential equation $y'' = f(x)y + g(x)$

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This paper describes a new one-step method based on the Gauss two-point rule for the numerical integration of the differential equation $y'' = f(x)y + g(x)$. Computational and theoretical comparison of the new method with other methods is given.

1. The numerical integration of ordinary differential equations by the use of Gaussian quadrature methods was introduced into the literature by Hammer and Hollingsworth (1955), for subsequent developments, see Morrison and Stoller (1958), Korganoff (1958), Kuntzmann (1961), Henrici (1962). In this paper we develop a one-step method for the numerical integration of the ordinary differential equation $y'' = f(x)y + g(x)$, $y(x_0) = y_0$, $y'(x_0) = y_0'$ based on the Gauss two-point rule (see Hildebrand, 1956). Theoretical and computational comparison of the new method with other methods is given.

2. By integrating the above differential equation from x_0 to $x_0 + h$ $(h > 0)$ we obtain

$$y'(x_0 + h) = y'(x_0) + \int_{x_0}^{x_0+h} [f(\tau)y(\tau) + g(\tau)]d\tau \quad (2.1)$$

$$y(x_0 + h) = y(x_0) + \int_{x_0}^{x_0+h} [f(\tau)y(\tau) + g(\tau)] (x_0 + h - \tau)d\tau + hy'(x_0). \quad (2.2)$$

If we approximate the integrals of (2.1) and (2.2) by the Gauss two-point rule on $[x_0, x_0 + h]$ we obtain

$$y'(x_0 + h) = y'(x_0) + h[f(x_p)y(x_p) + f(x_q)y(x_p)]/2 + h[g(x_p) + g(x_q)]/2 + h^5 y^{vi}(\xi_1)/4320 \quad (2.3)$$

$$x_0 < \xi_1 < x_0 + h$$

$$y(x_0 + h) = y(x_0) + hy'(x_0) + h^2[qf(x_p)y(x_p) + pf(x_q)y(x_q)]/2 + h^2[qg(x_p) + pg(x_q)]/2 + h^5[y''(\tau)(x_0 + h - \tau)]^{iv}_{\xi_2}/4320 \quad (2.4)$$

$$x_0 < \xi_2 < x_0 + h$$

where $x_p = x_0 + ph$, $x_q = x_0 + qh$

$$p = (3 - \sqrt{3})/6, \ q = 1 - p.$$

We note that we do not know $y(x_p)$, $y(x_q)$; thus if such an algorithm is to be of computational value we must obtain accurate approximate values for $y(x_p)$ and $y(x_q)$.

We obtain estimates for $y(x_p)$ and $y(x_q)$ by fitting a cubic polynomial $u(x)$ to the data $y(x_0)$, $y'(x_0)$ and the requirement that $u(x)$ satisfy the differential equation at the points x_p and x_q. We now give the details of this procedure.

Let $u(x) = y(x_0) + y'(x_0)(x - x_0) + a(x - x_0)^2 + b(x - x_0)^3$.

Set $u''(x_p) = f(x_p)u(x_p) + g(x_p)$

$u''(x_q) = f(x_q)u(x_q) + g(x_q)$ and solve for a and b.

We obtain

$$u_p = \frac{y_0(1 + h^2(2p - q^2)f(x_q)/6) + y_0'(ph + (2p - q)f(x_q)h^3/36)}{\Delta} + \frac{G_1}{\Delta}\left[1 + \frac{(3p - q)q^2h^2f(x_q)}{6(q - p)}\right] - \frac{2p^3h^2f(x_q)G_2}{6(q - p)\Delta} \quad (2.5)$$

$$u_q = \frac{y_0(1 + h^2(2q - p^2)f(x_p)/6) + y_0'(qh + (2q - p)f(x_p)h^3/36)}{\Delta} + \frac{G_1 2q^3 f(x_p)h^2}{6(q - p)\Delta} + \left[1 + \frac{(p - 3q)p^2h^2f(x_p)}{6(q - p)}\right]\frac{G_2}{\Delta} \quad (2.6)$$

in which

$$G_1 = \frac{h^2p^2}{6(q - p)}(3q - p)g(x_p) - \frac{2p^3h^2}{6(q - p)}g(x_q)$$

$$G_2 = \frac{h^2q^2}{6(q - p)}(q - 3p)g(x_q) + \frac{2q^3h^2}{6(q - p)}g(x_p)$$

$$\Delta = \frac{1 + h^2p^2f(x_p)(p - 3q)}{6(q - p)} + \frac{q^2(3p - q)h^2f(x_q)}{6(q - p)} + h^4f(x_p)f(x_q)/432. \quad (2.7)$$

It can be shown that

$$f(x_p)u(x_p) + g(x_p) = f(x_0)y(x_0) + g(x_0) + y_0^{iii}ph + y_0^{iv}p^2h^2/2 + y_0^{v}p^3h^3/6 + O(h^4). \quad (2.8)$$

Likewise a similar expression holds for $f(x_q)u(x_q) + g(x_q)$. Thus if we substitute these expressions into equations (2.3) and (2.4), we obtain, after making use of the properties of p and q,

$$y(x_0 + h) = y(x_0) + hy'(x_0) + h^2y''(x_0)/2 + h^3y^{iii}(x_0)/6 + h^4y^{iv}(x_0)/24 + h^5(qp^3 + pq^3)y^{v}/12$$

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$$+\,h^5[(x_0+h-\tau)(f(\tau)y(\tau)$$
$$+\,g(\tau))]^{\text{iv}}_{\xi_2}/4320+O(h^6) \qquad (2.9)$$
$$x_0<\xi_2<x_0+h$$

$$y'(x_0+h)=y'(x_0)+hy''(x_0)+h^2y^{\text{iii}}(x_0)/2$$
$$+\,h^3y^{\text{iv}}(x_0)/6+h^4y^{\text{v}}(x_0)/24+O(h^5). \qquad (2.10)$$

Equation (2.9) further simplifies to

$$y(x_0+h)=y(x_0)+hy'(x_0)+h^2y''(x_0)/2$$
$$+\,h^3y^{\text{iii}}(x_0)/6+h^4y^{\text{iv}}(x_0)/24$$
$$+\,h^5y^{\text{v}}/120+O(h^6). \qquad (2.11)$$

Thus the Gauss method agrees with the Taylor expansion about the point x_0 of $y(x)$ through the first six terms and with the derivative $y'(x)$ through the first five terms.

Briefly summarizing the Gauss method: To march from x_n to x_{n+1} one calculates u_p and u_q according to (2.5), (2.6) where $x_p=x_n+ph$, $x_q=x_n+qh$ and where y_n and y_n', respectively, replace y_0 and y_0' in equations (2.5), (2.6), (2.7) and in the definitions of G_1 and G_2. One then substitutes the resulting values for u_p and u_q into

$$y'_{n+1}=y'_n+h[f(x_p)u(x_p)+f(x_q)u(x_q)]/2$$
$$+\,h[g(x_p)+g(x_q)]/2 \qquad (2.12)$$
$$y_{n+1}=y_n+hy'_n+h^2[qf(x_p)u(x_p)$$
$$+\,pf(x_q)u(x_q)]/2+h^2[qg(x_p)+pg(x_q)]/2. \quad (2.13)$$

We investigate the stability and give further error analysis of the Gauss method. In this we follow the fundamental papers of Rutishauser (1952, 1960).

Consider the differential equation $y''=\alpha y$, α a real number. These are three cases of interest to us $\alpha=k^2$, $\alpha=0$, $\alpha=-k^2$.

After a brief calculation involving equations (2.5), (2.6), (2.7), and (2.12), (2.13), we obtain

$$y_{n+1}=y_n\left[1+\frac{\alpha h^2}{2\Delta}+\frac{\alpha^2h^4}{72\Delta}\right]+y'_n\left[h+\frac{\alpha h^3}{6\Delta}\right] \qquad (2.14)$$

$$y'_{n+1}=y_n\left[\alpha+\frac{\alpha^2h^2}{9}\right]h/\Delta+y'_n\left[1+\frac{\alpha h^2}{2\Delta}+\frac{\alpha^2h^4}{72\Delta}\right]. \qquad (2.15)$$

Equations (2.14) and (2.15) written in matrix notation are

$$\begin{bmatrix}y_{n+1}\\ y'_{n+1}\end{bmatrix}=\begin{bmatrix}c_{11} & c_{12}\\ c_{21} & c_{22}\end{bmatrix}\begin{bmatrix}y_n\\ y'_n\end{bmatrix} \qquad (2.16)$$

in which

$$c_{11}=1+\frac{\alpha h^2}{2\Delta}+\frac{\alpha^2h^4}{72\Delta} \qquad c_{12}=h+\frac{\alpha h^3}{6\Delta}$$

$$c_{21}=\left(1+\frac{\alpha h^2}{9}\right)\alpha h/\Delta \qquad c_{22}=c_{11}.$$

For $\alpha=0$ we obtain from (2.14) and (2.15)

$$y_{n+1}=y_n+hy'_n$$
$$y'_{n+1}=y'_n.$$

The solutions of these equations are

$$y'_n=y'_0$$
$$y_n=y_0+nhy'_0$$

which is of course what one expects in this case.

We treat the cases $\alpha=k^2$ and $\alpha=-k^2$ somewhat differently as they exhibit markedly different behaviour. The case we treat first is $\alpha=-k^2$; in this case of course we get oscillating solutions, so it is important for us to have the eigenvalues of the above matrix, equation (2.16), on or inside the unit circle.

The eigenvalues of the matrix (2.16) are

$$\lambda_{1,2}=1+\frac{\alpha h^2}{2\Delta}+\frac{\alpha^2h^4}{72\Delta}\pm\sqrt{\left[\frac{\alpha h^2}{\Delta}\left(1+\frac{\alpha h^2}{9}\right)\left(1+\frac{\alpha h^2}{6\Delta}\right)\right]}. \qquad (2.17)$$

Substituting in $-k^2$ for α in equation (2.17) we note that $1-\dfrac{h^2k^2}{6\Delta}>0$ for $0\leqslant h^2k^2\leqslant 12$, thus the roots are complex for $h^2k^2<9$. It is not difficult to see from the definition of Δ that the roots have unit modulus for $0\leqslant k^2h^2\leqslant 9$. Between 9 and 12 the roots are real and one of the roots is greater than 1 in absolute value.

The stability of the Gauss method compares quite favourably with other one-step methods now in use. Liniger (1957) finds that the Runge–Kutta method for the first-order equation $y'=ky$ is stable for $-2\cdot 785\leqslant kh\leqslant 0$, which for the above problem would be $0\leqslant h^2k^2\leqslant 7\cdot 756$. Ansorge and Törnig (1960) compute the stability range of the Runge–Kutta–Nystrom method for the same equation and find it to be $0\leqslant h^2k^2\leqslant 6\cdot 690$.

The methods of Cowell (1910) and Numerov (see Hamming (1960)) for the above equation $y''=-k^2y$ have their roots on the unit circle for all real $k, h>0$. For this reason, and the fact that they also have order six local error, they are usually recommended for the numerical integration of equations of the form $y''=f(x)y+g(x)$ in which $f(x)<0$. Furthermore, one does not need to carry values of y' along in the calculations. Weighted against this advantage is of course the disadvantage that they are not self-starting. Computational comparison of the Gauss method with these methods is given in a later paragraph.

Consider the case $y''=k^2y$. The analysis of this equation takes a somewhat different turn from that of the preceding equation $y''=-k^2y$. In the preceding case we have oscillating solutions; here our solutions are exponential in nature. For this case we rely on the analysis given by Rutishauser (1960). Therefore we make a few preliminary remarks.

The solution of the differential equation $y''=k^2y$ written in matrix form is

$$\begin{bmatrix}y(x)\\ y'(x)\end{bmatrix}=e^{(x-x_0)A}\begin{bmatrix}y_0\\ y'_0\end{bmatrix} \text{ where } A=\begin{bmatrix}0 & 1\\ k^2 & 0\end{bmatrix}. \qquad (2.18)$$

This is a special case of a general result found for example in Birkhoff and Rota (1962).

It is easy to convince oneself that the above equation for $x = x_0 + nh$ can be written in the form

$$\begin{bmatrix} y(x) \\ y'(x) \end{bmatrix} = \begin{bmatrix} 1 + h^2k^2/2 + h^4k^4/24 + h^6k^6/720 + \dots & h + h^3k^6/6 + h^5k^5/120 + \dots \\ hk^2 + h^3k^4/6 + h^5k^6/720 + \dots & 1 + h^2k^2/2 + h^4k^4/24 + h^6k^6/720 \end{bmatrix}^n \begin{bmatrix} y_0 \\ y_0' \end{bmatrix}. \quad (2.19)$$

In order to use the techniques of Rutishauser effectively we expand $1/\Delta$ in the elements of the matrix of (2.16) in power series. This series will converge provided that $h^2k^2/18 < 1$.

Denoting this matrix by the symbol C, it can be seen that its elements are:

$$\begin{aligned} c_{11} &= 1 + h^2k^2/2 + k^4h^4/24 + h^6k^6/864 + \dots \\ c_{22} &= c_{11} \\ c_{12} &= h + h^3k^2/6 + k^4h^5/108 + \dots \\ c_{21} &= hk^2 + h^3k^4/6 + 11h^5k^6/1296 + \dots . \end{aligned} \quad (2.20)$$

We easily obtain

$$\lim_{h \to 0} \frac{e^{Ah} - C}{h^5} = \begin{bmatrix} 0 & k^4/1080 \\ k^6/270 & 0 \end{bmatrix} = K.$$

Thus the Gauss method is of order four by the definition of Rutishauser.

For the Runge–Kutta–Nystrom method Rutishauser obtains the matrix (here $k = 1$)

$$K = \begin{bmatrix} 0 & -1/120 \\ 1/480 & 0 \end{bmatrix}.$$

We now treat the relative error of the Gauss method for the equation under discussion in case a large number of integration intervals (large x, small h) is to be considered.

The maximum eigenvalue of our matrix C is

$$\lambda = c_{11} + \sqrt{(c_{12}c_{22})} = 1 + hk + h^2k^2/2 + h^3k^3/6 + h^4k^4/24 + 23k^5h^5/2592 + \dots . \quad (2.21)$$

Thus the relative error F (in the sense of Rutishauser) of the Gauss method is

$$F_\infty \sim \frac{kh - 1n\lambda}{h} = \frac{\log(e^{hk}) - \log\lambda}{h} = \log\left(1 + \frac{(e^{hk} - \lambda)}{\lambda}\right) \approx 7k^5h^4/12960$$

for large x and small h. Rutishauser (1960) calculates the relative error for the Runge–Kutta–Nystrom method for the equation $y'' = k^2y$ and finds that $F_\infty \approx h^4k^5/320$; for the Runge–Kutta method he obtains $F_\infty \approx h^4k^5/120$. A similar calculation to that above yields for the method of Hammer and Hollingsworth $F_\infty \approx h^4k^5/720$.

We consider three computational examples. We have written programs in FORTRAN for the CDC 1604 computer for the following additional methods, Runge–Kutta and Numerov.

In each of the three examples we take the step size $h = 0{\cdot}02$.

Our first example is the differential equation $y'' = (x^2 + 1)y$ with the initial conditions taken at $x = 0$ so that the solution is $e^{x^2/2}$. We take all necessary starting values as exact (see Table 1).

Example two is a Mathieu differential equation $y'' + 100(1 - 0{\cdot}1 \cos(2x))y = 0$ with the initial conditions taken at $x = 0$ as $y(0) = 1$, $y'(0) = 0$. Starting value for Numerov's method is taken from Runge–Kutta calculation (see Table 2).

Our third example is the Bessel differential equation $y'' + (100 + 1/(4x^2))y = 0$ with initial conditions taken at $x = 1$ so that the solution is $\sqrt{x}J_0(10x)$. Starting values were taken from the tables of Bessel functions British Association for the Advancement of Science (1958) to 10D (see Table 3).

Thus our Gauss method compares quite favourably with the two other methods under consideration in the three computational examples we have considered.

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Table 1

Differential equation $y'' = (x^2 + 1)y$

X	GAUSS	RUNGE–KUTTA	NUMEROV	EXACT (10D) MACHINE
1·0	1·648721272	1·648721264	1·648721287	1·648721271
2·0	7·389056121	7·389055819	7·389056409	7·389056099
3·0	90·01713188	90·01710938	90·01714644	90·01713130
4·0	2980·957995	2980·954707	2890·959682	2980·957987
5·0	268337·2769	268336·2736	268337·7249	268337·2864

Table 2

Differential equation $y'' + 100(1 - 0\cdot1 \cos(2x))y = 0$

X	GAUSS	RUNGE–KUTTA	NUMEROV	EXACT (7D)
1·0	−0·9084191	−0·9084380	−0·9084107	−0·9084179
2·0	0·2309663	0·2308945	0·2309647	0·2309590
3·0	0·2057556	0·2053593	0·2058659	0·2057667
4·0	−0·4265191	−0·4260468	−0·4266454	−0·4265317
5·0	0·9417347	0·9415266	0·9417662	0·9417373

Table 3

Differential equation $y'' + (100 + 1/(4x^2))y = 0$

X	GAUSS	RUNGE–KUTTA	NUMEROV	EXACT (7D)
2·0	0·2362089	0·2362150	0·2362056	0·2362085
3·0	−0·1495953	−0·1496406	−0·1495801	−0·1495937
4·0	0·0147367	0·0148323	0·0147085	0·1047338
5·0	0·1247968	0·1246737	0·1248295	0·1248002
6·0	−0·2240571	−0·2239581	−0·2240786	−0·2240592
7·0	0·2511054	0·2510909	0·2510999	0·2511049
8·0	−0·1972648	−0·1973748	−0·1972238	−0·1972606
9·0	0·0798972	0·0801276	0·0798261	0·0798900
10·0	0·0631926	0·0628991	0·0632743	0·0632007

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