Construction of Variable-Stepsize Multistep Formulas

By Robert D. Skeel*

Abstract. A systematic way of extending a general fixed-stepsize multistep formula to a minimum storage variable-stepsize formula has been discovered that encompasses fixed-coefficient (interpolatory), variable-coefficient (variable step), and fixed leading coefficient as special cases. In particular, it is shown that the "interpolatory" stepsize changing technique of Nordsieck leads to a truly variable-stepsize multistep formula (which has implications for local error estimation and formula changing), and it is shown that the "variable-step" stepsize changing technique applicable to the Adams and backward-differentiation formulas has a reasonable generalization to the general multistep formula. In fact, it is shown how to construct a variable-order family of variable-coefficient formulas. Finally, it is observed that the first Dahlquist barrier does not apply to adaptable multistep methods if storage rather than stepnumber is the key consideration.

1. Introduction. Multistep methods have been the most successful numerical methods for solving initial-value problems in ordinary differential equations. The selection of a particular formula is often based on a theoretical analysis of fixed-stepsize formulas, and yet implementation normally requires the use of a variable-stepsize formula. The question of how to extend a formula to variable stepsize is the primary topic of this paper. Existing techniques for varying stepsize are studied, revealing interesting relationships and useful generalizations. At the same time, the results in Skeel [19] on the equivalence between multivalued methods and multistep methods are extended to variable stepsize. There are techniques for varying the stepsize other than the use of variable-stepsize formulas, and these are included in the survey of Krogh [13].

The question of how to extend a formula to variable stepsize has confronted a number of researchers. For example, Sand [15, p. 8] states:

Although there exist natural extensions of the two most common classes of fixed-step formulas to variable step-sizes, viz. the Adams LMF's and the BDF's... there exists no unique, and in general, no natural, variable-step version of a fixed-step formula.

The natural extensions referred to here are implemented in such codes as EPISODE (Byrne and Hindmarsh [1]) and ODE/DE/STEP, INTRP (Shampine and Gordon [17]), and have been named "variable-coefficient" formulas by Jackson and Sacks-Davis [11]. In Section 5 of this paper we present a systematic way of extending fixed-stepsize formulas to variable-stepsize formulas of which the natural variable-coefficient Adams and backward-differentiation formulas are particular cases. These

Received September 21, 1984; revised January 3, 1986.

1980 *Mathematics Subject Classification*. Primary 65L05.

Key words and phrases. Multistep formula, multistep method, multivalued method, variable stepsize, variable order.

*Work partially supported by the National Science Foundation under grant MCS 8107046 and by the U.S. Department of Energy under grant DEAC0276ERO2383.

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variable-coefficient formulas have attractive properties, that taken together are not possessed by other variable-stepsize extensions. They interpolate past data in some generalized sense *at previous meshpoints*, which suggests superior stability properties. Also, they require a minimum of storage.

The popular integrator LSODE (Hindmarsh [10]) does not use variable-coefficient formulas but rather “fixed-step interpolation” formulas based on an idea due to Nordsieck [14] and popularized by Gear [8]. This technique for varying the stepsize is applicable to general fixed-stepsize formulas. The precise nature of this type of variable-stepsize method has been somewhat of a mystery, but if there is a prevailing view, then it is most clearly expressed by Jackson and Sacks-Davis [11]:

If, in a fixed coefficient implementation, the stepsize is changed at every step, then the corrector equation . . . may be expressed in the form

$$(2.18) \quad \alpha_0 y_n + \sum_{j=1}^n \tilde{\alpha}_{n,j} y_{n-j} + h_n f_n + h_n \sum_{j=1}^{n-2} \tilde{\beta}_{n,j} f_{n-j} = 0,$$

provided, as well, that the order k is always kept greater than two. Thus the solution at t_n may depend on all of the previously computed values. Consequently, eq. (2.18) is not a “local formula” as are eqs. (2.6), (2.13), and (2.15). This gives one an intuitive understanding for the cause of the numerical instability of fixed coefficient formulas with respect to step-size changes.

These comments are specific to the backward-differentiation formulas; presumably they should apply also to other linear multistep formulas if the $n - 2$ in the limit of summation is changed to n . In Section 5 of this paper we show that the situation is not so bad, that fixed-coefficient formulas are true variable-stepsize formulas, meaning that the upper summation limits in (2.18) can be replaced by the stepnumber k and the formula coefficients depend on only the last $k - 2$ stepsize ratios. We expect that this information could be very important for the construction of local error estimates having a sound theoretical basis. There is little reason to believe that the local error estimators used in current implementations are asymptotically correct, even (for nonstiff problems) with slowly varying stepsize.

The variable-coefficient and fixed-coefficient extensions are related even more closely than has already been suggested. They are both specializations of a more general technique for variable-stepsize extension discussed in Section 2. This generic technique for extending formulas to variable stepsize is characterized by the fact that it creates methods having minimal storage requirements.

A fixed-stepsize linear k -step formula, $k \geq 2$, for the ODE $y'(t) = f(t, y(t))$ determines approximations y_n and y'_n to the solution and its derivative at a point t_n from the two equations

$$(1.1a) \quad \alpha_0 y_n + \alpha_1 y_{n-1} + \cdots + \alpha_k y_{n-k} = h(\beta_0 y'_n + \beta_1 y'_{n-1} + \cdots + \beta_k y'_{n-k}),$$

$$(1.1b) \quad y'_n = f(t_n, y_n),$$

assuming that approximations y_{n-j} , y'_{n-j} are available at previous meshpoints $t_{n-j} := t_n - jh$, $j = 1(1)k$. It is not necessary for our purposes that Eq. (1.1b) be satisfied exactly. We assume that $\alpha_0 \neq 0$ and that the polynomials

$$\rho(\xi) := \alpha_0 \xi^k + \alpha_1 \xi^{k-1} + \cdots + \alpha_k \quad \text{and} \quad \sigma(\xi) := \beta_0 \xi^k + \beta_1 \xi^{k-1} + \cdots + \beta_k$$

have no common factors, which is equivalent to the nonexistence of an “equivalent” formula of lower stepnumber. From the latter assumption it follows that $\alpha_k^2 + \beta_k^2 > 0$. Assume the formula is of order $\geq q$ where $k \leq q \leq 2k - 1$, which for linear

multistep methods is equivalent to requiring that the formula be exact if $y(t)$ is a polynomial of degree $\leq q$. The cases $q = k - 1$ and $q = 2k$ are excluded because they require special treatment. The order of the (fixed-step size) formula may exceed q , but we shall seek a variable-step size extension of order q only.

For nonstiff problems, stability considerations (strong stability) constrain the order to be $\leq k + 1$. The archetypal nonstiff formula is the Adams-Moulton formula (AMF)

$$y_n - y_{n-1} = h(\beta_0 y'_n + \beta_1 y'_{n-1} + \cdots + \beta_k y'_{n-k}),$$

which is of order $k + 1$. For stiff problems, stability considerations ($A(\alpha)$ -stability) constrain the order to be $\leq k$ (except for the trapezoidal rule), and the archetypal stiff formula is the backward-differentiation formula (BDF)

$$\alpha_0 y_n + \alpha_1 y_{n-1} + \cdots + \alpha_k y_{n-k} = h y'_n,$$

which is of order k . Both sets of formulas are attractive because of their simple derivation, but it is difficult to believe that they are the best for all special-purpose and general-purpose codes. We note that other formulas have been derived by many authors and that some of these have been used to solve practical problems, for example, the K -method of Kregel and Heimerl [12] used at the U.S. Army Ballistic Research Laboratory.

For various practical reasons (error control, efficiency, starting, solution of nonlinear systems) we want to use variable step size $h_n := t_n - t_{n-1}$. For a given fixed-step size formula we want a variable-step size extension

$$\sum_{j=0}^k \alpha_{jn} y_{n-j} = \beta_{0n} h_n y'_n + \sum_{j=1}^k \beta_{jn} h_{n-j+1} y'_{n-j}.$$

There are a number of restrictions that are clearly desirable. The coefficients α_{jn} , β_{jn} should depend only on $t_n, t_{n-1}, \dots, t_{n-k}$, and, in fact, they ought to be rational functions of the step size ratios $r_n, r_{n-1}, \dots, r_{n-k+2}$. Here, $r_n := h_n/h_{n-1}$. We will not require that the coefficients exist for all possible combinations of step size ratios, although this is desirable. It goes without saying that the variable-step size coefficients should be equal to the fixed-step size coefficients when the step size ratios are all one. The normalization

$$\alpha_{0n} = \alpha_0$$

will be assumed. Any other normalization may not always be applicable; for example, the more natural normalization $\sum \beta = 1$ sometimes fails for the f variant of the fixed leading coefficient formulas of Jackson and Sacks-Davis [11]. Requiring that the formula be exact for polynomials of degree at most q imposes another $q + 1$ linear conditions on the coefficients. However, we need yet another $2k - q$ conditions, which is the main topic of this paper.

Note. Our use of h_{n-j+1} instead of h_n as a coefficient for y'_{n-j} , $j \geq 2$, is unusual but for our purposes more convenient.

For the k -step AMF we need $k - 1$ auxiliary conditions and the most popular choice (variable coefficient) is

$$\alpha_{2n} = \alpha_{3n} = \cdots = \alpha_{kn} = 0.$$

For the k -step BDF we need k additional conditions and a popular choice (variable coefficient again) is

$$\beta_{1n} = \beta_{2n} = \cdots = \beta_{kn} = 0.$$

One motivation for these conditions, emphasized in the paper of Dill and Gear [7], is to keep down the number of saved values (more specifically, the number of values that must be saved between steps). For this variable-stepsize extension of AMF it is clear that only the $k + 1$ values $y_{n-1}, y'_{n-1}, \dots, y'_{n-k}$, are needed to determine y_n and y'_n , and for the BDF only k values are needed. However, this property is not unique to these choices of coefficients. It is shown in Skeel [19] that any fixed-stepsize k -step method requires only k values to be saved in order to advance the solution (and this is without reevaluating the right-hand side $f(t, y)$). This also follows from the equivalence between linear multistep and one-leg methods discovered by Dahlquist [3], as well as the modifier polynomial formalism of Wallace and Gupta [21]. In practice we want to use a predictor of order q at least, so that we get a good initial guess for the nonlinear equation solver, so that the Milne device can be used to estimate local errors, and so that interpolation to off-mesh points can be performed with an error of only $O(h^{q+1})$. Thus, we should save $q + 1$ values.

The same trick used to economize on storage for fixed-stepsize methods also works for variable-stepsize methods. Let us illustrate this with the 2-step Adams-Bashforth formula by choosing the $2k - q = 2$ auxiliary conditions plus the one normalization condition to be

$$\beta_{0n} = 0, \quad \beta_{1n} = \frac{3}{2}, \quad \beta_{2n} = -r_n/2.$$

Requiring that the formula be exact for second-degree polynomials yields

$$\alpha_{0n} = 2/(1 + r_n), \quad \alpha_{1n} = r_n - 2, \quad \alpha_{2n} = r_n(1 - r_n)/(1 + r_n).$$

If we are given the three values

$$y_{n-1}, \quad y'_{n-1}, \quad \tilde{s}_{n-2}^0 := -\alpha_{2n}y_{n-2} + \beta_{2n}h_{n-1}y'_{n-2},$$

we can determine $y_n, y'_n, \tilde{s}_{n-1}^0$ from

$$\begin{aligned} \tilde{s}_{n-1}^0 &= -\alpha_{2,n+1}y_{n-1} + \beta_{2,n+1}h_n y'_{n-1}, \\ \alpha_{0n}y_n + \alpha_{1n}y_{n-1} &= \beta_{1n}h_n y'_{n-1} + \tilde{s}_{n-2}^0, \\ y'_n &= f(t_n, y_n). \end{aligned}$$

There is a disturbing feature of this algorithm, that the reader may have noticed. It concerns the computation of $\tilde{s}_{n-1}^0$ at time t_n and the fact that this requires knowing the value of t_{n+1} . For adaptive methods, the value of t_{n+1} is determined, by trial and error, only after completely advancing to t_n .

The failure of our algorithm in this example is probably typical. For a second example, consider the constant- ρ variable-stepsize extension proposed by Gear and Watanabe [9], in which we require $\alpha_{jn} = \alpha_j$, $0 \leq j \leq k$, so that the variable-stepsize formula inherits the 0-stability properties of the fixed-stepsize formula. (This actually constitutes only $k - 1$ auxiliary conditions because a normalization is included and the formula is already exact for constant polynomials.) The result of applying the constant- ρ variable-stepsize extension to the third-order formula with

$$\alpha_0 = \frac{3}{2}, \quad \alpha_1 = -2, \quad \alpha_2 = \frac{1}{2},$$

has

$$\beta_{0n} = \frac{6r^3 + 9r^2 + 1}{12r^2(r+1)}, \quad \beta_{1n} = \frac{3r^3 + 9r^2 - 3r - 1}{12r^2}, \quad \beta_{2n} = -\frac{3r^3 + 3r + 2}{12(r+1)},$$

where $r = r_n$.

Therefore, in our search for auxiliary conditions we impose one more restriction:

The $2k - q$ auxiliary conditions should be such that only $q + 1$ values need be saved without knowing future meshpoints.

Such methods we call *adaptable* $(q + 1)$ -value methods. At the beginning of Section 2 we give generic auxiliary conditions that are sufficient and seem to be necessary in order that the storage be minimal without predetermined meshpoints.

It is convenient to introduce $m := (q + 1) - k$ and to use m rather than q in our discussion. Thus we are seeking $k - m + 1$ auxiliary conditions for a $(k + m)$ -value method of order $k + m - 1$. The assumption $k \leq q \leq 2k - 1$ implies $1 \leq m \leq k$. Typically, $m = 1$ for a stiff formula, and $m = 2$ for a nonstiff formula.

An auxiliary condition proposed by Jackson and Sacks-Davis [11] is to fix $\beta_{0n} = \beta_0$. Such *fixed leading coefficient* variable-step size formulas have certain practical advantages for stiff ODEs, and these formulas are considered in Section 6. On the other hand, there is some suggestion, namely, the equivalence of fixed leading coefficient to fixed-coefficient for the second-order BDF, that *variable leading coefficient* formulas have better stability properties.

If the meshpoints were known in advance, we could express the unique variable-step size k -step formula of order $2k$ in such a way that only k values need to be saved. However, if the new meshpoint t_n is not known in advance, we cannot expect the order of a q -value method to exceed q , because there are only $q + 1$ items of information available to determine the solution at t_n : the k saved values plus the differential equation at t_n . (Consider, in particular, the problem $y' = f(t)$.) Moreover, the q th order Adams-Moulton formula can be expressed as an adaptable q -value method, and thus there exist strongly 0-stable q -value methods of optimal order. Therefore, the first Dahlquist [2] barrier does not exist for adaptable variable-step size formulas, if we consider the number of saved values rather than the stepnumber of the formula. In Section 3 we construct an adaptable q th-order q -value variable-step size extension for any q th-order fixed-step size formula with stepnumber $< q$.

In the fixed-step size case, Skeel [19] shows how to formulate a $(k + m)$ -value method using a polynomial $p_n(t)$ that interpolates $k + m$ values as follows:

$$\begin{aligned} p_n(t_{n-j}) &= y_{n-j}, & j &= 0(1)m - 1, \\ p'_n(t_{n-j}) &= y'_{n-j}, & j &= 0(1)m - 1, \\ \sum_{i=0}^j &(-\alpha_{k-j+i} p_n(t_{n-m-i}) + h\beta_{k-j+i} p'_n(t_{n-m-i})) \\ &= \sum_{i=0}^j (-\alpha_{k-j+i} y_{n-m-i} + h\beta_{k-j+i} y'_{n-m-i}), & j &= 0(1)k - m - 1. \end{aligned}$$

In advancing from $p_{n-1}(t)$ to $p_n(t)$ we obtain one new item of information, namely, the derivative value at t_n . (This is obviously the case for the ODE $y' = f(t)$.) Hence, the polynomials $p_{n-1}(t)$ and $p_n(t)$ interpolate nearly the same data and so we

expect the difference to be especially simple. In fact,

$$(1.2) \quad p_n(t) = p_{n-1}(t) + \frac{1}{\alpha_0} (y'_n - p'_{n-1}(t_n)) \Lambda\left(\frac{t - t_n}{h}\right),$$

where the modifier polynomial $\Lambda(x)$ is determined by the formula through the conditions

$$(1.3a) \quad \Lambda(-j) = \begin{cases} \beta_0, & j = 0, \\ 0, & j = 1(1)m - 1, \end{cases}$$

$$(1.3b) \quad \Lambda'(-j) = \begin{cases} \alpha_0, & j = 0, \\ 0, & j = 1(1)m - 1, \end{cases}$$

$$(1.3c) \quad \sum_{i=0}^j \{-\alpha_{k-j+i} \Lambda(-m-i) + \beta_{k-j+1} \Lambda'(-m-i)\} = 0,$$

$$j = 0(1)k - m - 1.$$

It is shown (Skeel [19, Corollary to Theorem 2.1]) that these conditions uniquely determine $\Lambda(x)$. As an example, the k -step BDF has

$$\Lambda(x) = \binom{x+k}{k}.$$

The modifier polynomial was discovered in special cases by Descoux [6] and Byrne and Hindmarsh [1] and in general by Wallace and Gupta [21] and Skeel [19].

Equation (1.2) is an alternative way of expressing a linear multistep formula and has a number of advantages. First, a k th degree modifier polynomial $\Lambda(x)$ is a convenient parameterization of a linear k -step formula because the number of free coefficients after a normalization (such as $\Lambda'(0) = 1$ or $\Lambda^{(k)}(0) = 1$ which corresponds to $\alpha_0 = 1$ or $\sum \beta = 1$, respectively) exactly equals the k degrees of freedom in a normalized, linear multistep formula of order $\geq k$ and stepnumber $\leq k$. Second, the minimum storage implementation is obvious from (1.2). The coefficients are easily calculated from $\Lambda(x)$; for example, a divided-difference implementation would use divided differences of $\Lambda((t - t_n)/h)$. Third, there is a built-in predictor. Fourth, there is a built-in interpolation to off-mesh points. However, there is a disadvantage to the form (1.2), and that is that it seems to be less convenient for the analysis of stability and accuracy.

The modifier polynomial $\Lambda(x)$ is used in Section 5 to give the auxiliary conditions for the variable-coefficient extension. There is another more direct way of constructing the variable-coefficient formula, which we give here:

For the values y_{n-j} and y'_{n-j} , $j = 0(1)m - 1$,

$$(1.4) \quad s_{n-m}^j := \sum_{i=0}^j \{-\alpha_{k-j+i} y_{n-m-i} + \beta_{k-j+1} h_{n-m-i+1} y'_{n-m-i}\},$$

$$j = 0(1)k - m,$$

we determine $k + m$ coefficients α_{jn} , β_{jn} , γ_{jn} , such that the formula

$$\alpha_0 y_n - \beta_0 h_n y'_n = \sum_{j=1}^{m-1} \{-\alpha_{jn} y_{n-j} + \beta_{jn} h_{n-j+1} y'_{n-j}\} + \sum_{j=m}^k \gamma_{jn} s_{n-m}^{j-m}$$

is exact for polynomials of degree $\leq k + m - 1$.

The auxiliary conditions for the fixed-coefficient case are given in Section 7 in terms of the modifier polynomial $\Lambda(x)$. But again there is another, more direct way of describing this method. Assume we are given

$$y_{n-1,-j} \approx y(t_{n-1} - jh_{n-1}), \quad y'_{n-1,-j} \approx y'(t_{n-1} - jh_{n-1})$$

for $j = 0(1)k - 1$. Let $p_{n-1}(t)$ be the unique polynomial of degree at most $k + m - 1$ which interpolates (as before) the following equally spaced data:

$$y_{n-1,-j}, \quad y'_{n-1,-j}, \quad j = 0(1)m - 1,$$

$$\sum_{i=0}^j \{ -\alpha_{k-j+i} y_{n-1,-m-i} + h_{n-1} \beta_{k-j+i} y'_{n-1,-m-i} \}, \quad j = 0(1)k - m - 1.$$

Then, evaluate $p_{n-1}(t)$ and its derivative at the k points from t_{n-1} backwards with uniform spacing h_n ,

$$y_{n,-j} = p_{n-1}(t_n - jh_n), \quad y'_{n,-j} = p'_{n-1}(t_n - jh_n),$$

$j = 1(1)k$, and apply the fixed-stepsize formula (1.1) to those values in order to obtain y_n and y'_n .

As previously stated, a fixed-coefficient method can be expressed as a true variable-stepsize formula, and as an example, the fixed-coefficient second-order BDF has the form

$$\frac{3}{2}y_n - \frac{3+r_n^2}{2}y_{n-1} + \frac{r_n^2}{2}y_{n-2} = h_n y'_n + \frac{1-r_n}{2}h_n y'_{n-1}.$$

We have been considering fixed-formula methods only. For variable-formula methods the idea of the number of saved values still applies, although this number might have to be greater because of the possibility of changing formulas. Clearly, the various formulas ought to be related in such a way that the number of saved values is low. More specifically, if we want a family of variable-coefficient formulas indexed by $k = m(1)K$, such that the k th formula has stepnumber k and order $k + m - 1$, then we should begin by choosing the K th formula to be whatever we like, and for the k th formula, $k = m(1)K - 1$, we should use the unique formula of order $k + m - 1$ that relates the values

$$y_{n-j}, \quad y'_{n-j}, \quad j = 0(1)m - 1, \quad s'_{n-m}, \quad j = 0(1)k - m,$$

where the latter are defined using the coefficients of the K th formula. This is further discussed in Section 4 in greater generality.

Sections 2 through 7 appear in the supplements section at the end of this issue.

We conclude this section by offering some opinions about the various ideas sparked by Nordsieck [14] and pursued by a number of authors, especially Gear [8]. These ideas have had a profound practical impact but have otherwise been resisted by most researchers in numerical ODEs. As shown in this and previous papers, all interesting multivalued methods can be expressed as genuine multistep methods, although for blended methods this can be complicated [20]. The multistep form seems to be best for the analysis of errors and of stability. Nonetheless both the “number of saved values” and the “modifier polynomial” seem to be useful ideas worth retaining.

There is significant experimental and theoretical evidence in the case of Adams and backward-differentiation formulas that variable-coefficient methods are stable for a greater variety of stepsize sequences than are the fixed-coefficient methods.

Stability is a very important consideration, more so than the complexity of coefficient calculation (or the representation of saved values), and for this reason the fixed-coefficient schemes should be abandoned in favor of either variable-coefficient or fixed leading coefficient schemes, which, in this paper, have been defined for general linear multistep formulas. Even these may have inadequate stability properties compared to the second-order 2-step one-leg formulas of Dahlquist, Liniger, and Nevanlinna [5].

Department of Computer Science
University of Illinois at Urbana-Champaign
240 Digital Computer Laboratory
1304 W. Springfield Avenue
Urbana, Illinois 61801

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Supplement to Construction of Variable-Stepsize Multistep Formulas

By Robert D. Skeel

2. Generic Auxiliary Conditions

We are seeking $k-m+1$ auxiliary conditions on variable stepsize formula coefficients so that only $k+m$ values need be saved between steps without knowing future meshpoints. It is believed that such conditions can always be put in the form

$$[-\alpha_{1n}, \dots, \beta_{kn}] E^j \mathbf{g}_{n-j} = 0, \quad j = 0(1)k-m, \quad (2.1)$$

where $[-\alpha_{1n}, \dots, \beta_{kn}]$ is an abbreviation for $[-\alpha_{1n}, \beta_{1n}, \dots, -\alpha_{kn}, \beta_{kn}]$,

$$E := \begin{bmatrix} 0 & & & & \\ 0 & \bigcirc & & & \\ 1 & & & & \\ & \bigcirc & & & \\ & & 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{g}_n := [0, \dots, 0, c_{mn}, d_{mn}, \dots, c_{kn}, d_{kn}]^T,$$

$$c_{jn} := \text{function}(r_n, r_{n-1}, \dots, r_{n-j+2}),$$

and

$$d_{jn} := \text{function}(r_n, r_{n-1}, \dots, r_{n-j+2}).$$

We assume that these functions are rational functions that are well defined for all positive stepsize ratios and that the coefficients α_{jn} and β_{jn} are uniquely determined to be α_j and β_j when the stepsize ratios are all one. The complete set of $2k+2$ conditions that determine the formula coefficients will be called the *v.l.c. conditions*.

The mere existence of c_{jn} and d_{jn} such that (2.1) holds does impose substantial restrictions on the coefficients of the variable stepsize formula. For example, from (2.1) with $j=k-m$ we get

$$-c_{m,n-k+m} \alpha_{kn} + d_{m,n-k+m} \beta_{kn} = 0. \quad (2.2)$$

Our assumptions imply that for uniform stepsize

$$-c_m \alpha_k + d_m \beta_k = 0 \quad (2.3)$$

and

$$c_m^2 + d_m^2 > 0.$$

Taking $d_m \alpha_k + c_m \beta_k$ times (2.2) and subtracting $d_{m,n-k+m} \alpha_{kn} + c_{m,n-k+m} \beta_{kn}$ times (2.3) yields

$$\frac{-\beta_k \alpha_{kn} + \alpha_k \beta_{kn}}{\alpha_k \alpha_{kn} + \beta_k \beta_{kn}} = \frac{d_m c_{m,n-k+m} - c_m d_{m,n-k+m}}{c_m c_{m,n-k+m} + d_m d_{m,n-k+m}},$$

which implies that the left-hand side must be a rational function of $r_{n-k+m}, r_{n-k+m-1}, \dots, r_{n-k+2}$ only. If $m < k$, this is a real restriction, not satisfied by the two examples of Section 1. In fact, if $m = 1$, the numerator of the left-hand side must be identically zero, and as a corollary we get that $\alpha_{kn} \equiv 0$ if $\alpha_k = 0$ and $\beta_{kn} \equiv 0$ if $\beta_k = 0$.

and

- (ii) $\phi_n(t)E^{j+1}\mathbf{g}_{n-j} \equiv 0, \quad j = 0(1)k-m-1.$

These $2k$ conditions will be called the ϕ_n conditions.

The role of $\phi_n(t)$ is to provide a basis-free specification of the set of saved values. This set of $k+m$ saved values at t_n is given by

$$P_n(t) := \phi_n(t) [y_n, \dots, h_{n-k+2}y_{n-k+1}]^T,$$

where $[y_n, \dots, h_{n-k+2}y_{n-k+1}]$ is an abbreviation for $[y_n, h_n y_n, y_{n-1}, h_n y_{n-1}, \dots, y_{n-k+1}, h_{n-k+2}y_{n-k+1}]$. Note that the coefficients of $\phi_n(t_n + z h_n)$ depend only on $r_n, r_{n-1}, \dots, r_{n-k+3}$.

The elements of $\phi_n(t)$ form a set of Lagrange-like spanning functions. One can show that the difference $\mathbf{e}_i^T \text{tab}_n - \mathbf{e}_i^T$, where $\mathbf{e}_i$ denotes the i -th unit vector, satisfies the homogeneous ϕ_n conditions for $i = 1(1)2m$, and consequently

$$\mathbf{e}_i^T \text{tab}_n \phi_n = \mathbf{e}_i^T, \quad i = 1(1)2m, \quad (2.4)$$

which further implies

$$P_n(t_{n-j}) = y_{n-j}, \quad P_n'(t_{n-j}) = y'_{n-j}, \quad j = 0(1)m-1.$$

If the ϕ_n conditions are linearly dependent, then $\phi_n(t)$ is undefined. This is the concern of

THEOREM 2.2. Assume the v.l.c. conditions are linearly independent. Then $\phi_n(t)$ is well defined if and only if $\alpha_{kn}^2 + \beta_{kn}^2 > 0$, and in either case

$$\lambda_n(t) = \phi_n(t) [\beta_{0n}, \alpha_0, 0, \dots, 0]^T.$$

Moreover $\phi_n(t)$ is well defined for $r_n = r_{n-1} = \dots = r_{n-k+3} = 1$.

Proof. If $\alpha_{kn} = \beta_{kn} = 0$, then $[-\alpha_0, \beta_{0n}, \dots, -\alpha_{k-1,n}, \beta_{k-1,n}]$ satisfies the homogeneous ϕ_n conditions, which implies that $\phi_n(t)$ is not well defined. Assume $\alpha_{kn} + \beta_{kn}^2 > 0$. Let $[v_1, \dots, v_{2k}]$ satisfy the homogeneous ϕ_n conditions. Then

$$[v_1, \dots, v_{2k}, 0, 0] + \frac{v_1}{\alpha_0} [-\alpha_0, \dots, \beta_{k-1,n}, -\alpha_{kn}, \beta_{kn}] = 0$$

because it satisfies the homogeneous v.l.c. conditions. Because of our assumptions on the trailing coefficients, $v_1 = 0$, from which it follows that $v_2 = \dots = v_{2k} = 0$, demonstrating that $\phi_n(t)$ is well defined. The expression for $\lambda_n(t)$ is obtained using

$$\text{tab}_n \lambda_n = \beta_{0n} \mathbf{e}_1 + \alpha_0 \mathbf{e}_2 + \sum_{j=0}^{k-m-1} w_j E^{j+1} \mathbf{g}_{n-j}.$$

For $r_n = r_{n-1} = \dots = r_{n-k+3} = 1$, we know that $\alpha_{kn}^2 + \beta_{kn}^2 > 0$ and the result follows because $\phi_n(t)$ does not depend on r_{n-k+2} .

Q.E.D.

If $\phi_{n-1}(t)$ exists, then $\lambda_n(t)$ and the formula coefficients can be constructed from it.

THEOREM 2.3. Assume $\phi_{n-1}(t)$ is well defined. Then the v.l.c. conditions are linearly independent if and only if

In Sections 5 and 7 we present ways of choosing appropriate c_{jn} and d_{jn} . In this section we demonstrate that a variable stepsize multistep formula satisfying the given conditions can be implemented as an adaptable $(k+m)$ -value method.

First we need some definitions. Begin with

$$\text{tab}_n p := [p(t_n), h_n p'(t_n), p(t_{n-1}), h_n p'(t_{n-1}), \dots, p(t_{n-k+1}), h_n p'(t_{n-k+1})]^T$$

for any polynomial $p(t)$ of degree $\leq k+m-1$. (The tab symbol is adapted from Dahlquist and Björck [4, p. 88].) The linear operator tab_n becomes a $2k$ by $k+m$ matrix if we choose a particular basis for polynomials of degree $\leq k+m-1$. We refrain from doing so because any such choice would be arbitrary, although the Nordsieck basis

$$[1, (t-t_n)/h_n, \dots, ((t-t_n)/h_n)^{k+m-1}]$$

would not be a bad choice, in which case one can regard a polynomial p as a column vector of $k+m$ scaled derivatives at t_n and $p(t)$ as the product of the Nordsieck basis vector times p .

The following theorem serves to define a modifier polynomial for variable stepsizes.

THEOREM 2.1. Assume the v.l.c. conditions are linearly independent. Then there exists a unique polynomial $\lambda_n(t)$ of degree $\leq k+m-1$ such that

$$h_n \lambda_n'(t_n) = \alpha_0$$

and

$$R_n \text{tab}_{n-1} \lambda_n = \text{linear combination of } \mathbf{g}_n, E \mathbf{g}_{n-1}, \dots, E^{k-m} \mathbf{g}_{n-k+m}$$

where $R_n = \text{diag}(1, r_n, 1, 1, \dots, 1, 1)$. Moreover,

$$\lambda_n(t_n) = \beta_{0n}$$

and

$$\lambda_n(t_{n-j}) = \lambda_n'(t_{n-j}) = 0, \quad j = 1(1)m-1.$$

Proof. The conditions on $\lambda_n(t)$ can be restated as

$$\begin{bmatrix} h_n \lambda_n'(t_n) \\ R_n \text{tab}_{n-1} \lambda_n \end{bmatrix} = \begin{bmatrix} 0 \\ \sum_{j=0}^{k-m} w_j [E^j \mathbf{g}_{n-j}] \end{bmatrix} = \begin{bmatrix} \alpha_0 \\ 0 \end{bmatrix},$$

which is a system $2k+1$ equations for $2k+1$ unknown coefficients. The columns of the coefficient matrix arise from the v.l.c. conditions and hence are linearly independent. Premultiplying this system by $[\beta_{0n}, -\alpha_{1n}, \dots, \beta_{kn}]$ and using the fact that the formula is exact for $\lambda_n(t)$ gives the equation for $\lambda_n(t_n)$. The last equation is a consequence of the zero elements of $\mathbf{g}_n$.

Q.E.D.

The form $\lambda_n(t_n + z h_n)$ plays the role of the modifier polynomial for variable stepsizes. Its coefficients are now functions of $r_n, r_{n-1}, \dots, r_{n-k+2}$. Theorem 2.1 extends (1.3a) and (1.3b) to variable stepsizes.

Definition. Let $\phi_n(t)$ be the $2k$ -dimensional row vector which satisfies

- (i) $\phi_n(t) \text{tab}_n p \equiv p(t)$ for any polynomial $p(t)$ of degree $\leq k+m-1$,

$$= p_n(t) + \phi_n(t)[p_{n-1}(t_n) - y_n, h_n p'_{n-1}(t_n) - h_n y'_n, 0, \dots, 0]^T.$$

Because of (2.9) we have

$$\alpha_0 y_n - \beta_{0n} h_n y'_n = \alpha_0 p_{n-1}(t_n) - \beta_{0n} h_n p'_{n-1}(t_n)$$

and so

$$[y_n - p_{n-1}(t_n), h_n y'_n - h_n p'_{n-1}(t_n), 0, \dots, 0]^T \phi_n(t) = \frac{h_n}{\alpha_0} (y_n - p_{n-1}(t_n)) \lambda_n(t).$$

and

Q.E.D.

3. Methods of Optimal Order

For auxiliary conditions of a more restricted form it is possible to obtain an adaptable q -value method of order q , the highest possible order. Equivalently, it is possible to implement our $(k+m-1)$ -th order formula using only $k+m-1$ saved values rather than $k+m$ values.

We assume, in this section, that $m \geq 2$ and that

$$c_{jn} = \text{function}(r_{n-1}, r_{n-2}, \dots, r_{n-j+2}),$$

$$d_{jn} = \text{function}(r_{n-1}, r_{n-2}, \dots, r_{n-j+2}),$$

$j = m(1)k$. Hence there is no dependence of $\mathbf{g}_n$ on r_n .

Definition. Let $\hat{\phi}_n(t)$ be the $2k$ -dimensional row vector which satisfies

$$(i) \quad \hat{\phi}_n(t) \text{tab}_{n,p} = p(t) \text{ for any polynomial of degree } \leq k+m-2,$$

and

$$(ii) \quad \hat{\phi}_n(t) E^j \mathbf{g}_{n+1-j} \equiv 0, j = 0(1)k-m.$$

These $2k$ conditions will be called the $\hat{\phi}_n$ conditions.

Note that the coefficients of $\hat{\phi}_n(t_n + z h_n)$ depend only on $r_n, r_{n-1}, \dots, r_{n-k+3}$. The interpolation properties (2.4) hold only for $i = 1(1)2m-2$.

One result concerning the existence of $\hat{\phi}_n(t)$ is given by

THEOREM 3.1. Assume that the v.l.c. conditions are linearly independent. Then $\hat{\phi}_{n-1}(t)$ is well defined if and only if $\lambda_n(t)$ is of degree $k+m-1$ exactly, and in particular $\hat{\phi}_{n-1}(t)$ is well defined for $r_{n-1} = r_{n-2} = \dots = r_{n-k+2} = 1$.

Proof. Since $m \geq 2$, (2.8) becomes

$$\text{tab}_{n-1} \lambda_n = \sum_{j=0}^{k-m} w_j E^j \mathbf{g}_{n-j}. \quad (3.1)$$

Assume that $\hat{\phi}_{n-1}(t)$ is well defined. If we premultiply (3.1) by $\hat{\phi}_{n-1}(t)$ we conclude either that $\lambda_n(t) \equiv 0$, which is not possible since $h_n \lambda'_n(t_n) = \alpha_0 \neq 0$, or that $\lambda_n(t)$ is of degree $> k+m-2$. Assume that $\lambda_n(t)$ is of degree $k+m-1$ exactly, and let $\mathbf{v}^T$ satisfy the homogeneous $\hat{\phi}_{n-1}$ conditions. Thus $\mathbf{v}^T$ annihilates $\text{tab}_{n-1} p$ for arbitrary polynomials $p(t)$ of degree $\leq k+m-2$ and also, because of (3.1), annihilates $\text{tab}_{n-1} \lambda_n$. Since $\lambda_n(t)$ is of degree $k+m-1$, $\mathbf{v}^T$ must annihilate $\text{tab}_{n-1} p$ for any polynomial of degree $\leq k+m-1$, and

$$\phi'_{n-1}(t_n) R_n^{-1} \mathbf{g}_n \neq 0,$$

and in either case

$$\lambda_n(t) = \frac{\alpha_0 \phi'_{n-1}(t) R_n^{-1} \mathbf{g}_n}{h_n \phi'_{n-1}(t_n) R_n^{-1} \mathbf{g}_n}, \quad (2.5)$$

$$\beta_{0n} = \lambda_n(t_n), \quad (2.6)$$

and

$$[-\alpha_{1n}, \dots, \beta_{kn}] R_n = \alpha_0 \phi_{n-1}(t_n) - \beta_{0n} h_n \phi'_{n-1}(t_n). \quad (2.7)$$

Proof. If $\phi'_{n-1}(t_n) R_n^{-1} \mathbf{g}_n = 0$, then $[0, 1, -h_n \phi'_{n-1}(t_n) R_n^{-1}]$ satisfies the homogeneous v.l.c. conditions. Assume $\phi_{n-1}(t_n) R_n^{-1} \mathbf{g}_n \neq 0$. Let $[0, \beta_{0n}, -\alpha_{1n}, \dots, \beta_{kn}]$ satisfy the homogeneous v.l.c. conditions (α_{0n} must be zero). Then

$$\beta_{0n} h_n \phi'_{n-1}(t_n) + [-\alpha_{1n}, \dots, \beta_{kn}] R_n = 0$$

because the left-hand side satisfies the homogeneous ϕ_{n-1} conditions. Postmultiplying by $R_n^{-1} \mathbf{g}_n$ implies $\beta_{0n} = 0$, which in turn implies that the other coefficients are zero. To obtain (2.5), premultiply the equation

$$R_n \text{tab}_{n-1} \lambda_n = \sum_{j=0}^{k-m} w_j E^j \mathbf{g}_{n-j} \quad (2.8)$$

by $\phi_{n-1}(t) R_n^{-1}$ and use the fact that $h_n \lambda'_n(t_n) = \alpha_0$. Equation (2.6) is from Theorem 2.1. To get (2.7), note that the difference between the left and right-hand sides satisfies the homogeneous ϕ_{n-1} conditions.

Q.E.D.

THEOREM 2.4. Assume that the v.l.c. conditions are linearly independent and that ϕ_n and ϕ_{n-1} are well defined. Then the variable stepsize multistep formula given by the v.l.c. conditions can be implemented as an adaptable $(k+m)$ -value method. More specifically,

$$\alpha_0 p_{n-1}(t_n) - \beta_{0n} h_n p'_{n-1}(t_n) = \sum_{j=1}^k \{-\alpha_{jn} y_{n-j} + \beta_{jn} h_{n-j+1} y'_{n-j}\} \quad (2.9)$$

and so y_n and y'_n can be determined from $p_{n-1}(t)$, and furthermore,

$$p_n(t) = p_{n-1}(t) + \frac{h_n}{\alpha_0} (y'_n - p'_{n-1}(t_n)) \lambda_n(t),$$

and so the set of saved values at t_n can be computed from y'_n and the saved values at t_{n-1} .

Proof. Postmultiplying (2.7) by $[y_{n-1}, \dots, h_{n-k+1} y'_{n-k}]^T$ establishes (2.9). It can be shown, using the ϕ_{n-1} conditions, that

$$\phi_{n-1}(t) = \phi_n(t)(\mathbf{e}_1 \phi_{n-1}(t_n) + \mathbf{e}_2 h_n \phi'_{n-1}(t_n) + E R_n). \quad (2.10)$$

Postmultiplying this by $[y_{n-1}, \dots, h_{n-k+1} y'_{n-k}]^T$ yields

$$p_{n-1}(t) = \phi_n(t)[p_{n-1}(t_n), y_{n-1}, h_n y'_{n-1}, \dots, y_{n-k+1}, h_{n-k+2} y'_{n-k+1}]^T$$

$\hat{\phi}_{n-1}(t) = \phi_n(t)(\mathbf{e}_1 \hat{\phi}_{n-1}(t_n) + \mathbf{e}_2 h_n \hat{\phi}_{n-1}'(t_n) + ER_n)$, which follows from the linear independence of the $\hat{\phi}_{n-1}$ conditions. Postmultiply by $[y_{n-1}, \dots, h_{n-k+1}y_{n-k}]^T$ to get

$$\hat{p}_{n-1}(t) = \hat{\phi}_n(t) [\hat{p}_{n-1}(t_n) - y_n, h_n \hat{p}_{n-1}'(t_n) - h_n y_n', 0, \dots, 0]^T + p_n(t).$$

Because

$$\alpha_0 y_n - \beta_{0n} h_n y_n' = \alpha_0 \hat{p}_{n-1}(t_n) - \beta_{0n} h_n \hat{p}_{n-1}'(t_n)$$

we get

$$\hat{p}_{n-1}(t) = \frac{h_n}{\alpha_0} (\hat{p}_{n-1}'(t_n) - y_n') \lambda_n(t) + p_n(t)$$

which together with Theorem 3.3 establishes the result.

Q.E.D.

The following is a variable stepsize version of Steel [19, Theorem 3.1].

THEOREM 3.4 Assume the v.l.c. conditions are linearly independent and that $\phi_n(t)$, $\hat{\phi}_{n-1}(t)$, and $\hat{\phi}_{n-1}'(t)$ are well defined. Then

$$\hat{\lambda}_{n-1}(t) = \lambda_{n-1}(t) - \omega_n' \lambda_n(t)$$

where ω_n is chosen so that $\hat{\lambda}_{n-1}(t)$ is of degree at most $k+m-2$.

Proof. Take (2.7) and subtract (3.2) obtaining

$$\phi_{n-1}(t_n) - \hat{\phi}_{n-1}(t_n) = \frac{h_n \beta_{0n}}{\alpha_0} (\phi_{n-1}'(t_n) - \hat{\phi}_{n-1}'(t_n)).$$

This is substituted into (2.10) and subtracted from (3.3) to yield

$$\phi_{n-1}(t) - \hat{\phi}_{n-1}(t) = \frac{h_n}{\alpha_0} (\phi_{n-1}'(t_n) - \hat{\phi}_{n-1}'(t_n)) \lambda_n(t),$$

and the theorem follows from postmultiplying by $[\beta_{0n}, \alpha_0, 0, \dots, 0]^T$.

Q.E.D.

An example of this is given at the end of Section 5.

Remark. Under the assumptions of this section, (2.5) becomes

$$\lambda_n(t) = \frac{\alpha_0 \phi_{n-1}(t) \mathbf{g}_n}{h_n \phi_{n-1}(t_n) \mathbf{g}_n}$$

where $\mathbf{g}_n$ does not depend on r_n , and we see why $\omega_n \lambda_n(z)$ is independent of r_n for some ω_n .

4. Families of Formulas

Given a $(K+m)$ -value method of order $K+m-1$, we can generate a $(k+m)$ -value method of order $k+m-1$ for $k = m(1)/K$. In this section we describe the formula of one order lower and one stepnumber less and give a prescription for changing the order.

The coefficients α_{jn}^* , β_{jn}^* , $j = 0(1)k$, of the $(k-1)$ -step formula would be determined by requiring that $\alpha_{kn}^* = \beta_{kn}^* = 0$, that the formula be exact for polynomials of degree

therefore the coefficients $[0, 0, 0, \mathbf{v}^T]$ satisfy the homogeneous v.l.c. conditions. This implies that $\mathbf{v}^T = 0$ and we conclude that $\hat{\phi}_{n-1}$ is well defined. For $r_{n-1} = r_{n-2} = \dots = r_{n-k+2} = 1$, it follows from Steel [19, Eq. (4.3)] that the leading coefficient of $\lambda(t_n + z h_n)$ is $\sigma(1)/q! \neq 0$ when the stepsizes are uniform.

Q.E.D.

The central result of this section is the analog of Theorem 2.4 where

$$\hat{\lambda}_n(t) := \hat{\phi}_n(t) [\beta_{0n}, \alpha_0, 0, \dots, 0]^T$$

and

$$\hat{p}_n(t) := \hat{\phi}_n(t) [y_n, \dots, h_{n-k+2} y_{n-k+1}]^T.$$

THEOREM 3.2. Assume that the v.l.c. conditions are linearly independent and that $\hat{\phi}_n(t)$ and $\hat{\phi}_{n-1}(t)$ are well defined. Then

$$\alpha_0 \hat{p}_{n-1}(t_n) - \beta_{0n} h_n \hat{p}_{n-1}'(t_n) = \sum_{j=1}^k \{ -\alpha_{jn} y_{n-j} + \beta_{jn} h_n \hat{p}_{n-j+1}'(t_n) \}$$

and

$$\hat{p}_n(t) = \hat{p}_{n-1}(t) + \frac{h_n}{\alpha_0} (y_n - \hat{p}_{n-1}'(t_n)) \hat{\lambda}_n(t).$$

Proof. We use the linear independence of the $\hat{\phi}_{n-1}$ conditions to show that

$$[-\alpha_{1n}, \dots, \beta_{kn}] R_n = \alpha_0 \hat{\phi}_{n-1}(t_n) - \beta_{0n} h_n \hat{\phi}_{n-1}'(t_n) \quad (3.2)$$

and

$$\hat{\phi}_{n-1}(t) = \hat{\phi}_n(t) (\mathbf{e}_1 \hat{\phi}_{n-1}(t_n) + \mathbf{e}_2 h_n \hat{\phi}_{n-1}'(t_n) + ER_n) \quad (3.3)$$

and proceed as in Theorem 2.4.

Q.E.D.

We conclude this section by examining how $\hat{p}_n(t)$ is related to $p_n(t)$ and $\hat{\lambda}_n(t)$ to

$\lambda_n(t)$. First we note that

$$\hat{\phi}_n(t) \text{tab}_n \phi_n \equiv \hat{\phi}_n(t)$$

because the difference between left and right-hand sides satisfies the $\hat{\phi}_n$ conditions. Hence

$$\hat{p}_n(t) = \hat{\phi}_n(t) \text{tab}_n p_n,$$

$$\hat{\lambda}_n(t) = \hat{\phi}_n(t) \text{tab}_n \lambda_n.$$

Next is a result in the other direction, showing how to determine $p_n(t)$ from $\hat{p}_n(t)$.

THEOREM 3.3. Assume that the v.l.c. conditions are linearly independent and that $\phi_n(t)$, $\hat{\phi}_n(t)$, and $\hat{\phi}_{n-1}(t)$ are well defined. Then

$$p_n(t) = \hat{p}_n(t) + \frac{h_n}{\alpha_0} (y_n - \hat{p}_{n-1}'(t_n)) (\lambda_n(t) - \hat{\lambda}_n(t)).$$

Proof. We begin with

$\leq k+m-2$, that (2.1) hold for $j = 0(1)k-1-m$, and that $\alpha_{0n}^* = \alpha_0$. For convenience we continue to work with $2k$ -dimensional vectors rather than $(2k-2)$ -dimensional vectors.

Definition. Let $\phi_n^*(t)$ be the $2k$ -dimensional row vector which satisfies

- (i) $\phi_n^*(t) \operatorname{tab}_n p = p(t)$ for any polynomial $p(t)$ of degree $\leq k+m-2$,
- (ii) $\phi_n^*(t) E^{j+1} \mathbf{g}_{n-j} \equiv 0, j = 0(1)k-m-2$,

and

- $$(iii) \quad \phi_n^*(t)e_i \equiv 0, \quad j = 2k-1, 2k.$$

Consider the problem of lowering the order by one. Using the ϕ_n conditions, we can verify that

$$\phi_n^*(t) = \phi_n^*(t) \operatorname{tab}_n \phi_n$$

and hence

$$p_n^*(t) = \phi_n^*(t) \text{ tab}_n p_n$$

where, of course,

$$p_n^*(t) := \phi_n^*(t) [y_n, \dots, h_{n-k+2} y_{n-k+1}]^T.$$

Increasing the order by one is the subject of

THEOREM 4.1. Assume that the v.l.c. conditions are linearly independent and that $\phi_n(t)$, $\phi_n^+(t)$, and $\phi_{n-1}^-(t)$ are well defined. Then

$$p_n(t) = p_n^*(t) + \frac{h_n}{\alpha_n} (y_n' - p_{n-1}'(t_n))(\phi_n(t) - \phi_n^*(t))[\beta_{0n}^*, 0]^T.$$

Proof. The relation

$$\dot{\phi}_{n-1}^*(t) = \dot{\phi}_n(t)(e_1 \phi_{n-1}^*(t_n) + e_2 h_n \phi_{n-1}^{*'}(t_n) + ER_n)$$

follows from the linear independence of the ϕ_{n-1}^* conditions. By an argument like that in the proof of Theorem 3.3 we get

$$p_{n-1}^*(t) = \frac{h_n}{\alpha_n} (p_{n-1}^{s'}(t_n) - y_n) \phi_n(t) [\beta_n^*, \alpha_n, 0, \dots, 0]^T + p_n(t),$$

and the result follows from a lower-order version of Theorem 2.4.

Q.E.D.

The code DIFSUB and its derivatives do not change order properly, as noted by Shampine [16].

The development in this section is applicable also to the minimal storage methods of the preceding section.

5. Variable Coefficient Extensions

We present auxiliary conditions which lead to what we believe is the most natural variable-stepsize extension of a general linear multistep formula.

For uniform stepsise it follows from (1.3) that

$$\sum_{i=0}^j \{-\alpha_{k-j+i} \Lambda(-m-i) + \beta_{k-j+i} \Lambda'(-m-i)\} = 0, \quad j = 0(1)k-m.$$

The case $j = k - m$ follows from (1.3a), (1.3b), and the fact that the formula with meshpoints $0, -1, \dots, -k$ is exact for $d(z)$. That these auxiliary conditions together with the other conditions are linearly independent is shown in the corollary to Theorem 5.1. A simple extension of these conditions to variable stepsize is given below:

Definition. The variable coefficient extension of a fixed-stepwise linear k -step formula of order $k+m-1$, where $k \geq 2$ and $1 \leq m \leq k$, is obtained by fixing $\alpha_{0n} = \alpha_0$, requiring that it be exact for polynomials of degree $\leq k+m-1$, and imposing condition (2.1) where

$$c_{in} := \Lambda(-j), d_{in} = \Lambda'(-j), \quad j = m(1)k.$$

We note that the c_{jn} and d_{jn} have the form required for minimum storage (alternatively, optimal order) methods; that is, for $m \geq 2$ the number of saved values can be reduced from $k+m$ to $k+m-1$ as described in Section 3.

Another nice property is that if the trailing α_j 's or β_j 's are all zero, then they remain zero for the variable coefficient extension. To see this, suppose $\alpha_j = \alpha_{j+1} = \dots = \alpha_k = 0$ where $j > m$. This implies

$$\Lambda'(-m) = \Lambda'(-m-1) = \dots = \Lambda'(-k+j-m) = 0,$$

which in turn implies $\alpha_{in} = \alpha_{i+1,n} = \dots = \alpha_{kn} = 0$.

A complete treatment of the simplest case, $k = 2$ and $m = 1$, is not difficult. A convenient parametrisation of such formulas is via the modifier polynomial $A(x) = \beta_0 + \alpha_0 x + \frac{1}{2}x^2$. Our normalisation is equivalent to $\sum \beta = 1$, which is always possible since $\rho(\xi)$ and $\sigma(\xi)$ are assumed to have no common factors. Since $\phi_n(t)$ is independent of r_n , it always exists. The existence of the variable coefficient extension depends on the denominator in (2.5) being nonzero. There are regions of the (α_0, β_0) -plane such that this expression does not vanish for any $r_n > 0$, and there are other regions for which it vanishes for one or two positive values of r_n . For example with $\alpha_0 = \frac{3}{2}$ and $\beta_0 = \frac{5}{6}$ the variable coefficient formula "blows up" at $r_n = 1 + \sqrt{3/2}$.

The polynomial $p_n(t)$ for variable coefficient methods possesses interpolation properties in addition to those stemming from (2.4). Using an argument based on the linear independence of the ϕ_n conditions, we get the equality $Q \text{ tab}_n \phi_n = Q$ where

$$[0, \dots, 0, -\alpha_m, \dots, \beta_k] R_n \text{ tab}_{n-1} \lambda_n = 0.$$

Proof. Because the formula of Theorem 5.2 is exact for $\lambda_n(t)$ we have

$$\begin{aligned} \alpha_0 \lambda_n(t_n) - \beta_0 \lambda_n \lambda_n'(t_n) &= \sum_{j=1}^{m-1} \{-\alpha_j \lambda_n(t_{n-j}) + \beta_j \lambda_n \lambda_n'(t_{n-j})\} \\ &\quad + \sum_{j=m}^i \gamma_j \sum_{i=0}^j \{-\alpha_{k-j+1} \lambda_n(t_{n-m-i}) \\ &\quad + \beta_{k-j+1} \lambda_n \lambda_n'(t_{n-m-i})\} \end{aligned}$$

and the result follows from Eq. (5.2).

Q.E.D.

The characterisation of $\lambda_n(t)$ given by this theorem and Eq. (5.2) is useful for constructing $\lambda_n(t)$, as Byrne and Hindmarsh [1] have done. The k -th order BDF has

$$\lambda_n(t) = \frac{(t-t_{n-1}) \cdots (t-t_{n-k})}{(t_n-t_{n-1}) \cdots (t_n-t_{n-k})}$$

and the $(k+1)$ -th order Adams-Moulton formula has

$$\lambda_n(t) = \frac{1}{h_n} \int_{t_{n-1}}^t \frac{(r-t_{n-1}) \cdots (r-t_{n-k})}{(t_n-t_{n-1}) \cdots (t_n-t_{n-k})} dr.$$

The relation $\hat{\lambda}_n(t) = \lambda_n(t) - \omega_{n+1} \lambda_{n+1}(t)$ for minimum storage methods is applicable to the $(k+1)$ -th order Adams-Moulton formula, for which we have

$$\hat{\lambda}_n(t) = \lambda_n(t) - \frac{h_{n+1}(t_{n+1}-t_n) \cdots (t_{n+1}-t_{n+1-k})}{h_n(t_n-t_{n-1}) \cdots (t_n-t_{n-k})} \lambda_{n+1}(t)$$

$$= \dots = \beta_0 n - \beta_0^* + \lambda_n^*(t)$$

where $\beta_0 n$ and $\lambda_n^*(t)$ are the leading coefficient and modifier polynomial, respectively, for the $(k+1)$ -value implementation of the $(k+1)$ -step k -th order Adams-Moulton formula.

6. Fixed Leading Coefficient Extensions

For a fixed leading coefficient formula the condition

$$\beta_0 n = \beta_0$$

is substituted for the case $j = 0$ of (2.1). Thus the auxiliary conditions are limited to

$$[-\alpha_1 n, \dots, \beta_k n] E^j \mathbf{g}_{n-j} = 0, \quad j = 1(1)k-m,$$

with the same assumptions as in Section 2. The complete set of conditions in this case will be called the *f.l.c. conditions*.

The omitted v.l.c. condition has the form

$$-\alpha_{mn} c_{mn} + \beta_{mn} d_{mn} - \dots - \alpha_{kn} c_{kn} + \beta_{kn} d_{kn} = 0.$$

Since the coefficients c_{kn} and d_{kn} do not occur in the other auxiliary conditions, we are free to define them in such a way that the above condition is satisfied, except that they would be undefined whenever $\alpha_{kn}^2 + \beta_{kn}^2$ vanishes. Thus f.l.c. is essentially a special case of v.l.c. The fixed coefficient formulas described in the next section are notable examples of this.

We define $\phi_n(t)$ and $p_n(t)$ exactly as in Section 2 and define

$$\lambda_n(t) := \phi_n(t) \beta_0, \quad \alpha_0, 0, \dots, 0]^T.$$

Note that the f.l.c. conditions are linearly independent if and only if $\phi_{n-1}(t)$ is well defined. The modifier polynomial $\lambda_n(t_n + z h_n)$ has coefficients that depend on only $r_n, r_{n-1}, \dots, r_{n-k+3}$ because $\beta_0 n = \beta_0$ does not depend on r_{n-k+2} . The central result Theorem 2.4 holds for the f.l.c. extensions. The coefficients of an f.l.c. formula can be obtained from (2.7) with $\beta_0 n = \beta_0$.

The material in Section 3 on minimal storage methods is not applicable to f.l.c. extensions because of the omitted v.l.c. condition.

For the remainder of this section we consider variable coefficient f.l.c. extension. The linear independence of the f.l.c. conditions for $r_{n-1} = r_{n-2} = \dots = r_{n-k+2} = 1$ follows from the existence of $\phi_{n-1}(t)$, which is a consequence of Theorem 5.1 and the linear independence of conditions (1.3).

The result in Section 5 concerning vanishing trailing coefficients applies only for $j \geq m+1$ in the case of f.l.c. formulas.

A result similar to Theorem 5.2 holds for the f.l.c. variant:

THEOREM 6.1. *The coefficients of the formula*

$$\alpha_0 y_n - h_n \beta_0 y_n' = \sum_{j=1}^m \{-\alpha_j n y_{n-j} + \beta_j y_n h_{n-j+1} y_{n-j}'\} + \sum_{j=m+1}^k \gamma_j n s_j^{j-m-1}$$

are uniquely determined by the condition that the formula be exact for polynomials of degree $\leq k+m-1$ if and only if the variable coefficient f.l.c. conditions are linearly independent. In either case the two formulas are equivalent.

Proof. A combination of the proofs of Theorem 5.1 and Theorem 5.2.

Q.E.D.

Our variable coefficient f.l.c. extensions of the BDFs are the f variants of the f.l.c. formulas proposed by Jackson and Sacks-Davis [11]. Their y variant requires increasing the stepnumber of the formula.

7. Fixed Coefficient Extensions

The auxiliary conditions used in this approach can be expressed in such a way that they look quite similar to those for the variable coefficient approach:

Definition. The fixed coefficient extension of a fixed stepsize linear k -step formula of order $k+m-1$, where $1 \leq m \leq 2 \leq k$, is obtained by fixing $\alpha_0 n = \alpha_0$, requiring that it be exact for polynomials of degree $\leq k+m-1$, and imposing condition (2.1) where

$$c_{jn} := A\left(\frac{t_{n-j}-t_n}{h_n}\right), d_{jn} := \frac{h_{n-j+1}}{h_n} A\left(\frac{t_{n-j}-t_n}{h_n}\right), \quad j = m(1)k.$$

Note the restriction $m \leq 2$. The situation for $m > 2$ is rather complicated and, in any case, not of practical interest.

An example of a nonexistent fixed coefficient extension occurs with $A(x) = (x+1)(x+\frac{3}{2})(x+2)$ when $r_n = \frac{1}{5}$.

We show below that there are no separate f.l.c. and v.l.c. variants of this approach and that the modifier polynomial is simple to compute.

THEOREM 7.1. *For a fixed coefficient method the v.l.c. and f.l.c. conditions are equivalent, and if the v.l.c. conditions are linearly independent, then*

$$\lambda_n(t) = A\left(\frac{t-t_n}{h_n}\right).$$

Proof. Since the multistep formula is exact for polynomials of degree $\leq k+m-1$,

$$-\alpha_{0n}A(0) + \beta_{0n}A(0) + \sum_{j=1}^k \left\{ -\alpha_{jn}A\left(\frac{t_{n-j}-t_n}{h_n}\right) + \beta_{jn} \frac{h_{n-j+1}}{h_n} A\left(\frac{t_{n-j}-t_n}{h_n}\right) \right\} = 0.$$

Using (1.3) and $\alpha_{0n} = \alpha_0$, we get

$$\alpha_0(-\beta_0 + \beta_{0n}) + [-\alpha_{1n}, \dots, \beta_{kn}] \mathbf{g}_n = 0,$$

which indicates that the f.l.c. condition is satisfied if and only if the v.l.c. condition is. With

$$\bar{\lambda}_n(t) := A\left(\frac{t-t_n}{h_n}\right)$$

we note that

$$R_n \text{tab}_{n-1} \bar{\lambda}_n = \mathbf{g}_n$$

so that by Theorem 2.1 we must have $\lambda_n(t) = \bar{\lambda}_n(t)$.

Q.E.D.

THEOREM 7.2. *The fixed coefficient formula described near the end of Section 1 is equivalent to that defined in this section in the sense that if $p_{n-1}(t)$ is the same in both cases then $p_n(t)$ is the same, and in particular, y_n and $\bar{y}_n$ are the same.*

Proof. Let overbars denote values computed by the procedure in Section 1. Thus $\bar{y}_n$ and $\bar{y}_n$ are determined by the fixed stepsize formula applied to values of $p_{n-1}(t)$ at equally spaced points $t_n - jh_n$. Because the formula is exact for $p_{n-1}(t)$, we have

$$\alpha_0 \bar{y}_n - \beta_0 h_n \bar{y}'_n = \alpha_0 p_{n-1}(t_n) - \beta_0 h_n p'_{n-1}(t_n)$$

and hence $\bar{y}_n = y_n$ and $\bar{y}'_n = y'_n$. The new polynomial $\bar{p}_n(t)$ is defined to be the unique (recall (1.3)) polynomial of degree $\leq k+m-1$ satisfying

$$Q \text{tb}_n \bar{p}_n$$

$$= Q(\text{tb}_n p_{n-1} + (y_n - p_{n-1}(t_n)) \mathbf{e}_1 + h_n (y'_n - p'_{n-1}(t_n)) \mathbf{e}_2)$$

where tb_n is simply tab_n for meshpoints $t_n - jh_n$, $j = 0(1)k-1$. However, we also have

$$Q \text{tb}_n p_n = Q(\text{tb}_n p_{n-1} + \frac{h_n}{\alpha_0} (y'_n - p'_{n-1}(t_n)) \text{tb}_n \lambda'_n),$$

$$\text{tb}_n \lambda'_n = \beta_0 \mathbf{e}_1 + \alpha_0 \mathbf{e}_2,$$

and

$$\frac{\beta_0}{\alpha_0} h_n (y'_n - p'_{n-1}(t_n)) = y_n - p_{n-1}(t_n).$$

By Theorem 5.2, $Q \text{tb}_n$ is nonsingular, and hence $\bar{p}_n(t) = p_n(t)$.

Q.E.D.

It is because of the use of the fixed stepsize formula in this procedure that the Nordstieck interpolatory technique has been referred to as a "fixed step" procedure. And it is for this reason that Jackson and Sacks-Davis [11] have named it "constant coefficient." We would suggest another reason for this name, and that is that $A_n(x) := \lambda_n(t_n + xh_n)$ has constant coefficients not depending on the stepsize ratios.

A minimum storage implementation is not possible for fixed coefficient variable stepsize methods because c_{jn} and d_{jn} depend on r_n . However, for the case $m = 2$, if the auxiliary conditions are modified to become

$$c_{jn} := A\left(\frac{t_{n-j}-t_{n-1}}{h_{n-1}} - 1\right),$$

$$d_{jn} := \frac{h_{n-j+1}}{h_{n-1}} A\left(\frac{t_{n-j}-t_{n-1}}{h_{n-1}} - 1\right),$$

then the appropriate conditions are satisfied. For $k = 2$ (only) this gives a variable coefficient formula. With $\bar{\lambda}_n(t) := A(\frac{t-t_{n-1}}{h_{n-1}} - 1)$ we note that

$$R_n \text{tab}_{n-1} \bar{\lambda}_n = \mathbf{g}_n$$

and

$$h_n \bar{\lambda}'_n(t_n) = r_n A'(r_n - 1),$$

and therefore by Theorem 2.1

$$\lambda_n(t) = \frac{A(0)}{r_n A'(r_n - 1)} A\left(\frac{t-t_{n-1}}{h_{n-1}} - 1\right).$$

With this we can construct adaptable multivalued methods of optimal order.