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Some A-Stable Methods for Stiff Ordinary Differential Equations

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Abstract. This paper gives some A-stable methods of order $2n$, with variable coefficients, based on Hermite interpolation polynomials, for the stiff system of ordinary differential equations, making use of n starting values. The method is exact if the problem is of the form $y'(t) = Py(t) + Q(t)$, where P is a constant and $Q(t)$ is a polynomial of degree $2n$.

1. Introduction. Many physical problems lead to ordinary differential equations with a property given by the following definition:

Definition 1. A system of ordinary differential equations $y'(t) = f(t, y)$, $y(a) = \mathcal{Y}$ is said to be stiff if the eigenvalues of the matrix $\partial f(t, y)/\partial y$ have negative real parts at every time t and differ greatly in magnitude.

A linear k-step method with constant coefficients for the numerical solution of ordinary differential equations is given by

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i y'_{n+i}, \quad \text{where } \alpha_k \neq 0 \text{ and } |\alpha_0| + |\beta_0| > 0. \tag{1.1}$$

Stiff equations present a difficulty in numerical integration, since the integration interval is determined by the fastest rate and the region of integration is determined by the slowest rate. Conventional methods of the form (1.1) are unstable if the step size used is much greater than the smallest time constant. Dahlquist [1] introduced the concept of A-stability in connection with the integration of stiff systems of differential equations. A-stability is defined as:

Definition 2. A k-step method is called A-stable if all the solutions of (1.1) tend to zero as $n \to \infty$, when the method is applied with fixed positive h to any differential equation of the form $dy/dt = \lambda y$, where λ is a complex constant with negative real part.

Dahlquist [1] has also shown that if (1.1) is to be stable for all λ, such that $\operatorname{Re}(h\lambda) \leq 0$, then the order of the method cannot exceed two. He also showed that the best method in this sense is the trapezoidal rule. In order to achieve greater accuracy and order, we study nonlinear methods (see Treanor [2]) or methods with variable coefficients. Norsett [3] derived a class of A-stable methods with variable coefficients of order n using Lagrangian interpolation polynomials passing through the n starting values.

In this paper, we have derived an integration method of order $2n$ with variable

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coefficients using Hermite interpolation polynomials passing through the n starting values. A proof that the present method is A-stable in the sense of Dahlquist [1] is included in Section 3.

2. Derivation of the Method. Let the problem be defined by the equation

$$y'(t) = f(t, y), \qquad y(a) = \mathcal{Y} \tag{2.1}$$

over the interval $I = [a, b]$. Choose $t_n \in I$ and define $t_{n-i} = t_n - ih$. It is assumed that the solution of (2.1) is known at the n starting values ($i = 0, 1, \cdots, n-1$).

Instead of considering the equation $y'(t) = f(t, y)$, we consider the function $y'(t) + Py(t)$. The main steps in the argument are as follows:

1. Approximate the function $y'(t) + Py(t)$ by the Hermite interpolation polynomial $T(t)$ at the points t_{n-i}, $i = 0, 1, \cdots, n-1$.
2. Integrate the exact differential equation $y'(t) + Py(t) = T(t)$ between the limits t_n to t_{n+1}.
3. Choose P as an approximation to $-(\partial f/\partial y)_n$.
4. Determine the order of the method and show that it is A-stable.

Thus approximating the function $y'(t) + Py(t)$ by the Hermite interpolation polynomial, we obtain

$$y'(t) + Py(t) = \sum_{i=1}^{n} h_i(t)(f_i + Py_i) + \sum_{i=1}^{n} \bar{h}_i(t)(f_i' + Pf_i) + TE, \tag{2.2}$$

where $h_i(t)$ and $\bar{h}_i(t)$ are the standard Hermite functions of degree $2n$ (see Ralston [4, p. 62]), $f_i = f(t_i, y_i)$ and $f_i' = f'(t_i, y_i)$.

$$TE = \frac{1}{2n!} F^{(2n)}(\xi)\pi^2(t), \quad \text{where } F(t) = f(t) + Py(t),$$

and $a < \xi < b$.

Obviously, (2.2) is an exact differential equation. Integrating (2.2) from t_n to t_{n+1}, we obtain

$$y_{n+1} = \bar{e}^{Ph} y_n + \bar{e}^{Pt_{n+1}} \left[\sum_{i=1}^{n} (H_i F_i + \bar{H}_i F_i') \right] + R_n, \tag{2.3}$$

where

$$H_i = \int_{t_n}^{t_{n+1}} e^{Pt} h_i(t)\, dt, \qquad \bar{H}_i = \int_{t_n}^{t_{n+1}} e^{Pt} \bar{h}_i(t)\, dt,$$

$$R_n = \frac{\bar{e}^{Pt_{n+1}}}{(2n)!} \int_{t_n}^{t_{n+1}} e^{Pt} F^{(2n)}(\xi)\pi^2(t)\, dt.$$

Since P is an approximation to $-(\partial f/\partial y)_n$ for a single differential equation, a natural choice of P is

$$P = -\frac{f_n - f(t_n, y_{n-1})}{y_n - y_{n-1}}. \tag{2.4}$$

For a system of equations, the choice of P may depend on the efficiency of the routine to evaluate $\bar{e}^{Ph}$, where P is a matrix. A simple choice of P is the diagonal matrix

$$P_{ii} = -\frac{f_n^i - f^i(t_n, y_n^1, \cdots, y_{n-1}^i, \cdots, y_n^s)}{y_n^i - y_{n-1}^i}. \tag{2.5}$$

3. The A-Stability and Order of the Method (2.3). We shall show here that (2.3) is of order $2n$ and is A-stable.

THEOREM. *The method* (2.3) *is A-stable and of order* $2n$ *with the usual definition of A-stability given by Dahlquist* [1].

Proof. Let $f(t, y) = \lambda y$, where λ is a complex constant and Re $\lambda < 0$. Thus, $P = -\lambda$. Obviously, $F_i = f_i + Py_i = \lambda y_i - \lambda y_i$ is zero for every i. Similarly, $F_i' = f_i' + Pf_i = \lambda y_i' - \lambda y_i'$ is also zero for every i. Hence, (2.3) reduces to $y_{n+1} = e^{\lambda h} y_n$. Since Re $\lambda < 0$, $y_n \to 0$ as $n \to \infty$ for any fixed h and hence (2.3) is A-stable.

Taking $s = (t - t_n)/h$, (2.3) can be rewritten as

$$y_{n+1} = \bar{e}^{Ph} y_n + h\bar{e}^{Ph}\left[\sum_{i=1}^{n} (H_i F_i + \bar{H}_i F_i')\right] + R_n, \tag{3.1}$$

where

$$H_i = \int_0^1 e^{Phs} h_i(s)\, ds, \qquad \bar{H}_i = \int_0^1 e^{Phs} \bar{h}_i(s)\, ds, \qquad i = 1, 2, \cdots, n,$$

$$\begin{aligned} R_n &= \frac{h^{2n+1}}{2n!} \bar{e}^{Ph} \int_0^1 e^{Phs} F^{(2n)}(\xi) \pi^2(s)\, ds \\ &= \frac{h^{2n+1}}{2n!} \bar{e}^{Ph} \int_0^1 F^{(2n)}(\xi) \pi^2(s)\, ds + O(h^{2n+2}) \\ &= \frac{h^{2n+1}}{2n!} \bar{e}^{Ph} F^{(2n)}(\xi) \int_0^1 \pi^2(s)\, ds + O(h^{2n+2}) \\ &= h^{2n+1} \bar{e}^{Ph} F^{(2n)}(\xi) \Lambda_n + O(h^{2n+2}), \end{aligned}$$

where $\Lambda_n = (1/2n!) \int_0^1 \pi^2(s)\, ds$ and hence the method (2.3) is of order $2n$.

4. A Few Particular Cases. If we look at (3.1), we find that the integrations involved to determine H_i, $\bar{H}_i$ and R_n are of the form

$$I_n = \int_0^1 e^{Phs}\left(\sum_{i=1}^{N} A_i s^i\right) ds,$$

where N is a positive integer depending on n. The coefficients H_i and $\bar{H}_i$ are of the form

$$H_i = \sum_{r=1}^{2n} a_r \left(\frac{1}{Ph}\right)^r e^{Ph} + h \sum_{r=1}^{2n} b_r \left(\frac{1}{Ph}\right)^r,$$

$$\bar{H}_i = \sum_{r=1}^{2n} \alpha_r \left(\frac{1}{Ph}\right)^r e^{Ph} + h \sum_{r=1}^{2n} \beta_r \left(\frac{1}{Ph}\right)^r.$$

Taking a simple case $n = 1$, we have

$$h_1(t) = 1; \qquad \bar{h}_1(t) = t - t_1; \qquad \pi(t) = t - t_1;$$

$$h_1(s) = 1; \qquad \bar{h}_1(s) = s; \qquad \pi(s) = s;$$

$$H_1 = \int_0^1 e^{Phs}\, ds = \frac{1}{Ph}(e^{Ph} - 1),$$

$$\bar{H}_1 = \int_0^1 s e^{Phs}\, ds = \left(\frac{1}{Ph} - \frac{1}{P^2h^2}\right)e^{Ph} + \frac{1}{P^2h^2},$$

$$\Lambda_1 = \frac{1}{2}\int_0^1 s^2\, ds = \frac{1}{6},$$

$$a_1 = 1; \quad a_2 = 0; \quad b_1 = -1; \quad b_2 = 0;$$

$$\alpha_1 = 1; \quad \alpha_2 = -1; \quad \beta_1 = 0; \quad \beta_2 = 1.$$

Similarly, for $n = 2$,

$$h_1(t) = \left\{1 + \frac{2}{h}(t - t_1)\right\}\frac{(t - t_2)^2}{h^2}$$

$$h_2(t) = \left\{1 - \frac{2}{h}(t - t_2)\right\}\frac{(t - t_1)^2}{h^2}$$

$$\bar{h}_1(t) = \frac{1}{h^2}(t - t_1)(t - t_2)^2,$$

$$\bar{h}_2(t) = \frac{1}{h^2}(t - t_1)^2(t - t_2),$$

$$\pi(t) = (t - t_1)(t - t_2).$$

Using $t - t_2 = hs$, we obtain

$$h_1(s) = (2s + 3)s^2,$$

$$h_2(s) = (1 - 2s)(s + 1)^2,$$

$$\bar{h}_1(s) = (s + 1)s^2,$$

$$\bar{h}_2(s) = (s + 1)^2 s,$$

$$\pi(s) = s(s + 1).$$

The simple integration gives the required coefficients. The values of a_r, b_r, α_r, β_r and Λ_n are given in Table 1 for $n = 0(1)4$.

5. Numerical Comparison. A simple example

$$Y'(t) = -100ty^2, \qquad Y(1) = 1/51 \tag{5.1}$$

has been chosen to show the advantages of the present method over the method developed by Norsett [3]. The exact solution of (5.1) is

$$Y(t) = 1/(1 + 50t^2).$$

We have solved (5.1) with the method of Norsett and the present method for different values of n and for different step sizes, on an IBM 360 in single precision. Some of the results are given in Table 2. Our results are closer to the exact solution, even when a smaller number of starting values are used.

TABLE 1-a

n	i	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8
1	1	1	0						
2	1	5	−12	18	−12				
	2	−4	12	−18	12				
3	1	10	−33	83	−148.5	168	−90		
	2	9	−24	44	−48	24	0		
	3	−18	57	−127	196.5	−192	90		
4	1	$\frac{47}{3}$	$\frac{-550}{9}$	$\frac{10523}{54}$	$\frac{-8891}{18}$	$\frac{8620}{9}$	$\frac{-12020}{9}$	$\frac{10740}{9}$	$\frac{-4620}{9}$
	2	64	−240	728	−1734	3120	−3990	3240	−1260
	3	−36	150	$\frac{-1009}{2}$	$\frac{2643}{2}$	−2580	3540	−3060	1260
	4	$\frac{-128}{3}$	$\frac{1360}{9}$	$\frac{-11296}{27}$	$\frac{8158}{9}$	$\frac{-13480}{9}$	$\frac{16070}{9}$	$\frac{-12360}{9}$	$\frac{4620}{9}$

TABLE 1-b

n	i	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8
1	1	−1	0						
2	1	0	0	−6	12				
	2	−1	0	6	−12				
3	1	0	0	−3.5	25.5	−78	90		
	2	0	0	−8	24	−24	0		
	3	−1	0	11.5	−49.5	102	−90		
4	1	0	0	$-\frac{8}{3}$	$\frac{238}{9}$	$-\frac{400}{3}$	$\frac{3590}{9}$	$-\frac{2040}{3}$	$\frac{1540}{3}$
	2	0	0	−13.5	121.5	−540	1380	−1980	1260
	3	0	0	0	−54	360	−1110	1800	−1260
	4	−1	0	$\frac{97}{6}$	$-\frac{1691}{18}$	$\frac{940}{3}$	$-\frac{6020}{9}$	$\frac{2580}{3}$	$-\frac{1540}{3}$

TABLE 1-c

n	i	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	Λ_n
1	1	1	-1							$1/3$
2	1	2	-5	8	-6					$31/30$
	2	4	-8	10	-6					
3	1	3	-10	25.5	-46.5	54	-30			$\frac{869}{105}$
	2	18	-57	136	-228	240	-120			
	3	9	-24	48.5	-70.5	66	-30			
4	1	4	$-\frac{47}{3}$	$\frac{452}{9}$	$-\frac{769}{6}$	$\frac{752}{3}$	$-\frac{1060}{3}$	320	-140	$\frac{74113}{630}$
	2	48	-184	574	-1416	2658	-3570	3060	-1260	
	3	72	-264	781	-1813.5	3192	-4020	3240	-1260	
	4	16	$-\frac{152}{3}$	$\frac{1178}{9}$	$-\frac{1624}{6}$	$\frac{1298}{3}$	$-\frac{1510}{3}$	380	-140	

TABLE 1-d

n	i	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8
1	1	0	1						
2	1	0	0	-2	6				
	2	0	1	-4	6				
3	1	0	0	-1	$\frac{15}{2}$	-24	30		
	2	0	0	-8	48	-120	120		
	3	0	1	-6	$\frac{39}{2}$	-36	30		
4	1	0	0	$\frac{-2}{3}$	$\frac{20}{3}$	-34	$\frac{310}{3}$	-180	140
	2	0	0	-9	$\frac{171}{2}$	-408	1140	-1800	1260
	3	0	0	-18	144	-582	1410	-1980	1260
	4	0	1	$\frac{-22}{3}$	$\frac{193}{6}$	-96	$\frac{580}{3}$	-240	140

TABLE 2

h	$Y(t)$	*Norsett's Method* $n = 3$	*Present Method* $n = 2$	*Exact*
$\frac{1}{16}$	$Y(10)$	.19995554(−3)	.19996018(−3)	.19996001(−3)
$\frac{1}{8}$	$Y(10)$	.19991486(−3)	.19996310(−3)	.19996001(−3)
	$Y(20)$	.49994562(−4)	.49997695(−4)	.49997500(−4)
$\frac{1}{4}$	$Y(10)$	.19906134(−3)	.20000938(−3)	.19996001(−3)
	$Y(20)$	.49940176(−4)	.50000607(−4)	.49997500(−4)

6. Remarks. In order to apply (2.3), we need to know the first derivative of $f(t, y)$. If the exact derivative is not available, the numerical differentiation may be used. But in such a case, we are not sure whether the order of this method is preserved or not. It is also hoped that some generating functions and recurrence relations may be derived to obtain H_i, and H_i directly.

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