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Linearly Implicit Variable Coefficient Methods of Lambert–Sigurdsson Type

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Lambert & Sigurdsson's linear multistep formulae with variable matrix coefficients for the numerical integration of stiff systems are analysed. The maximum attainable order of an A-stable formula of this type is determined. We associate with a given linear multistep method a variable coefficient formula which has the same order and stability properties and does not require the solution of nonlinear systems. Some numerical examples are presented.

1. Introduction

VARIABLE COEFFICIENT METHODS for the numerical solution of initial value problems in ordinary differential equations go back to Brunner (1967) and Lambert (1970). In 1972, Lambert & Sigurdsson developed a class of methods

$$\sum_{j=0}^{k}\left[a_j^{(0)}I+\sum_{s=1}^{S}a_j^{(s)}h^sQ_n^s\right]\mathbf{y}_{n+j}=h\sum_{j=0}^{k}\left[b_j^{(0)}I+\sum_{s=1}^{S-1}b_j^{(s)}h^sQ_n^s\right]\mathbf{f}_{n+j}, \tag{1.1}$$

for the problem

$$\mathbf{y}'=\mathbf{f}(x,\mathbf{y}),\qquad \mathbf{y}(x_0)=\mathbf{y}_0, \tag{1.2}$$

where $\mathbf{y}$ and $\mathbf{f}$ are N-vectors, I is the $N\times N$ unit matrix and Q_n is an $N\times N$ matrix coefficient which varies with n. The real coefficients $a_j^{(s)}$, $b_j^{(s)}$ are constants and it is assumed that $a_k^{(0)}=1$. In practice Q_n is an approximation to the negative Jacobian $-\partial f/\partial y$ over $[x_n, x_{n+k}]$, although Lambert & Sigurdsson are able to carry out their analysis under much weaker assumptions (see their work).

A method of class (1.1) (henceforth an LS method) is said to be *linearly implicit* if $b_k^{(s)}=0$, $s=0,1,\ldots,S-1$, otherwise is said to be *fully implicit*. Fully implicit methods require the solution at each step of a *non-linear* system, whilst for a linearly implicit method the system to be solved is *linear*.

When (1.2) is stiff, LS formulae enjoy the following potential advantages:

(1) There exist A-stable LS methods with orders $2, 4, 6, \ldots$ as opposed to the situation in the linear multistep case.
(2) Furthermore such high order A-stable methods can be found even if we require them to be linearly implicit to avoid the expensive Newton iteration.
(3) The order of the method, being independent of the choice of Q_n, does not suffer if Q_n is a poor approximation to the negative Jacobian.

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On the other hand note that the computational complexity will clearly increase significantly with increasing S.

Of course there are a host of LS methods. Lambert & Sigurdsson (1972) focus their attention on so-called "stabilized" methods. Skeel & Kong (1977) have studied an implementation of what they call a "blend" of the Adams–Moulton and backward differentiation formulae. They point out that such a blend is an LS method which is not stabilized.

In this paper, which was inspired by the "blending approach", we shall analyse the stability properties of LS methods, without making the restriction that the methods should be stabilized. Let us quote the main results. (See the next section for more precise definitions of the terms involved.)

THEOREM 1. *A convergent, A-stable LS method has order* $p \leqslant 2S$.

This result was proved by Lambert & Sigurdsson for the particular case of stabilized methods. In fact they established that $p \leqslant 2S$ for *any* stabilized method.

As a consequence of Theorem 1, if we are not prepared to take $S > 1$ the method cannot both be A-stable and have order greater than two. When facing this dilemma in the linear multistep case, the usual practice is to choose high order formulae with "large" regions of absolute stability (Lambert, 1973). Thus we are led to the question: are there high order A_0-, $A(\alpha)$- or stiffly stable LS methods with $S = 1$? Fortunately one can prove:

THEOREM 2. *Given a convergent linear k-step method of order* $p \leqslant k+1$, *there exist convergent, linearly implicit LS methods with the same order and stability region,* $S = 1$ *and at most* $k+1$ *steps.*

So LS methods with minimum computational effort can mimic the stability properties of the commonest linear multistep methods. Furthermore Theorem 2 can be sharpened in a very important instance to yield:

THEOREM 3. *Given a convergent linear k-step method of order k (such as the backward differentiation formulae,* $k \leqslant 6$), *there exists a convergent, linearly implicit LS method with* $S = 1$, *and the same step number and order, such that both methods generate the same numerical solution when applied to the test system*

$$\mathbf{y}' = A\mathbf{y}, \tag{1.3}$$

when Q_n *is chosen to be* $-A$. (*And hence they have the same region of absolute stability.*)

Note that stabilized LS methods cannot enjoy the favourable properties referred to in Theorems 2 and 3, since their order would necessarily be restricted to two.

2. An Analysis of LS Methods

We shall have to deal with k-step m-derivative (Obrechkoff) methods of the form

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+j} = \sum_{i=1}^{m} h^i \sum_{j=0}^{k} \beta_{ij} \mathbf{y}^{(i)}_{n+j}, \tag{2.1}$$

where α_j, β_{ij}, $i = 1, 2, \ldots, m$; $j = 0, 1, \ldots, k$ are real constants. We introduce the characteristic polynomials $\rho(r)$, $\sigma_i(r)$, $i = 1, 2, \ldots, m$, as in Lambert (1973) or Stetter

(1973), and denote (2.1) by $(\rho(r), \sigma_1(r), \ldots, \sigma_m(r))$. For notational convenience and contrary to the usual practice, we do not assume $\alpha_k = 1$ or

$$|\alpha_k| + \sum_{i=1}^{m} |\beta_{ik}| \neq 0,$$

so that (2.1) may have less than k steps. Neither shall we suppose that $\rho(r), \sigma_1(r), \ldots, \sigma_m(r)$ have no non-constant common factor.

We associate with formula (1.1) polynomials

$$\rho^{(s)}(r) = \sum_{j=0}^{k} a_j^{(s)} r^j, \quad s = 0, 1, \ldots, S,$$

$$\sigma^{(s)}(r) = \sum_{j=0}^{k} b_j^{(s)} r^j, \quad s = 0, 1, \ldots, S-1,$$

$$\sigma^{(S)}(r) \equiv 0,$$

and use $\{\rho^{(0)}(r), \ldots, \rho^{(S)}(r); \sigma^{(0)}(r), \ldots, \sigma^{(S-1)}(r)\}$ to symbolize (1.1).

Some results of Lambert & Sigurdsson (1972) are easily stated with this notation, for instance,

Proposition 1. Formula (1.1) is zero-stable if and only if $(\rho^{(0)}(r), \sigma^{(0)}(r))$ is a zero-stable linear multistep method.

Proposition 2. Formula (1.1) has order $p \geqslant S$ if and only if the linear multistep method $(\rho^{(s)}(r), \sigma^{(s)}(r))$, $s = 0, 1, \ldots, S$, has order $p - s$.

In order to study the (weak) stability properties of formula (1.1) we apply it with $Q_n = -A$ to the system (1.3), where it is assumed that the matrix A has a complete set of eigenvectors. (It should be pointed out that Lambert & Sigurdsson do not make this assumption and correspondingly their $\bar{A}$-stability is a property slightly stronger than our A-stability.)

Setting $Q_n = -A$ in (1.1), applying the resulting formula to (1.3) and uncoupling, one sees that the growth of a component in the uncoupled system is governed by the difference equation

$$\sum_{j=0}^{k} \left[a_j^{(0)} + \sum_{s=1}^{S} \{a_j^{(s)} + b_j^{(s)}\}(-1)^s \lambda^s h^s \right] \mathbf{z}_{n+j} = 0, \tag{2.2}$$

where λ is an eigenvalue of A. With $\bar{h} = h\lambda$ the corresponding characteristic equation can be written

$$\rho^{(0)}(r) + \sum_{s=1}^{S} \bar{h}^s (-1)^s [\rho^{(s)}(r) + \sigma^{(s-1)}(r)] = 0. \tag{2.3}$$

Definition 1. The set (or "region") of absolute stability of (1.1) is the set of all complex values $\bar{h}$ for which all the roots r_s of (2.3) satisfy $|r_s| < 1$, $s = 1, 2, \ldots, \alpha$. The method (1.1) is A-stable if its set of absolute stability contains the left half-plane $\operatorname{Re} \bar{h} < 0$.

This is consistent with the original definition of A-stability (Dahlquist, 1963). Analogously we can define $A(\alpha)$-, A_0-, L-, ..., stability (Lambert, 1973).

Clearly (2.3) is also the characteristic equation of the k-step, S-derivative method $(\rho(r), \sigma_1(r), \ldots, \sigma_S(r))$ where

$$\begin{aligned} \rho(r) &\equiv \rho^{(0)}(r), \\ (-1)^{i-1}\sigma_i(r) &\equiv \rho^{(i)}(r)+\sigma^{(i-1)}(r), \quad i = 1, 2, \ldots, S. \end{aligned} \tag{2.4}$$

We say that $(\rho(r), \sigma_1(r), \ldots, \sigma_S(r))$ is the *companion* (Obrechkoff) method of the LS method (1.1).

Proposition 3. An LS method has at most the same order as its companion Obrechkoff method.

Proof. Apply the linear operators associated with the methods $(\rho^{(i)}(r), \sigma^{(i)}(r))$, $i = 0, \ldots, S$, to the ith derivative of the test function $\mathbf{y}(x)$ and combine the results (see Lambert, 1973, paragraphs 2.6 and 7.2).

Proof of Theorem 1. Assume that (1.1) is A-stable, is convergent and has order $p > 2S$. It follows that the companion method given by (2.4) is also A-stable and has order $p > 2S$, in contradiction with a result of Wanner, Hairer & Norsett (1978) (proof of the conjecture of Daniel & Moore). [We may need to suppress common factors amongst $\rho(r)$, $\sigma_1(r)$, ..., $\sigma_S(r)$; convergence implies that $(r-1)$ is not such a factor, and so the order is not decreased in that process.]

Proof of Theorem 3. Let $(\rho(r), \sigma(r))$ be the multistep method. Set

$$\sigma^*(r) = \sigma(r)-\beta_{1k}(r-1)^k,$$

so that $\sigma^*(r)$ has degree $k-1$. Then the LS method $\{\rho(r), \beta_{1k}(r-1)^k; \sigma^*(r)\}$ is found to possess all the required properties. [Note that its companion method is $(\rho(r), \sigma(r))$.] To prove that its order is k, write

$$\frac{\rho(r)}{\log r} - \sigma(r) = O((r-1)^k), \quad r \to 1, \tag{2.5}$$

which yields

$$\frac{\rho(r)}{\log r} - \sigma^*(r) = O((r-1)^k), \quad r \to 1, \tag{2.6}$$

so that $(\rho(r), \sigma^*(r))$ has order k. Now $(\beta_{1k}(r-1)^k, 0)$ has order $k-1$, and Proposition 2 applies. Of course $(\beta_{1k}(r-1)^k, 0)$ is not zero-stable, but this fact is irrelevant.)

Proof of Theorem 2. It is similar to the previous one. The method we seek is of the form

$$\{\rho(r)(r-\alpha), \beta_{1k}(r-1)^{k+1}; \sigma(r)(r-\alpha)-\beta_{1k}(r-1)^{k+1}\}$$

where α is real, $|\alpha| < 1$. Of course we have to increase the step number because there is no method of the form $(\rho^{(1)}(r), 0)$ which has order k and step number $\leqslant k$.

Note. Given a linear multistep method as in Theorem 2 and provided that we are prepared to increase the step number, it is possible to obtain LS methods which have $S = 1$, and the same stability set, order and *principal truncation error*. Take

$$\rho^{(0)}(r) = r^2\rho(r), \qquad \sigma^{(0)}(r) = r^2\sigma(r)-\beta_{1k}(r-1)^{k+2}$$

and

$$\rho^{(1)}(r) = \beta_{1k}(r-1)^{k+2}.$$

Now $(\rho^{(0)}(r), \sigma^{(0)}(r))$ and $(\rho^{(1)}(r), 0)$ have both the same order.

This suggests a way of controlling the step size analogous to Milne's device for predictor–corrector algorithms. In fact the theories of order for LS and PC methods appear to be very much alike.

3. Numerical Results

The basic idea in Theorems 2 and 3 is, as Skeel & Kong (1977) put it, "to take a linear multiderivative multistep formula and convert it into a variable matrix coefficient, linear multistep formula so that the region of absolute stability and the order of accuracy are unaffected". They also note that "there is no reason to suspect that this transformation would either improve or degrade the performance of the transformed formula". Extensive experimental tests would be necessary in order to obtain an assessment of that performance. The following numerical examples, although very limited, might throw some light on this matter.

We consider the third order backward differentiation method

$$\mathbf{y}_{n+3}-\tfrac{18}{11}\mathbf{y}_{n+2}+\tfrac{9}{11}\mathbf{y}_{n+1}-\tfrac{2}{11}\mathbf{y}_n = h\tfrac{6}{11}\mathbf{f}_{n+3}, \tag{3.1}$$

whose principal truncation error is $(-3/22)h^4\mathbf{y}^{(4)}$. The proof of Theorem 3 associates with this formula the LS method

$$\mathbf{y}_{n+3}-\tfrac{18}{11}\mathbf{y}_{n+2}+\tfrac{9}{11}\mathbf{y}_{n+1}-\tfrac{2}{11}\mathbf{y}_n+\tfrac{6}{11}hQ_n(\mathbf{y}_{n+3}-3\mathbf{y}_{n+2}+3\mathbf{y}_{n+1}-\mathbf{y}_n) = h(\tfrac{18}{11}\mathbf{f}_{n+2}-\tfrac{18}{11}\mathbf{f}_{n+1}+\tfrac{6}{11}\mathbf{f}_n). \tag{3.2}$$

The principal local truncation error is now $(9/22)h^4\mathbf{y}^{(4)}+(12/22)h^4Q_n\mathbf{y}^{(3)}$. When (3.2) is applied to the linear system (1.3), it is identical to (3.1) (provided $Q_n=-A$).

We applied (3.2) to the following well-known stiff systems (Liniger & Willoughby, 1967):

(I) The linear variable coefficient problem

$$\begin{aligned} y_1' &= 10{\cdot}0y_2-(60{\cdot}0-0{\cdot}125x)y_1+0{\cdot}125x,\\ y_2' &= 0{\cdot}2(y_1-y_2),\\ y_1'(0) &= y_2(0)=0, \quad 0\leqslant x\leqslant 400. \end{aligned}$$

(II) The non-linear problem

$$\begin{aligned} y_1' &= 0{\cdot}01-[1+(y_1+1000)(y_1+1)](0{\cdot}01+y_1+y_2),\\ y_2' &= 0{\cdot}01-(1+y_2^2)(0{\cdot}01+y_1+y_2),\\ y_1(0) &= y_2(0)=0, \quad 0\leqslant x\leqslant 100. \end{aligned}$$

The step length used was 1·0 for system I and 0·1 for system II; in both cases Q_n was chosen to be the negative Jacobian evaluated at $x=x_{n+2}$. The results are displayed in Tables 1 and 2, respectively. A fourth-order Runge–Kutta method provided us with the "theoretical solution" and the necessary starting values. In order to assess the effect of the choice of Q_n, we performed some runs keeping that matrix fixed over a number of consecutive steps. The parameter NUP in the tables refers to that number; for instance NUP = 50 means that the Jacobian was updated every 50 steps.

It appears that (3.2) has more difficulties in integrating accurately fast transients

TABLE 1

X	Theoretical	Error = Theoretical − Numerical		
		NUP = 1	NUP = 50	NUP = ∞
10	$y_1 = 0{\cdot}23448858 \times 10^{-1}$	-61×10^{-8}	-66×10^{-8}	-66×10^{-8}
	$y_2 = 0{\cdot}13015276 \times 10^{-1}$	-47×10^{-7}	-47×10^{-7}	-47×10^{-7}
100	0·32754980	28×10^{-8}	32×10^{-8}	37×10^{-8}
	0·30630032	26×10^{-8}	29×10^{-8}	34×10^{-8}
200	0·98104589	13×10^{-7}	16×10^{-7}	26×10^{-7}
	0·93463309	12×10^{-7}	14×10^{-7}	23×10^{-7}
300	$0{\cdot}28638768 \times 10^{1}$	17×10^{-6}	23×10^{-6}	60×10^{-6}
	$0{\cdot}26973467 \times 10^{1}$	14×10^{-6}	19×10^{-6}	50×10^{-6}
400	$0{\cdot}27110713 \times 10^{2}$	74×10^{-4}	18×10^{-3}	10×10^{-2}
	$0{\cdot}22242220 \times 10^{2}$	44×10^{-4}	11×10^{-3}	64×10^{-3}

TABLE 2

X	Theoretical	Error × 10^6		
		NUP = 1	NUP = 100	NUP = 500
10	$y_1 = -0{\cdot}109754$	12	12	12
	$y_2 = 0.099777$	−12	−12	−12
20	$y_1 = -0{\cdot}209508$	12	12	12
	$y_2 = 0{\cdot}199533$	−13	−13	−13
40	$y_1 = -0{\cdot}408862$	12	12	13
	$y_2 = 0{\cdot}398896$	−12	−12	−12
60	$y_1 = -0{\cdot}607812$	12	12	12
	$y_2 = 0{\cdot}597862$	−12	−12	−12
80	$y_1 = -0{\cdot}805642$	12	12	12
	$y_2 = 0{\cdot}795743$	−12	−12	−12
100	$y_1 = -0{\cdot}991642$	8	12	36
	$y_2 = 0{\cdot}983336$	−9	−12	−29

than other third-order methods for stiff systems. [Performances of some of these are reported by Lambert & Sigurdsson (1972).] On the other hand (3.2) enjoys the potential advantages referred to in the Introduction; in particular the Jacobian can be held fixed over large intervals without drastic losses in accuracy. At any rate a meaningful, practical comparison between LS and other methods is only possible on the basis of using variable step implementations and no study in that direction has been made by the present author.

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