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A Seventh Order Method for the Numerical Solution of Ordinary Differential Equations*

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Abstract. Modified multistep methods which combine some of the properties of Runge-Kutta methods and of linear multistep methods are capable of yielding stable high order algorithms with some useful properties. In this paper a two-step method requiring five derivative calculations per step and with seventh order accuracy is found. The order for a one-step method with the same number of derivative calculations would be no more than four. The coefficients in the method are given in exact (surd) form and also as 20D approximations.

In searching for high order formulae for the numerical solution of the initial value problem in ordinary differential equations, one naturally considers either linear multistep methods or Runge-Kutta methods. For an order of seven or more neither of these alternatives is attractive since, in the one case, we would need a six-step method and in the other we would need to use a method requiring nine derivative evaluations per step. However, modified multistep methods are available.[1],[2],[3],[4] These are methods which utilize information from previous steps as do linear multistep methods and which involve intermediate calculations as do Runge-Kutta methods.

For stable k-step methods requiring r intermediate calculations per

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step (that is, a total of $r + 2$ derivative calculations per step) a worthwhile target to aim for is an order $2k + r$. For $r = 0$ this was shown by Dahlquist[5] to be possible only for $k < 3$. It appears that for $r = 1$ it is possible up to $k = 7$ and for $r = 2$ up to $k = 15$. $r = 3$ is a particularly interesting case as the Runge-Kutta case, $k = 1$, does not exist.[6]

However, there is no reason to suspect that for some $k > 1$ such methods might not exist. Owing to the great labour of the manipulations involved, only the single case $k = 2$ is investigated here. The interesting result is that there is indeed a method of order seven. In fact, there is at least a two-parameter family, although only one of its members will be shown explicitly here. However, the method of derivation is given and, in fact, can easily be extended to cases of higher k.

Let $y' = f(x,y)$ be the differential equation for which a solution is sought and for our present purposes we suppose that f is differentiable arbitrarily often with respect to x and (the elements of the vector) y. We suppose that the solution is known at points x_{n-1}, $x_n = x_o + nh$. Denote $y_n = y(x_n)$ and $f_n = f(x_n, y_n)$. We seek a method for computing y_{n+1} in the form

$$y_{n+u} = a_1^0 y_n + a_1^{-1} y_{n-1} + h(b_1^0 f_n + b_1^{-1} f_{n-1})$$

$$y_{n+v} = a_2^0 y_n + a_2^{-1} y_{n-1} + h(b_2^1 f_{n+u} + b_2^0 f_n + b_2^{-1} f_{n-1})$$

$$y_{n+w} = a_3^0 y_n + a_3^{-1} y_{n-1} + h(b_3^2 f_{n+v} + b_3^1 f_{n+u} + b_3^0 f_n + b_3^{-1} f_{n-1})$$

$$\hat{y}_{n+1} = a_4^0 y_n + a_4^{-1} y_{n-1} + h(b_4^3 f_{n+w} + b_4^2 f_{n+v} + b_4^1 f_{n+u} + b_4^0 f_n + b_4^{-1} f_{n-1})$$

$$y_{n+1} = a^0 y_n + a^{-1} y_{n-1} + h(b^4 \hat{f}_{n+1} + b^3 f_{n+w} + b^2 f_{n+v} + b^1 f_{n+u} + b^0 f_n + b^{-1} f_{n-1})$$

where u, v, w are three numbers distinct from each other and from -1, 0, 1 and $a_1^0, a_1^{-1}, \ldots, b^{-1}$ are the constant coefficients for the method.

It is now our purpose to choose the various parameters so that y_{n+u}, y_{n+v}, y_{n+w}, $\hat{y}_{n+1}$ agree with their exact values with error $O(h^4)$ and so that y_{n+1} agrees with its exact value with error $O(h^8)$. As in [4], we shall identify the various coefficients as the numerators in the partial fraction expressions of certain rational functions $\varphi_1(z)$, $\varphi_2(z)$, $\varphi_3(z)$, $\varphi_4(z)$, $\varphi(z)$. We shall suppose that these functions are related by

$$b^1\varphi_1(z) + b^2\varphi_2(z) + b^3\varphi_3(z) + b^4\varphi_4(z) + (z-1)\varphi(z) = 0$$

and that φ_1, φ_2, φ_3, φ take the forms

$$\varphi_1(z) = \frac{-K_1}{(z-u)z^2(z+1)^2}$$

$$\varphi_2(z) = \frac{-K_2}{(z-v)z^2(z+1)^2}\left\{1 + \frac{L_{21}}{z-u}\left(1 + \frac{M_{21}}{z-u}\right)\right\}$$

$$\varphi_3(z) = \frac{-K_3}{(z-w)z^2(z+1)^2}\left\{1 + \frac{L_{31}}{z-u}\left(1 + \frac{M_{31}}{z-u}\right) + \frac{L_{32}}{z-v}\left(1 + \frac{M_{32}}{z-v}\right)\right\}$$

$$\varphi(z) = \frac{-1}{(z-1)^2z^2(z+1)^2}\left\{\frac{L_1}{z-u}\left(1 + \frac{M_1}{z-u}\right) + \frac{L_2}{z-v}\left(1 + \frac{M_2}{z-v}\right) + \frac{L_3}{z-w}\left(1 + \frac{M_3}{z-w}\right)\right\}$$

Let B denote the set of functions bounded in $\{z:|z| \geqq R\}$ where R is some real constant satisfying $R > \max\{1,|u|,|v|,|w|\}$. Then, using the type of analysis used in [4] we see that K_1, K_2, L_{21}, ... , M_3 must be chosen so that the following conditions are satisfied.

(1) The residue of $\varphi_1(z)$ at $z=u$ is -1,

(2) The residue of $\varphi_2(z)$ at $z=u$ is 0,

(3) The residue of $\varphi_2(z)$ at $z=v$ is -1,

(4) The residue of $\varphi_3(z)$ at $z=u$ is 0,

(5) The residue of $\varphi_3(z)$ at $z=v$ is 0,

(6) The residue of $\varphi_3(z)$ at $z=w$ is -1,

(7) The residue of $\varphi(z)$ at $z=u$ is 0,

(8) The residue of $\varphi(z)$ at $z=v$ is 0,

(9) The residue of $\varphi(z)$ at $z=w$ is 0,

(10) The residue of $\varphi(z)$ at $z=1$ is -1,

(11) $z^8\varphi(z)\epsilon B$,

(12) $z^9\varphi(z)\epsilon B$,

(13) $z^6\left\{b^1(1-u)\varphi_1(z) + b^2(1-v)\varphi_2(z) + b^3(1-w)\varphi_3(z)\right\}\epsilon B$,

(14) $z^7\left\{b^1(1-u)\varphi_1(z) + b^2(1-v)\varphi_2(z) + b^3(1-w)\varphi_3(z)\right\}\epsilon B$,

(15) $z^6\left\{b^1(1-u)u\varphi_1(z) + b^2(1-v)v\varphi_2(z) + b^3(1-w)w\varphi_3(z)\right\}\epsilon B$,

(16) $z^6\left\{\left(b^2(1-v)b_2^1 + b^3(1-w)b_3^1\right)\varphi_1(z) + b^3(1-w)b_3^2\varphi_2(z)\right\}\epsilon B$.

These constitute 16 independent conditions on u, v, w and the 15 constants $K_1, K_2, \ldots, M_3$. Hence, u, v, w cannot be chosen independently. A tedious calculation yields the following relationship between these numbers

$$3 + 7(uv + vw + wu) = (5 \pm 2\sqrt{22})(u + v + w + 3uvw)$$

where either value of the surd may be chosen. We select the values $v = \frac{1}{3}$, $w = \frac{2}{3}$, resulting in $u = (-493 + 4\sqrt{22})/819$ or its conjugate. As it happens, the conjugate value leads to an unstable method, so only the one value of u need be considered.

We are now in a position to compute K_1, K_2, ... , M_3 and, hence, the coefficients a_1^0, a_1^{-1}, ... , b^{-1}. First, we use (7), (8), (9) to compute M_1, M_2, M_3 and then (10), (11), (12) to find L_1, L_2, L_3. We now determine $b_1 = \lim_{z \to u}(z-u)^2\varphi(z)$, b_2 and b_3. M_{21}, M_{31}, M_{32} are now found from (2), (4), (5); K_1 is found from (1) and then K_2 and K_3 from the simultaneous equations (13) and (15). L_{21} is now given from (3) and L_{31}, L_{32} from the system (14) and (6). We are now in a position to compute the remaining coefficients and to substitute into (16) as a check. For the calculations performed by the author this check was indeed satisfied.

Values of the coefficients are given in Table I in algebraic and in decimal form. For the number $(\alpha+\beta\sqrt{22})/\gamma$ the integers α, β, γ are given as is the decimal value rounded to 20D. That a method of the form we are considering should be (asymptotically) stable, it is necessary that $|b^{-1}| \leqq 1$ and sufficient that $|b^{-1}| < 1$. In our case, it is found that $b^{-1} = -751 + 160\sqrt{22} \approx -0.53$ so that the method is stable.

To see how the method performs in the solution of real problems, two examples were selected. The equations were (a) $dy/dx = y$, (b) $dy/dx = -y^2/(1+x^2)$ in each case with initial value $y(o) = 1$. Using a step size $h = 1/n$ where n took on a number of integral values, the highest being 1000, the solutions were evaluated at $x = 1$. At this point the exact solutions are (a) $y(1) = e$, (b) $y(1) = 4/(4+\pi)$. Double length accuracy (26 octal digits) was used in the computations so that for most values of n used, rounding errors were insignificant compared with the truncation errors. The results found indicated that the truncation errors had the asymptotic forms (a) $1.7 \times 10^{-2} \cdot h^7$ (b) $-1.6 \times 10^{-3} \cdot h^7$ so that in either case, 30 decimal accuracy, for example, could be achieved with something like 10000 steps.

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TABLE I

	α	β	γ	
a_1^{-1}	3573 48727	-38 54416	5493 53259	0.61758 05966 20588 02121
a_1^{0}	1920 04532	38 54416	5493 53259	0.38241 94033 79411 97879
b_1^{-1}	790 01654	-3 12140	5493 53259	0.14114 34015 44339 82287
b_1^{0}	-523 38100	-8 59232	5493 53259	-0.10260 83933 98362 64633
a_2^{-1}	-73 05815	6 59016	5 31657	-7.92758 48293 62169 12157
a_2^{0}	78 37472	-6 59016	5 31657	8.92758 48293 62169 12157
b_2^{-1}	-4 47520	13878	5 31657	-0.71931 04014 15142 55364
b_2^{0}	-1769 07184	207 90000	675 20439	-1.17584 30710 62836 24075
b_2^{1}	-248 73684	22 64538	25 00757	-5.69909 80235 50856 99385
a_3^{-1}	-2307 00032	248 08500	49 68243	-23.01373 99926 73556 40526
a_3^{0}	2356 68275	-248 08500	49 68243	24.01373 99926 73556 40526
b_3^{-1}	-539 51980	-22 81995	198 72972	-3.25343 81526 74812 15826
b_3^{0}	-4 37253 79630	22536 17550	44167 68027	-7.50661 48265 39844 05295
b_3^{1}	-588 30744 33970	74 77481 18375	17 56892 17074	-13.52288 38441 74063 47633
b_3^{2}	13 53320	13 93235	40 74756	1.93586 34973 81829 94895

TABLE I (cont'd)

	α	β	γ	
a_4^{-1}	-3609 66187	1943 56296	49 58737	111.04554 38107 13772 93095
a_4^{0}	3659 24924	-1943 56296	49 58737	-110.04554 38107 13772 93095
b_4^{-1}	210 94684	741 45132	247 93685	14.87742 46203 01035 56676
b_4^{0}	-6 31513 79588	4 62481 58232	44083 17193	34.88217 92792 85014 55736
b_4^{1}	-2 71216 34824 37940	1 24595 63159 44878	4655 62378 75273	67.27110 69634 10131 18380
b_4^{2}	41 87502	-133 65846	91 50659	-6.39340 54062 96196 43986
b_4^{3}	-11 22984	8 86248	21 54385	1.40823 83540 13788 06289
a^{-1}	-751	160	1	-0.53347 84282 51271 26950
a^{0}	752	-160	1	1.53347 84282 51271 26950
b^{-1}	-2 42355	51629	2910	-0.06650 33457 30637 63826
b^{0}	-8 63124	1 84040	2667	0.03753 89718 42510 39455
b^{1}	-10 42768 14958 67067	2 22142 25284 35759	2404 08358 09774	-0.34467 43420 54428 78832
b^{2}	43371	-9225	358	0.28467 76972 87325 02551
b^{3}	-6 99300	1 50984	19765	0.44916 43349 95228 32616
b^{4}	5787	-1207	1182	0.10631 82554 08731 41086