

In Sections 5 and 7 we present ways of choosing appropriate e_{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

$$\text{tab}_n p := [p(t_n), h_n p'(t_n), p(t_{n-1}), h_n p'(t_{n-1}), \dots, p(t_{n-k+1}), h_{n-k+2} p'(t_{n-k+1})]^T$$

for any polynomial $p(t)$ of degree $\leq k+m-1$. (The tab symbol is adapted from Dahlquist and Björck [4, p. 83].) 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 Nordstieck 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 Nordstieck basis vector times p .

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

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 $\lambda_n(t_n + zh_n)$ plays the role of the modifier polynomial for variable stepsize. 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 stepsize.

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

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

and

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

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 $\phi_n(t_n + zh_n)$ 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 $e_i^T \text{tab}_n \phi_n - e_i^T$, where e_i denotes the i -th unit vector, satisfies the homogeneous ϕ_n conditions for $i = 1(1)2m$, and consequently

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

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

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

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

$$\text{tab}_n \lambda_n = \beta_{0n} e_1 + \alpha_0 e_2 + \sum_{j=0}^{k-m-1} w_j E^{j+1} \mathbf{g}_{n-j}.$$

For $r_n = r_{n-1} = \dots = r_{n-k+2} = 1$, 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*

$$= p_n(t) + \phi_n(t) [p_{n-1}(t_n) - y_n, h_n p_{n-1}(t_n) - h_n y_n, 0, \dots, 0]^T.$$

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

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

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 \mathfrak{g}_n on r_n .

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

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

and

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

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

Note that the coefficients of $\phi_n(t_n + zh_n)$ 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 $\phi_n(t)$ is given by

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

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

$$\text{tab}_{n-1} \lambda_n = \sum_{j=0}^{k-m} w_j E^j \mathfrak{g}_{n-j}. \tag{3.1}$$

Assume that $\phi_{n-1}(t)$ is well defined. If we premultiply (3.1) by $\phi_{n-1}(t)$ 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 v^T satisfy the homogeneous ϕ_{n-1} conditions. Thus 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 $k+m-1$, v^T must annihilate $\text{tab}_{n-1} p$ for any polynomial of degree $\leq k+m-1$, and

$$\phi_{n-1}'(t_n) R_n^{-1} \mathfrak{g}_n \neq 0,$$

and in either case

$$\lambda_n(t) = \frac{\alpha_0 \phi_{n-1}(t) R_n^{-1} \mathfrak{g}_n}{h_n \phi_{n-1}'(t_n) R_n^{-1} \mathfrak{g}_n}, \tag{2.5}$$

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

and

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

Proof. If $\phi_{n-1}'(t_n) R_n^{-1} \mathfrak{g}_n = 0$, then $[0, 1, -h_n \phi_{n-1}'(t_n) R_n^{-1}]$ satisfies the homogeneous v.l.c. conditions. Assume $\phi_{n-1}'(t_n) R_n^{-1} \mathfrak{g}_n \neq 0$. 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 $R_n^{-1} \mathfrak{g}_n$ implies $\beta_{0n} = 0$, which in turn implies that the other coefficients are zero. To obtain (2.5), premultiply the equation

$$R_n \text{tab}_{n-1} \lambda_n = \sum_{k-m}^{j=0} w_j E^j \mathfrak{g}_{n-j} \tag{2.8}$$

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,

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

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

$$\phi_{n-1}(t) = \phi_n(t) (e_1 \phi_{n-1}(t_n) + e_2 h_n \phi_{n-1}'(t_n) + E R_n). \tag{2.10}$$

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

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

therefore the coefficients $[0, 0, 0, \dots, v^T]$ satisfy the homogeneous v.l.c. conditions. This implies that $v^T = 0$ 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 Skeel [19, Eq. (4.3)] that the leading coefficient of $\lambda(t_n + xh_n)$ 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

$$\hat{\lambda}_n(t) := \hat{\phi}_n(t) [\beta_{0n}, \alpha_{00}, 0, \dots, 0]^T$$

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

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

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

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

and

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

and proceed as in Theorem 2.4.

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

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

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 $\hat{\phi}_n(t)$, $\hat{\phi}_{n-1}(t)$, 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

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

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 Skeel [19, Theorem 3.1].

THEOREM 3.4. Assume the v.l.c. conditions are linearly independent and that $\hat{\phi}_n(t)$, $\phi_{n-1}(t)$, 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

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

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

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

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

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

where \mathbf{g}_n does not depend on r_n , and we see why $\omega_n \lambda_n(x)$ 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 change 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

For uniform stepsize it follows from (1.3) that

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

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 $A(x)$. 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-stepsize 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

$$c_{jn} := A(-j), \quad d_{jn} = A(-j), \quad j = m(1)k.$$

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.

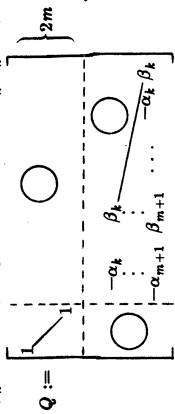
Another nice property is that if the trailing α_j 's or β_j 's are all zero, then they remain zero for the variable coefficient extension. To see this, suppose $\alpha_j = \alpha_{j+1} = \dots = \alpha_k = 0$ where $j \geq m$. This implies

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

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

A complete treatment of the simplest case, $k = 2$ and $m = 1$, is not difficult. A convenient parametrization 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 $\alpha_0 = \frac{5}{2}$ 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



$\leq k+m-2$, 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) $\phi_n^*(t) \text{ tab}_n p = p(t)$ for any polynomial $p(t)$ of degree $\leq k+m-2$,
 - (ii) $\phi_n^*(t) E^{j+1} \mathbf{e}_{n-j} \equiv 0, j = 0(1)k-m-2$,
- and
- (iii) $\phi_n^*(t) \mathbf{e}_j \equiv 0, j = 2k-1, 2k$.

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

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

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

$$p_n(t) = p_{n-1}(t) + \frac{h_n}{\alpha_0} (y_n - p_{n-1}(t_n)) (\phi_n(t) - \phi_n^*(t)) [\beta_{0n}, \alpha_{0n}, 0, \dots, 0]^T.$$

Proof. The relation

$$\phi_{n-1}^*(t) = \phi_n(t) (\mathbf{e}_1 \phi_{n-1}^*(t_n) + \mathbf{e}_2 h_n \phi_{n-1}^*(t_n) + E R_n)$$

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

$$p_{n-1}^*(t) = \frac{h_n}{\alpha_0} (p_{n-1}(t_n) - y_n) \phi_n^*(t) [\beta_{0n}, \alpha_{0n}, 0, \dots, 0]^T + p_n(t),$$

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 Shampline [16].

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

5. Variable Coefficient Extensions

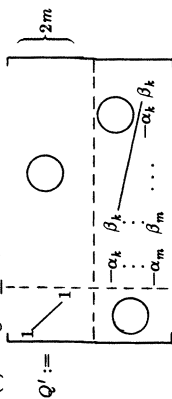
We present auxiliary conditions which lead to what we believe is the most natural variable-stepsize extension of a general linear multistep formula.

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 v.l.c. conditions are linearly independent. In either case the two formulas are equivalent.

Proof. The first set of conditions can be expressed as $\bar{\alpha}_{0n} = \alpha_0$ and

$$[-\bar{\alpha}_{0n}, \dots, \bar{\beta}_{m-1,n}, \gamma_{mn}, \dots, \gamma_{kn}] Q^T \text{Tab}_n p = 0$$

for any polynomial $p(t)$ of degree $\leq k+m-1$ where



and $\text{Tab}_n p := [\text{tab}_n p, p(t_{n-k}), h_{n-k+1} p'(t_{n-k})]$. Assume that the v.l.c. conditions are linearly independent. Consider w^T such that $w_1 = 0$ and $w^T Q^T \text{Tab}_n p = 0$ for all polynomials $p(t)$ of degree $\leq k+m-1$. Then $w^T Q^T e_1 = 0$, and

$$w^T Q^j = 0, \quad j = 0(1)k-m.$$

Hence $w^T Q^j = 0$, and since Q^j is of full rank, $w^T = 0$, and so the first set of conditions are linearly independent. The proof of the converse is similar to that of Theorem 5.1. In either case we have that

$$[-\bar{\alpha}_{0n}, \dots, \beta_{kn}] = [-\bar{\alpha}_{0n}, \dots, \bar{\beta}_{m-1,n}, \gamma_{mn}, \dots, \gamma_{kn}] Q^j$$

Q.E.D.

In the $(k+m)$ -value implementation the polynomial $p_{n-1}(t)$ actually interpolates

$$y_{n-1}, y_{n-1}, \dots, y_{n-m}, y_{n-m}, s_{n-m}^0, s_{n-m-1}^0, \dots, s_{n-m-1}^{k-m-1}$$

but to advance to the next meshpoint we need only $k+m-1$ linear combinations of these values, namely,

$$y_{n-1}, y_{n-1}, \dots, y_{n-m+1}, y_{n-m+1}, s_{n-m}^0, s_{n-m}^0, \dots, s_{n-m}^{k-m}.$$

This reduced set of values is used in the $(k+m-1)$ -value implementation to construct $\hat{p}_{n-1}(t)$.

An additional interpolation property of $\lambda_n(t)$ is given by

THEOREM 5.3. *If the variable coefficient v.l.c. conditions are linearly independent, then*

$$Q \text{tab}_n p_n = Q[y_{n-1}, \dots, h_{n-m+2} y_{n-m+1}, s_{n-m}^0, \dots, s_{n-m}^{k-m-1}]^T \tag{5.1}$$

$$Q \text{tab}_n \lambda_n = \beta_{0n} e_1 + \alpha_0 e_0. \tag{5.2}$$

Equation (5.1) is an alternative construction of $P_n(t)$, which is justified by

THEOREM 5.1. *The polynomial $P_n(t)$ is uniquely determined by condition (5.1) if and only if $\phi_n(t)$ is well defined. In either case*

$$\phi_n(t) = \psi_n(t) Q \tag{5.3}$$

where $\psi_n(t)$ is a $(k+m)$ -dimensional row vector uniquely determined by the requirement that

$$\psi_n(t) Q \text{tab}_n p = p(t)$$

for any polynomial $p(t)$ of degree $\leq k+m-1$.

Proof. Condition (5.1) can be expressed as

$$Q \text{tab}_n p = Q[y_{n-1}, \dots, h_{n-k+2} y_{n-k+1}]^T,$$

and so we must show that $Q \text{tab}_n$ is nonsingular as a mapping from polynomials of degree $\leq k+m-1$ if and only if $\phi_n(t)$ is well defined. Assume that $\phi_n(t)$ is well defined. Let w^T be such that $w^T Q \text{tab}_n p = 0$ for all polynomials $p(t)$ of degree $\leq k+m-1$. Also $w^T Q E^{j+1} \mathbf{g}_{n-j} = 0, j = 0(1)k-m-1$. The linear independence of the ϕ_n conditions implies that $w^T Q = 0$. Since Q is of full rank, $w^T = 0$, and so $Q \text{tab}_n$ is nonsingular. Assume that $Q \text{tab}_n$ is nonsingular as a mapping from polynomials of degree $\leq k+m-1$.

Let v^T satisfy the homogeneous ϕ_n conditions. From Skeel [19, Theorem 4.1] we have $\Delta(-m)^2 + \Delta(-m)^2 = \alpha_k^2 + \beta_k^2 > 0$ and so the $E^{j+1} \mathbf{g}_{n-j}, j = 0(1)k-m-1$, are linearly independent, and thus the columns of Q span the $(k+m)$ -dimensional null space of this set of $k-m$ vectors. Hence $v^T = w^T Q$ for some w^T . But $v^T \text{tab}_n = 0$ which implies $w^T Q \text{tab}_n = 0$, and so $w^T = 0$ implying that $v^T = 0$. To establish (5.3), merely note that the right-hand side satisfies the ϕ_n conditions.

Q.E.D.

COROLLARY. *The variable coefficient v.l.c. conditions are linearly independent for $r_n = r_{n-1} = \dots = r_{n-k+2} = 1$.*

Proof. For uniform stepsize (5.1) reduces to (1.3), which is known to uniquely determine a polynomial. Since $P_{n-1}(t)$ is defined on a uniform mesh, it follows from the theorem that $\phi_{n-1}(t)$ is well defined. Thus according to Theorem 2.3 it is enough to show that $\phi_{n-1}(t_n) \mathbf{g}_n \neq 0$. But $\mathbf{g}_n = \text{tab}_n \bar{\lambda}_n$ where $\bar{\lambda}_n(t) = \Delta((t-t_n)/h_n)$ so that $\phi_{n-1}(t_n) \mathbf{g}_n = \lambda_n(t_n) \mathbf{g}_n = \lambda_n(0)/h_n = \alpha_0/h_n \neq 0$.

Q.E.D.

A more direct way of constructing the variable coefficient formula was given in Section 1, which is justified by

THEOREM 5.2. *The coefficients of the formula*

$$\alpha_0 y_n - \beta_{0n} h_n y_n = \sum_{j=1}^{m-1} \{-\alpha_j y_{n-j} + \beta_j y_n h_{n-j+1} y_{n-j}\} + \sum_{j=m}^k \gamma_j s_{n-m}^{j-m}$$

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

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

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

Note that the f.l.c. conditions are linearly independent if and only if $\phi_{n-1}(t)$ is well defined. The modifier polynomial $\lambda_n(t_n + zt_n)$ has coefficients that depend on only $r_n, r_{n-1}, \dots, r_{n-k+3}$ because $\beta_{0n} = \beta_0$ 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 $\beta_{0n} = \beta_0$.

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*

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

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 [1]. 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 $\alpha_{0n} = \alpha_0$, requiring that it be exact for polynomials of degree $\leq k+m-1$, and imposing condition (2.1) 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

$$\begin{aligned} \alpha_0 \lambda_n(t_n) - \beta_{0n} h_n \lambda_n'(t_n) &= \sum_{j=1}^{m-1} \{-\alpha_{jn} \lambda_n(t_{n-j}) + \beta_{jn} h_{n-j+1} \lambda_n'(t_{n-j})\} \\ &+ \sum_{j=m}^k \gamma_{jn} \sum_{i=0}^j \{-\alpha_{k-j+1} \lambda_n(t_{n-m-i}) \\ &+ \beta_{k-j+1} h_{n-m-i+1} \lambda_n'(t_{n-m-i})\} \end{aligned}$$

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

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

$$= \dots = \beta_{0n} - \beta_{0n}^*(t)$$

where β_{0n}^* and $\lambda_{n+1}^*(t)$ 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.

8. Fixed Leading Coefficient Extensions

For a fixed leading coefficient formula the condition

$$\beta_{0n} = \beta_0$$

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

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

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

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

$$\text{tb}_n \lambda_n = \beta_0 e_1 + \alpha_0 e_2,$$

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 Nordseick 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 $\Lambda_n(x) := \lambda_n(t_n + xh_n)$ 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

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

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

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

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

and

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

and therefore by Theorem 2.1

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

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

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

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

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

Proof. Since the multistep formula is exact for polynomials of degree $\leq k+m-1$, $-\alpha_0 n A(0) + \beta_0 n A'(0) + \sum_{j=1}^k \{-\alpha_{jn} A(\frac{t_n - j - t_n}{h_n}) + \beta_{jn} \frac{h_{n-j+1}}{h_n} A(\frac{t_n - j - t_n}{h_n})\} = 0$.

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

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

which indicates that the f.l.c. condition is satisfied if and only if the v.l.c. condition is. With $\bar{\lambda}_n(t) := A(\frac{t - t_n}{h_n})$ we note that

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

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 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

$$Q \text{tb}_n \bar{p}_n = Q(\text{tb}_n p_{n-1} + (y_n - p_{n-1}(t_n)) e_1 + h_n (y'_n - p'_{n-1}(t_n)) e_2)$$

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