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A CLASS OF MULTISTEP METHOD CONTAINING SECOND ORDER DERIVATIVES FOR SOLVING STIFF ORDINARY DIFFERENTIAL EQUATIONS*

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Abstract

In this paper a general k-step k-order multistep method containing derivatives of second order is given. In particular, a class of k-step $(k+1)th$-order stiff stable multistep methods for $k = 3 - 9$ is constructed. Under the same accuracy, these methods are possessed of a larger absolute stability region than those of Gear's [1] and Enright's [2]. Hence they are suitable for solving stiff initial value problems in ordinary differential equations.

§1. Introduction

For the initial value problem of first order ordinary differential equations

$$y' = f(x,y), \quad y(a) = \eta, \quad a \le x \le b, \tag{1}$$

we consider a k-step method which contains derivatives of second order

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i y'_{n+i} + h^2 \sum_{i=0}^{k} \gamma_i y''_{n+i}, \tag{2}$$

where $y_{n+i}, i = 0, 1, \cdots, k$, are numerical approximate solutions of solution $y(x)$ of (1) at $x = x_{n+i}$; further $y'_{n+i} = f(x_{n+i}, y_{n+i}), y''_{n+i} = f'_{n+i} = f'(x_{n+i}, y_{n+i})$. The characteristic polynomials of (2) are

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^i, \quad \sigma(\xi) = \sum_{i=0}^{k} \beta_i \xi^i, \quad \gamma(\xi) = \sum_{i=0}^{k} \gamma_i \xi^i.$$

Our purposes are: (i) construct a k-step, k-order method and give its error constants, (ii) construct for $k = 3 - 9$ a class of k-step, $(k+1)th$-order stiff stable method, which can be automatically generated by computer. For the same accuracy, the stability region of the methods in this paper is obviously larger than those of Gear's [1] and Enright's [2]. So they are suitable for solving initial value problems of stiff ordinary differential equations.

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§2. Construction of the Methods

Definition. *The method (2) is of order p, if for arbitrary function $y(x) \in C^{p+1}_{[a,b]}$, the following relation holds;*

$$L[y(x);h] = \sum_{i=0}^{k} \alpha_i y(x+ih) - h\sum_{i=0}^{k} \beta_i y'(x+ih) - h^2 \sum_{i=0}^{k} \gamma_i y''(x+ih)$$
$$= C_{p+1} h^{p+1} y^{(p+1)}(x) + O(h^{p+2}), \quad h \to 0, \tag{3}$$

where p and C_{p+1} are independent of $y(x)$, and $C_{p+1} \neq 0$ [3].

Lemma. *Let E be a shift operator such that $Ef(x) = f(x+h)$, and $\nabla f(x) = f(x) - f(x-h)$, $\Delta f(x) = f(x+h) - f(x)$, $Df(x) = \dfrac{df(x)}{dx}$. Suppose the function $f(x)$ is sufficiently differentiable. Then, the relations*

$$hD = \sum_{j=1}^{\infty} \frac{1}{j} \nabla^j, \quad (hD)^2 = \sum_{j=2}^{\infty} \sum_{i=1}^{j-1} \frac{1}{i(j-i)} \nabla^j \tag{4}$$

hold.

Proof. Because

$$E = e^{hD} = (1+\Delta) = (1-\nabla)^{-1}, \tag{5}$$

it follows, that

$$hD = -\ln(1-\nabla) = \sum_{j=1}^{\infty} \frac{1}{j} \nabla^j, \quad (hD)^2 = \sum_{j=2}^{\infty} \sum_{i=1}^{j-1} \frac{1}{i(j-i)} \nabla^j.$$

Theorem. *Suppose the coefficients in the k-step method*

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i y'_{n+i} + h^2 \sum_{i=0}^{k} \gamma_i y''_{n+i} \tag{6}$$

are

$$\alpha_{k-m} = (-1)^m \sum_{i=0}^{k} \left[\beta_i A_1^{(k-i)} + \sum_{j=2}^{k} (\beta_i A_j^{(k-i)} + \gamma_i B_j^{(k-i)}) \binom{j}{m} \right], \quad m = 0, 1;$$
$$\alpha_{k-m} = (-1)^m \sum_{j=m}^{k} \sum_{i=0}^{k} (\beta_i A_j^{(k-i)} + \gamma_i B_j^{(k-i)}) \binom{j}{m}, \quad m = 2(1)k. \tag{7}$$

Then the method (6) is of order k and possesses an error constant

$$C = \frac{1}{\sigma(1)} \sum_{i=0}^{k} (\beta_i A_{k+1}^{(k-i)} + r_i B_{k+1}^{(k-i)}), \tag{8}$$

where

$$A_j^{(l)} = \nabla^l A_j^{(0)}, \quad A_j^{(0)} = \frac{1}{j}, \quad j = 1(1)k;$$
$$B_j^{(l)} = \nabla^l B_j^{(0)}, \quad B_j^{(0)} = \sum_{i=1}^{j-1} \frac{1}{i(j-i)}, \quad j = 2(1)k, \ l = 0(1)k; \tag{9}$$
$$A_\nu^{(0)} = B_\nu^{(0)}, \quad \nu < 0.$$

Proof. In the same notation as in the lemma, there follows

$$L(y(x);h]=\Big[\sum_{i=0}^{k}\alpha_i E^i-(hD)\sum_{i=0}^{k}\beta_i E^i-(hD)^2\sum_{i=0}^{k}r_i E^i\Big]y(x).$$

From (1) one obtains

$$hD=\sum_{j=1}^{\infty}A_j^{(0)}\nabla^j,\quad (hD)^2=\sum_{j=2}^{\infty}B_j^{(0)}\nabla^j,$$

where

$$A_j^{(0)}=\frac{1}{j},\quad B_j^{(0)}=\sum_{i=1}^{j-1}\frac{1}{i(j-i)}.$$

Hence

$$L[y(x);h]=\Big[\sum_{i=0}^{k}\alpha_i E^i-E^k\Big(\sum_{j=1}^{\infty}\sum_{i=0}^{k}\beta_i A_j^{(0)}E^{-(k-i)}\nabla^j+\sum_{j=2}^{\infty}\sum_{i=0}^{k}r_i B_j^{(0)}E^{-(k-i)}\nabla^j\Big)\Big]y(x).$$

By the relations

$$\sum_{j=1}^{\infty}A_j^{(0)}E^{-(k-i)}\nabla^j=\sum_{j=1}^{\infty}A_j^{(k-i)}\nabla^j,\quad \sum_{j=2}^{\infty}B_j^{(0)}E^{-(k-i)}\nabla^j=\sum_{j=2}^{\infty}B_j^{(k-i)}\nabla^j,$$

where $A_j^{(l)}\triangleq\nabla^l A_j^{(0)},\quad B_j^{(l)}=\nabla^l B_j^{(0)},\quad A_\nu^{(0)}=B_\nu^{(0)}=0,\quad \nu\le 0,\quad l=0,1,\cdots,$

it holds that

$$L[y(x);h]=\Big[\sum_{i=0}^{k}\alpha_i E^i-E^k\Big(\sum_{j=1}^{\infty}\sum_{i=0}^{k}\beta_i A_j^{(k-i)}\nabla^j+\sum_{j=2}^{\infty}\sum_{i=0}^{k}r_i B_j^{(k-i)}\nabla^j\Big)\Big]y(x).$$

Let

$$\sum_{i=0}^{k}\alpha_i E^i=E^k\sum_{i=0}^{k}\Big[\sum_{j=1}^{k}\beta_i A_j^{(k-i)}\nabla^j+\sum_{j=2}^{k}r_i B_j^{(k-i)}\nabla^j\Big].\tag{10}$$

By the relation

$$E^k\nabla^{k+1}=O((hD)^{k+1}),\quad h\to 0,$$

we obtain

$$L[y(x);h]=O((hD)^{k+1}),\quad h\to 0.$$

So by definition the method (6) is of order k and the error constant is (8).
From (10) one obtains

$$\sum_{i=0}^{k}\alpha_i E^i=\sum_{m=0}^{j}(-1)^m\sum_{i=0}^{k}\Big[\sum_{j=1}^{k}\beta_i A_j^{(k-i)}+\sum_{j=2}^{k}r_i B_j^{(k-i)}\Big]\binom{j}{m}E^{k-m}.$$

Comparing the coefficients of E^{k-m}, E^k and E^{k-1} automatically leads to (7).

Corollary. If the coefficients of the k-step method

$$\sum_{i=0}^{k}\alpha_i y_{n+i}=hy'_{n+k}\tag{11}$$

are

$$\alpha_{k-m}=(-1)^m\sum_{j=1}^{k}A_j^{(0)}\binom{j}{m},\quad m=0,1;\quad \alpha_{k-m}=(-1)^m\sum_{j=m}^{k}A_j^{(0)}\binom{j}{m},\quad m=2(1)k,\tag{12}$$

then the method (11) is of order k.

§3. Construction of k-step $(k+1)$th-order Stiff Stable Method for $k = 3 - 9$

Suppose the k-step method is written as

$$\sum_{i=0}^{k} y_{n+i} = hy'_{n+k} + rh^2(y''_{n+k} + r_1 y''_{n+k-1} + r_2 y''_{n+k-2}). \tag{13}$$

From (7) one can obtain

$$\begin{aligned} \alpha_{k-m} &= (-1)^m \Big[1 + \sum_{j=2}^{k} (A_j^{(0)} + r(B_j^{(0)} + r_1 B_j^{(1)} + r_2 B_j^{(2)})\binom{j}{m}\Big], \quad m = 0, 1; \\ \alpha_{k-m} &= (-1)^m \sum_{j=m}^{k} \Big[\frac{1}{j} + r(B_j^{(0)} + r_1 B_j^{(1)} + r_2 B_j^{(2)})\Big]\binom{j}{m}, \quad m = 2(1)k. \end{aligned} \tag{14}$$

Let $C = 0$ in (8). Then, there follows

$$r = -1/(k+1)(B_{k+1}^{(0)} + r_1 B_{k+1}^{(1)} + r_2 B_{k+1}^{(2)}) \tag{15}$$

and the order of (13) is $k+1$. The characteristic polynomials of (13) are

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^i, \quad \sigma(\xi) = \xi^k \quad \gamma(\xi) = \gamma \xi^{k-2}(\xi^2 + \gamma_1 \xi + r_2).$$

Let the test equation be $y' = \lambda y$, Re $\lambda < 0$. The absolutely stable polynomial is then

$$\pi(\xi, \mu) = \rho(\xi) - \mu\sigma(\xi) - \mu^2\gamma(\xi), \quad \mu = h\lambda,$$

and the absolute stability region is

$$\Omega = \{\mu \in C | \pi(\xi, \mu) = 0 \text{ module of all roots less then } 1\}. \tag{16}$$

Let

$$\gamma(\xi) = r\xi^{k-2}(\xi^2 + r_1\xi + r_2) = r\xi^{k-2}(\xi - a)(\xi - b).$$

Then,

$$r_1 = -(a+b), \quad r_2 = ab,$$

where a, b are parameters. To make the method (13) stable at infinity[2], $|a| < 1$ and $|b| < 1$ should be fulfilled.

For the constructed method to be stiff stable, assume $a = -0.9(0.1)0.9$, $b = -0.9(0.1)0.9$ for the given k, a and b and calculate r in (15) and α_i in (14), respectively. Then, decide by using Schur's rule the zeros of polynomial $\frac{\rho(\xi)}{\xi - 1}$, and whether the module of all the zeros are less than 1. If they did be, then the boundary curve of the absolute stability region will be calculated, so that the method possesses the least D (see the figure); otherwise, change the parameter a or b and repeat the procedure. For $k = 3 - 9$, we obtain a class of stiff stable methods. Their coefficients are listed in Table 1. Letting $r = 0$ in the method (13), one obtains Gear's method[1]. Table 2 is a comparison of D among the methods (13), Gear's [1] and Enright's [2] methods.

Table 1. The coefficients of $\sum_{i=0}^{k} \alpha_i y_{n+i} = h y'_{n+k} + r h^2 (y''_{n+k} + r_1 y''_{n+k-1} + r_2 y''_{n+k-2})$

k	order	a	b	r_1	r_2	r	α_0	α_1	α_2
3	4	0.2	0.2	-0.4	0.4	-0.264084337	-0.0798123479	0.570423126	-0.190140915
4	5	0.5	0.2	-0.7	0.1	-0.224299014	0.0331776738	-0.264174938	1.00373840
5	6	0.9	0.6	-1.5	0.54	-0.190379441	-0.0175530910	0.148020744	-0.662310839
6	7	0.9	0.9	-1.8	0.81	-0.174428642	0.0096614957	-0.0864475369	0.363031983
7	8	0.9	0.9	-1.8	0.81	-0.166893125	-0.006171703	0.059642488	-0.264160156
8	9	0.9	0.9	-1.8	0.81	-0.161096334	0.0043417811	-0.045653220	0.219666839
9	10	0.9	0.9	-1.8	0.81	-0.156390250	-0.003245949	0.0370801091	-0.194560230

α_3	α_4	α_5	α_6	α_7	α_8	α_9
1.41079807						
-2.34766388	1.574942161					
1.76672173	-3.05083084	1.81595135				
-1.08107376	2.28283787	-3.40031338	1.91230392			
0.725362659	-1.53838730	2.63782978	-3.55582428	1.94170475		
-0.644005477	1.30801105	-2.13331795	3.03248119	-3.71018600	1.96866322	
0.622236431	-1.36136627	2.19001484	-2.88896370	3.46972752	-3.86471748	1.99379539

Table 2. Comparing of least D.

order	method (13)		Gear method [1]		Enright method [2]	
	k	min D	k	min D	k	min D
4	3	0.05	4	0.7	2	A-stability
5	4	0.05	5	2.4	3	0.1
6	5	0.05	6	6.1	4	0.52
7	6	0.1	—	—	5	1.4
8	7	0.25	—	—	6	2.7
9	8	0.55	—	—	7	5.3
10	9	1.0	—	—	—	—

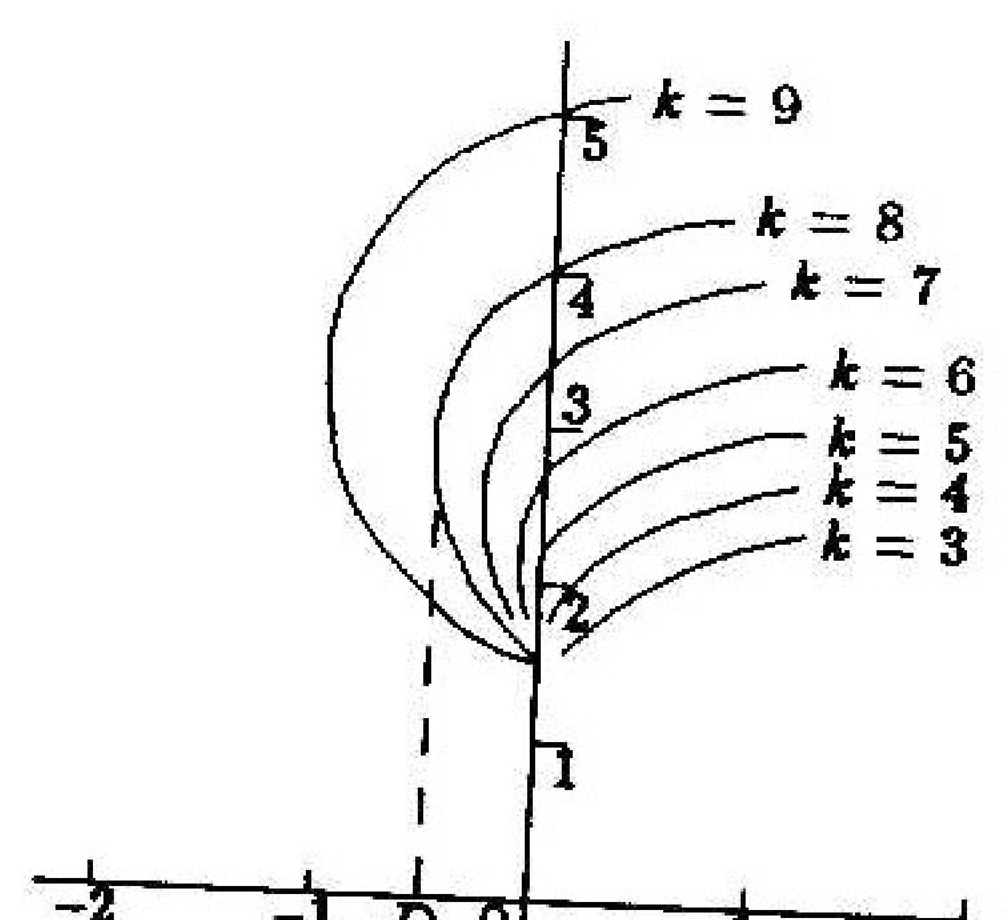

Fig. Stability regions for methods (13)

References

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