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OPTIMAL ORDER MULTISTEP METHODS WITH AN ARBITRARY NUMBER OF NONSTEPPOINTS

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Abstract.

In this paper optimal order, k-step methods with one nonstep point for the numerical solution of $y' = f(x,y)$ $y(a) = \eta$, introduced by Gragg and Stetter (1) are extended to an arbitrary number s of nonstep points. These methods have order $2k + 2s$, are proved stable for $k \leq 8$, $s \geq 2$, and not stable for large k.

1. Introduction.

A linear k-step method for the numerical solution of $y' = f(x,y)$ $y(a) = \eta$, can be written in the form

$$y_{n+k} = \sum_{i=0}^{k-1} \alpha_i y_{n+i} + h \sum_{i=0}^{k} \beta_i f_{n+i} \tag{1.1}$$

where y_n is a numerical approximation to the solution y at the point $x_n = a + nh$, $n=0,1,2,..$ and $f_n = f(x_n,y_n)$.

(1.1) is called stable if the polynomial

$$\rho(z) = z^k - \sum_{i=0}^{k-1} \alpha_i z^i$$

has all its roots on the unit disc and the roots of modulus one are simple.

To the method (1.1) we can associate an operator L_0 defined on the class of continously differentiable functions by

$$L_0[y(x);h] = y(x+kh) - \sum_{i=0}^{k-1} \alpha_i y(x+ih) - h \sum_{i=0}^{k} \beta_i y'(x+ih) \tag{1.3}$$

Suppose y is $p+2$ times continously differentiable. Then the method is of order p if

$$L_0[y(x);h] = C_{p+1} h^{p+1} y^{(p+1)}(x) + O(h^{p+2})$$

and $C_{p+1} \neq 0$.

Using sufficiently accurate startingvalues a stable method of order p produces a discretization error of order $O(h^p)$ where the $O(h^p)$ term increases with the error constant $C_{p+1}/\Sigma\beta_i$.

It therefore seems advantageous to use stable methods whose order p is as high as possible and errorconstant as small as possible. There exists k-step methods (1.1) of order $2k$. However Dahlquist has shown that the order of a stable linear method (1.1) cannot exceed $k+2$.

One way to get stable methods of optimal order is to introduce in (1.1) the value of f in a nonsteppoint x_{n+r} where $k-1<r<k$.Then

$$y_{n+k} = \sum_{i=0}^{k-1} \alpha_i y_{n+i} + h \sum_{i=0}^{k} \beta_i f_{n+i} + h\beta_r f_{n+r}$$

It has been proved by Gragg and Stetter (1) and Danchick (2) that r can be chosen so that these methods have the optimal order $2k + 2$ and are stable for $k \leq 6$.

It is the purpose of this paper to show that we can introduce in (1.1) the values of f in s nonsteppoints $x_{n+r_1}, \dots, x_{n+r_s}$ and obtain a $2k + 2s$ order method which in addition to the results for $s = 1$ is stable for $s \geq 2$ and $k \leq 8$.
The method can be written in the form

$$y_{n+k} = \sum_{i=0}^{k-1} \alpha_i y_{n+i} + h \sum_{i=0}^{k} \beta_i f_{n+i} + h \sum_{j=1}^{s} \beta_{r_j} f_{n+r_j} \qquad (1.4)$$

The values of y in the nonsteppoints will generally not be known and have to be supported by an accurate, independent method. This gives at least s extra functionevaluations pr. integrationstep and restricts the number of nonsteppoints to be used in practice.

2. The existence and coefficients of the optimal order nonstepmethod.

To the method (1.4) we associate the operator L_s given by

$$L_s[y(x);h] = y(x+kh) - \sum_{i=0}^{k-1} \alpha_i y(x+ih) - h \sum_{i=0}^{k} \beta_i y'(x+ih) - h \sum_{j=1}^{s} \beta_{r_j} y'(x+r_j h) \qquad (2.1)$$

We also define

$$H_0 = 0 \quad H_i = H_{i-1} + \frac{1}{i} \quad i = 1,2,\dots \qquad (2.2)$$

$$p(i) = (-1)^{k-i} \cdot i! \cdot (k-i)!(k-r_1)\dots(k-r_s) \quad i = 0(1)k \qquad (2.3)$$

$$p(r_j) = \prod_{i=0}^{k} (r_j - i) \prod_{\substack{i=1 \\ i\neq j}}^{s} (r_j - r_i) \tag{2.4}$$

$$t(i) = H_{k-i} - H_i + \sum_{j=1}^{s} \frac{1}{r_j - i} \tag{2.5}$$

$$t(r_j) = \sum_{i=0}^{k} \frac{1}{r_j - i} + \sum_{\substack{i=1 \\ i\neq j}}^{s} \frac{1}{r_j - r_i} \tag{2.6}$$

Theorem 2.1.

Suppose

(i) k, s are given natural numbers

(ii) y is a $2k + 2s + 1$ times continously differentiable function on an interval $[a,b]$ and $x \in [a,b]$

Then we can find nonsteppoints $r_1, \ldots, r_s$ where $k-1<r_1<r_2<\ldots<r_s<k$ (unique in this interval) and a point $\xi \in (x, x+kh)$ such that

$$L_s[y(x);h] = \frac{-M}{(2k+2s+1)!} h^{2k+2s+1} y^{(2k+2s+1)}(\xi) \tag{2.7}$$

where

$$M = -\frac{p(k)^2}{2t(k)} \tag{2.8}$$

The coefficients in L_s are uniquely given by

$$b_i = \frac{M}{p(i)^2} \quad i = 0(1)k \quad b_{r_j} = \frac{M}{p(r_j)^2} \quad j = 1(1)s \tag{2.9}$$

$$a_i = 2t(i) \cdot b(i) \quad i = 0(1)k-1 \tag{2.10}$$

r_j $j = 1(1)s$ is the unique solution in $(k-1,k)$ of the system $t(r_j) = 0$ $j = 1(1)s$ of equations.

Proof.

Suppose $a_1, \ldots, a_N$ is N distinct real numbers, and let y be $2N-1$ continously differentiable on a set containing $a_1, \ldots a_N$. Then there exists unique constants A_j, B_j and a ξ in the smallest intervall containing $a_1, \ldots a_N$ such that

$$\sum_{j=1}^{N} A_j y(a_j) + \sum_{j=1}^{N} B_j y'(a_j) + \frac{y^{(2N-1)}(\xi)}{(2N-1)!} = 0 \tag{2.11}$$

The existence of this formulae follows from a generalization (similar to Danchick (2) p. 205) of the Hermite interpolation formulae. By inserting polynomials with suitable zeros we can find expressions for the coefficients A_j and B_j.

Letting $a_1 = x_n, a_2 = x_{n+1}, \ldots, a_k = x_{n+k-1}, a_{k+1} = x_{n+r_1}, \ldots, a_{k+s} = x_{n+r_s}$,

$a_{k+s+1} = x_{n+k}$, $N = k+s+1$ we get a formulae of the form

$$\sum_{i=0}^{k} \alpha_i y(x+ih) + \sum_{j=1}^{s} \alpha_{r_j} y(x+r_j h) + h \sum_{i=0}^{k} \beta_i y'(x+ih)$$

$$+ h \sum_{j=1}^{s} \beta_{r_j} y'(x+r_j h) = \frac{y^{(2k+2s+1)}(\xi)}{(2k+2s+1)!}$$

Now in order to obtain (2.7) we choose $r_1, \ldots, r_s$ so that $\alpha_{r_j} = 0$

$j = 1(1)s$. It turns out that this is equivalent to the system $t(r_j) = 0 \quad j = 1(1)s$ of equations, where $t(r_j)$ is given by (2.6). Let

$$D_i^0 = \{(r_1, \ldots, r_s) \mid i-1 < r_1 < r_2 < \ldots < r_s < i\}$$

Then we have the following result:

Lemma 2.1.

For $i = 1(1)k$ the system of equations $t(r_j) = 0 \quad j = 1(1)s$, where $t(r_j)$ is given by (2.6) has a unique solution in the set D_i^0. If $(r_1, \ldots, r_s)$ is a solution if $t(r_j) = 0 \quad j = 1(1)s$ then $r_j \in [0,k] \; j = 1(1)s$.

Proof of lemma 2.1.

Let the polynomial

$$g(r_1, \ldots, r_s) = \prod_{j=1}^{s} \{r_j(r_j-1)\ldots(r_j-k)(r_j-r_{j+1})\ldots(r_j-r_s)\}$$

be given on the set

$$D_i = \{(r_1, \ldots, r_s) \mid i-1 \le r_1 \le \ldots \le r_s \le i\}$$

D_i^0 is the interior of D_i, $g = 0$ on the boundary of D_i and $g = 0$ on D_i^0. It follows since D_i is compact that g has an extremum on D_i^0. So we can find $r_1,\ldots,r_s$ in D_i^0 such that $\frac{\partial g}{\partial r_j}(r_1,\ldots,r_s) = 0$. Then $\frac{\partial g}{\partial g_j}/g = t(r_j) = 0$ at the same point. This proves the existence part of the lemma. For reasons of space the proof for the uniqueness must be omitted. Suppose $(r_1,\ldots,r_s)$ is a solution of $t(r_j) = 0 \quad j = 1(1)s$. We can put $r_1 \leq r_2 \leq \cdots \leq r_s$. Then for $r_1 \in (-\infty,0)$ we have $t(r_1) < 0$, and for $r_s \in (k,\infty)$ we have $t(r_s) > 0$, a contradiction in both cases.

This completes the proof of lemma 2.1 and also establish theorem 2.1

3. Stability properties of the optimal order nonstepmethod.

Theorem 3.1.

The method given by (2.7) is stable for $k \leq 6$ if $s = 1$, for $k \leq 8$ if $s = 2$, and for $k \leq 12$ if $s \geq 3$.

To all $s \geq 1$ we can find a constant $K(s)$ so that $k \geq K(s)$ implies instability of the method given by (2.7).

Proof.

The result for $s = 1$ has been proved by Gragg and Stetter (1) and Danchick (2). Using $1/(r_j-i) < 1/(k-i) \quad i = 0(1)k-1$ we can prove by direct calculation of $t(i)$ that $\alpha_i \geq 0 \quad i = 0(1)k-1$ for $k \leq 8$ if $s = 2$ and for $k \leq 12$ for $s \geq 3$. It follows (see Danchick (2) p. 207) since $\Sigma\, \alpha_i = 1$ that the polynomial $\rho(z) = z^k - \sum_{i=0}^{k-1} \alpha_i z^i$ has all its roots except $z = 1$ in the interior of the unitdisc. Hence stability follows. By showing that $\alpha_i/\binom{k}{i}$ tends to infinity for some i when k tends to infinity the instability follows. (See Marden (3) p. 124).

4. Concluding remark.

We note that the methods given by (2.7) are stable for most practical values of k. The method has $2k + 2s + 1$ parameters that can be chosen freely. Therefore the order $2k + 2s$ is the maximum order that can normally be obtained with this number of parameters. We then look at the errorconstant $C_{2k+2s+1}/(\Sigma\,\beta_i + \Sigma\,\beta_{r_j}) \approx C_{2k+2s+1}$ for stable methods.

If the order is fixed we find by increasing the number of nonstep points that the errorconstant will decrease.

The formulae (2.7) is for $k > 1$ a generalization of Lobatto quadrature and should in many cases be well suited for numerical integration.

References.

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