Numer. Math. 45, 345–360 (1984)

Numerische Mathematik

Asymptotic Expansions of the Global Error of Fixed-Stepsize Methods

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Summary. In his fundamental paper on general fixed-stepsize methods, Skeel [6] studied convergence properties, but left the existence of asymptotic expansions as an open problem. In this paper we give a complete answer to this question. For the special cases of one-step and linear multistep methods our proof is shorter than the published ones.

Asymptotic expansions are the theoretical base for extrapolation methods.

Subject Classifications: AMS(MOS): 65LO5, CR: G1.7.

1. Introduction

Let us consider the system of differential equations

$$y' = f(x, y), \qquad y(x_0) = y_0 \tag{1.1}$$

where f is sufficiently differentiable. Our aim is to find for the global error of general discretization methods an asymptotic expansion in powers of the stepsize. Henrici [5] has given the leading term and Gragg [3] has derived the full asymptotic expansion for one-step and linear multistep methods. The proof, which is very technical and long, can also be found in the book of Stetter [7]. Later, many new classes of methods have been studied, such as predictor-corrector methods, hybrid methods, (A,B)-methods of Butcher [2], multistep-multistage-multiderivative methods [4, 1], and similar methods for higher order ordinary differential equations, ... etc. All these methods, together with the classical ones, fall into the class of fixed-stepsize methods, analysed in the paper of Skeel [6]. There, Skeel has given the principal error term and has conjectured the existence of an asymptotic expansion.

In Sect. 2 we first give a new proof of the asymptotic expansion of the global error of one-step methods. This case is simpler and shows the basic idea, which will be essential for the general case. In Sect. 3 we extend the proof to strictly stable fixed-stepsize methods. For stable methods, which are not strictly stable, the proof is carried out in Sect. 4 and in the appendix. In Sect. 5 we show that for symmetric fixed-stepsize methods h^2-expansions of the global error can be obtained.

2. One-Step Methods

For the numerical solution of (1.1) we consider one-step methods of the form

$$y_{n+1}=y_n+h\Phi(x_n, y_n, h) \tag{2.1}$$

where we assume that Φ is sufficiently differentiable. In the situation $x=x_0+nh$ with $n=0,1,2,\dots$ and $h\in[0,h_0]$ we also write $y(x,h)=y_n$. The existence of an asymptotic expansion of the global error is given by

Theorem 1 (Gragg [3]). *Assume the consistency condition*

$$\Phi(x,y,0)=f(x,y)$$

and the following expansion of the local error

$$y(x+h)-y(x)-h\Phi(x,y(x),h)=d_{p+1}(x)\,h^{p+1}+\dots+d_{N+1}(x)\,h^{N+1}+O(h^{N+2}) \tag{2.2}$$

with $p\geqq 1$ and $y(x)$ the exact solution of (1.1). *Then the global error has an asymptotic expansion of the form*

$$y(x,h)-y(x)=e_p(x)\,h^p+\dots+e_N(x)\,h^N+E(x,h)\,h^{N+1} \tag{2.3}$$

where

$$e_j'(x)=\frac{\partial f}{\partial y}(x,y(x))\,e_j(x)+\mathit{inhomogenity}(x), \qquad e_j(x_0)=0,$$

and $E(x,h)$ is bounded on compact sets.

Proof. a) The idea is to subtract the first term $e_p(x)\,h^p$ from the conjectured expansion (2.3) and to consider

$$y(x,h)-e_p(x)\,h^p=:y^*(x,h) \tag{2.4}$$

as the numerical solution of a new method

$$y^*_{n+1}=y^*_n+h\Phi^*(x_n, y^*_n, h).$$

By comparison with (2.1), one sees that the increment function for the new method must be given by

$$\Phi^*(x,y,h)=\Phi(x,y+e_p(x)\,h^p,h)-(e_p(x+h)-e_p(x))\,h^{p-1}. \tag{2.5}$$

Our task is thus to find a function $e_p(x)$, $e_p(x_0)=0$, such that the method with increment function Φ^* is convergent of order $p+1$.

b) Expanding the local error of the one-step method Φ^* into powers of h we obtain

$$y(x+h)-y(x)-h\Phi^*(x, y(x), h)$$
$$=\left[d_{p+1}(x)-\frac{\partial f}{\partial y}(x, y(x))\, e_p(x)+e_p'(x)\right] h^{p+1}+O(h^{p+2})$$

where we have used $\frac{\partial \Phi}{\partial y}(x, y, 0)=\frac{\partial f}{\partial y}(x, y)$. The expression in square brackets vanishes if $e_p(x)$ is defined as the solution of

$$e_p'(x)=\frac{\partial f}{\partial y}(x, y(x))\, e_p(x)-d_{p+1}(x), \qquad e_p(x_0)=0.$$

By the convergence theorem for one-step methods (see e.g. Henrici [5]) the method Φ^* is convergent of order $p+1$.

c) If $N=p$, the proof of (2.3) is complete. Otherwise, the increment function Φ^* satisfies the assumptions of the theorem with p replaced by $p+1$. Therefore the construction of Φ^{**}, $\Phi^{***}, \ldots$ etc. according to a) and b) can be repeated until $p=N$ is reached. □

3. Multistep and General Fixed-Stepsize Methods (Strictly Stable Methods)

In order to apply the techniques of Sect. 2 to multistep methods, it is useful to write them as a "one-step" method in a higher dimensional space. We therefore follow the lines of Butcher [2] and Skeel [6] and consider methods, which consist of:

(I) a *forward step procedure*, i.e. a formula

$$u_{n+1}=Su_n+h\Phi_n(x_n, u_n, h) \tag{3.1a}$$

where S is a square matrix; the increment functions Φ_n are sufficiently differentiable.

(II) a *correct value function* $z(x, h)$, which is sufficiently smooth. The quantities $z_n=z(x_n, h)$ are to be approximated by u_n, so that the global error is given by u_n-z_n. It is assumed that the exact solution $y(x)$ of (1.1) can be recovered from $z(x, h)$.

(III) a smooth *starting procedure* $\phi(h)$, which specifies the starting value

$$u_0=\phi(h). \tag{3.1b}$$

($\phi(h)$ approximates $z_0=z(x_0, h)$).

Example. For the special case of linear multistep methods

$$\sum_{j=0}^{k} \alpha_j y_{n+j}=h\sum_{j=0}^{k} \beta_j f_{n+j}, \qquad \alpha_k=1$$

we have

$$S=\begin{pmatrix} -\alpha_{k-1} & -\alpha_{k-2} & \dots & -\alpha_0 \\ 1 & 0 & \dots & 0 \\ 0 & 1 & & \vdots \\ \vdots & & & \\ 0\dots & 0 & 1 & 0 \end{pmatrix}$$

$$\Phi_n(x,u,h)=e_1\psi(x,u,h), \qquad e_1=(1,0,\dots,0)^T, \tag{3.2}$$

where for $u=(v_{k-1},\dots,v_0)^T$ the value $\psi=\psi(x,u,h)$ is implicitly defined by

$$\psi=\sum_{j=0}^{k-1}\beta_j f(x+jh,v_j)+\beta_k f\left(x+kh,h\psi-\sum_{j=0}^{k-1}\alpha_j v_j\right).$$

The correct value function is given by

$$z(x,h)=(y(x+(k-1)h),\dots,y(x+h),y(x))^T. \tag{3.3}$$

In this example and in all methods of practical interest the increment functions Φ_n do not depend on n. We have introduced this additional dependence, because the iterative proof for the asymptotic expansion leads to methods of this type.

In order to formulate and prove the asymptotic expansion of (3.1) we recall some definitions (cf. Skeel [6]).

Method (3.1) is called *stable*, if S^n is bounded uniformly for all $n\geqq 0$. It is called *strictly stable*, if

$$E=\lim_{n\to\infty} S^n \tag{3.4}$$

exists. These concepts are equivalent to RC and MSRC of Skeel [6], respectively. We assume in this section that the method (3.1) is strictly stable. The more general case will be treated in Sects. 4 and 5.

The *local error* of (3.1) is defined by

$$\begin{aligned} d_0&=z_0-\phi(h)\\ d_{n+1}&=z_{n+1}-Sz_n-h\Phi_n(x_n,z_n,h). \end{aligned} \tag{3.5}$$

The iterative proof of Theorem 2 below will lead us to increment functions of the form

$$\Phi_n(x,u,h)=\Phi(x,u+h\alpha_n(h),h)+\beta_n(h) \tag{3.6}$$

with smooth Φ and polynomials α_n, β_n, whose coefficients satisfy $\alpha_n^j, \beta_n^j=O(\rho^n)$. Here ρ is some number lying between the spectral radius of $S-E$ and 1, i.e. $\rho(S-E)<\rho<1$. By Taylor expansion we obtain for the local error of such methods

$$\begin{aligned} d_0&=\gamma_0+\gamma_1 h+\dots+\gamma_N h^N+O(h^{N+1})\\ d_{n+1}&=(d_0(x_n)+\delta_n^0)+\dots+(d_{N+1}(x_n)+\delta_n^{N+1})\,h^{N+1}+O(h^{N+2})\\ &\quad\text{for } nh\leqq \text{const}. \end{aligned} \tag{3.7}$$

where $d_j(x)$ are smooth and $\delta_n^j = O(\rho^n)$. This expansion (extension of (2.2)) is unique, because $\delta_n^j \to 0$ for $n \to \infty$.

Method (3.1) with Φ_n given by (3.6) is called *consistent of order p*, if

$$\begin{aligned} &d_n = O(h^p) \quad \text{for } nh \leqq \text{const.} \\ &E d_p(x) = 0. \end{aligned} \tag{3.8}$$

The conditions (3.8) clearly imply

$$d_{n+1} + E(d_n + \ldots + d_0) = O(h^p) \quad \text{for } nh \leqq \text{const.},$$

which is equivalent to quasi-consistency of order p in the terminology of Skeel [6]. As a consequence of Theorem 3.8 of [6], strict stability and consistency of order p imply convergence of order p, i.e.

$$u_n - z_n = O(h^p) \quad \text{for } nh \leqq \text{const.}$$

In the following theorem we again use the notation $u(x,h) = u_n$ when $x = x_0 + nh$.

Theorem 2. *Let the method* (3.1) *with* Φ_n *given by* (3.6) *be strictly stable and consistent of order* $p (p \geqq 1)$. *Then the global error has an asymptotic expansion of the form*

$$u(x,h) - z(x,h) = e_p(x)\,h^p + \ldots + e_N(x)\,h^N + E(x,h)\,h^{N+1} \tag{3.9}$$

where $e_j(x)$ *are given in the proof* (*cf. formula* (3.21)) *and* $E(x,h)$ *is bounded uniformly in* $h \in [0, h_0]$ *for* x *in compact intervals not containing* x_0.

More precisely than (3.9), *there is an expansion*

$$u_n - z_n = (e_p(x_n) + \varepsilon_n^p)\,h^p + \ldots + (e_N(x_n) + \varepsilon_n^N) h^N + \tilde{E}(n,h)\,h^{N+1} \tag{3.10}$$

where $\varepsilon_n^j = O(\rho^n)$ *and* $\tilde{E}(n,h)$ *is bounded for* $nh \leqq \text{const.}$

Remarks. a) We obtain from (3.10) and (3.9)

$$E(x_n, h) = \tilde{E}(n,h) + h^{-1}\varepsilon_n^N + h^{-2}\varepsilon_n^{N-1} + \ldots + h^{p-N-1}\varepsilon_n^p,$$

such that the remainder term $E(x,h)$ is in general not uniformly bounded in h for x varying in an interval $[x_0, \bar{x}]$. This is in contrast to the situation for one-step methods. However, if x is bounded away from x_0, $x \geqq x_0 + \delta$ ($\delta > 0$ fixed), the sequence ε_n^j goes to zero faster than any power of $\frac{\delta}{n} \leqq h$.

b) The special case $N = p$ is Theorem 6.1 of Skeel [6].

Proof. a) Similar as in the proof of Theorem 1 we construct a new method, which has as numerical solution

$$u_n^* = u_n - (e(x_n) + \varepsilon_n)\,h^p \tag{3.11}$$

for a given smooth function $e(x)$ and sequence ε_n satisfying $\varepsilon_n = O(\rho^n)$. Such a method is given by

$$u_{n+1}^* = S u_n^* + h \Phi_n^*(x_n, u_n^*, h), \qquad u_0^* = \phi^*(h) \tag{3.12}$$

where $\phi^*(h)=\phi(h)-(e(x_0)+\varepsilon_0)\,h^p$ and

$$\Phi_n^*(x,u,h)=\Phi_n(x,u+(e(x)+\varepsilon_n)\,h^p,h)-(e(x+h)-Se(x))\,h^{p-1}$$
$$-(\varepsilon_{n+1}-S\varepsilon_n)\,h^{p-1}. \tag{3.13}$$

By assumption, this increment function is again of the form (3.6), so that its local error has an expansion (3.7). We shall now determine $e(x)$ and ε_n in such a way that the method (3.12) is consistent of order $p+1$.

b) The local error d_n^* of (3.12) can be expanded

$$\begin{aligned} d_0^* &= z_0-u_0^*=(\gamma_p+e(x_0)+\varepsilon_0)\,h^p+O(h^{p+1})\\ d_{n+1}^* &= z_{n+1}-Sz_n-h\Phi_n^*(x_n,z_n,h)\\ &= d_{n+1}+[(I-S)\,e(x_n)+(\varepsilon_{n+1}-S\varepsilon_n)]\,h^p\\ &\quad +[-G(x_n)(e(x_n)+\varepsilon_n)+e'(x_n)]\,h^{p+1}+O(h^{p+2}). \end{aligned}$$

Here

$$G(x)=\frac{\partial\Phi_n}{\partial u}(x,z(x,0),0), \tag{3.14}$$

which is independent of n by (3.6). The method (3.12) is thus consistent of order $p+1$, if

(i) $\varepsilon_0=-\gamma_p-e(x_0)$
(ii) $d_p(x)+(I-S)\,e(x)+\delta_n^p+\varepsilon_{n+1}-S\varepsilon_n=0$
(iii) $Ee'(x)=EG(x)\,e(x)-Ed_{p+1}(x)$.

We assume for the moment that the system (i)–(iii) can be solved for $e(x)$ and ε_n. This will actually be demonstrated in part d) of the proof. By the convergence theorem (cf. Skeel [6] and the remark after formula (3.8)) the method (3.12) is convergent of order $p+1$. Hence

$$u_n^*-z_n=O(h^{p+1})\qquad\text{uniformly for } nh\leqq\text{const.},$$

which yields the statement (3.10) for $N=p$.

c) The method (3.12) satisfies the assumptions of the theorem with p replaced by $p+1$. As in Theorem 1 an induction argument yields the result.

d) It remains to find a solution of the system (i)–(iii). Condition (ii) is satisfied if

(iia) $d_p(x)=(S-I)(e(x)+c)$
(iib) $\varepsilon_{n+1}-c=S(\varepsilon_n-c)-\delta_n^p$

hold for some constant c. Using $(I-S+E)^{-1}(I-S)=(I-E)$, formula (iia) is equivalent to

$$(I-S+E)^{-1}\,d_p(x)=-(I-E)(e(x)+c). \tag{3.15}$$

From (i) we obtain $\varepsilon_0-c=-\gamma_p-(e(x_0)+c)$, so that by (3.15)

$$(I-E)(\varepsilon_0-c)=-(I-E)\,\gamma_p+(I-S+E)^{-1}\,d_p(x_0). \tag{3.16}$$

Since $Ed_p(x_0)=0$, this relation is satisfied if in particular

$$\varepsilon_0-c=-(I-E)\,\gamma_p+(I-S+E)^{-1}\,d_p(x_0). \tag{3.17}$$

The numbers $\varepsilon_n - c$ are now determined by the recurrence relation (iib)

$$\begin{aligned}\varepsilon_n - c &= S^n(\varepsilon_0 - c) - \sum_{j=1}^{n} S^{n-j}\,\delta_{j-1}^p \\ &= E(\varepsilon_0 - c) + (S-E)^n(\varepsilon_0 - c) - E\sum_{j=0}^{\infty}\delta_j^p + E\sum_{j=n}^{\infty}\delta_j^p - \sum_{j=1}^{n}(S-E)^{n-j}\,\delta_{j-1}^p,\end{aligned}$$

where we have used $S^n = E + (S-E)^n$. If we put

$$c = E\sum_{j=0}^{\infty}\delta_j^p \tag{3.18}$$

the above defined sequence $\{\varepsilon_n\}$ satisfies $\varepsilon_n = O(\rho^n)$, since $E(\varepsilon_0 - c) = 0$ by (3.17).

In order to find $e(x)$ we define

$$v(x) = Ee(x).$$

With the help of formulas (3.18) and (3.15) we can recover $e(x)$ from $v(x)$ by

$$e(x) = v(x) - (I - S + E)^{-1}\,d_p(x). \tag{3.19}$$

Equation (iii) can now be rewritten as the differential equation

$$v'(x) = EG(x)[v(x) - (I - S + E)^{-1}\,d_p(x)] - Ed_{p+1}(x), \tag{3.20}$$

and condition (i) yields the starting value $v(x_0) = -E(\gamma_p + \varepsilon_0)$. This initial value problem can be solved for $v(x)$ and we obtain $e(x)$ by (3.19). This function and the above defined ε_n represent a solution of (i)–(iii). □

Remark. a) It follows from (3.18)–(3.20) that the principal error term satisfies

$$\begin{aligned} e_p'(x) &= EG(x)\,e_p(x) - Ed_{p+1}(x) - (I - S + E)^{-1}\,d_p(x) \\ e_p(x_0) &= -E\gamma_p - E\sum_{j=0}^{\infty}\delta_j^p + (I - S + E)^{-1}\,d_p(x_0). \end{aligned} \tag{3.21}$$

b) Since $e_{p+1}(x)$ is just the principal error term of method (3.12), it satisfies the differential equation (3.21) with d_j replaced by d_{j+1}^*. By an induction argument we therefore have for $j \geqq p$

$$e_j'(x) = EG(x)\,e_j(x) + \text{inhomogenity } (x). \tag{3.22}$$

Let us illustrate the above definitions and results for strictly stable multistep methods (cf. Skeel [6]). By (3.2) and (3.3) the local error (3.5) satisfies

$$d_{n+1} = (\mathbb{1} - S\mathbb{1})\,y(x_n) + (\mathbb{1} + (I - S)\,a - e_1\sigma(1))\,hy'(x_n) + O(h^2)$$

where $\mathbb{1} = (1, \ldots, 1)^T$, $e_1 = (1, 0, \ldots, 0)^T$, $a = (k-1, \ldots, 1, 0)^T$, $\sigma(1) = \sum_{j=0}^{k}\beta_j$ and $y(x)$ is the exact solution of (1.1). Hence the method is consistent of order 1, if and only if $d_0 = O(h)$ and

$$S\mathbb{1}=\mathbb{1} \quad \left(\text{i.e. } \sum_{j=0}^{k} \alpha_j = 0\right)$$
$$E\mathbb{1}=Ee_1 \cdot \sigma(1). \tag{3.23}$$

Formula (3.2) together with (3.3) yields

$$G(x)=\frac{\partial \Phi_n}{\partial u}(x, z(x,0), 0)=e_1 b^T \frac{\partial f}{\partial y}(x, y(x))$$

where $b=(\beta_{k-1}-\beta_k\alpha_{k-1}, \ldots, \beta_0-\beta_k\alpha_0)^T$. The consistency conditions (3.23) imply $E\mathbb{1}=\mathbb{1}$, $b^T\mathbb{1}=\sigma(1)$ and hence also

$$EG(x)\,\mathbb{1}=\mathbb{1}\,\frac{\partial f}{\partial y}(x, y(x)). \tag{3.24}$$

For a $p-th$ order multistep method the local error has the form

$$d_{n+1}=e_1\{\delta_{p+1}(x_n)\,h^{p+1}+\ldots+\delta_{N+1}(x_n)\,h^{N+1}+O(h^{N+2})\}$$

where in particular

$$\delta_{p+1}(x)=C_{p+1}\,y^{(p+1)}(x).$$

Since $\mathbb{1}$ is the unique eigenvector of S corresponding to the eigenvalue 1, Ev is for every v a multiple of $\mathbb{1}$. The solution of (3.21) is therefore given by

$$e_p(x)=\mathbb{1}\,\varepsilon_p(x)$$

where

$$\varepsilon_p'(x)=\frac{\partial f}{\partial y}(x, y(x))\,\varepsilon_p(x)-C y^{(p+1)}(x)$$

and $C=C_{p+1}/\sigma(1)$ is the error constant.

4. Multistep and General Fixed-Stepsize Methods (Stable Methods)

We demonstrate in this section, how the results and techniques of Sect. 3 can be extended to stable methods (3.1), which are not strictly stable.

Stability implies that all eigenvalues of S have absolute value less or equal to 1 and those of modulus 1, say $1=\zeta_1, \zeta_2, \ldots, \zeta_l$, are simple roots of the minimal polynomial of S. Thus, S can be decomposed in the form

$$S=\zeta_1 E_1+\ldots\zeta_l E_l+R \tag{4.1}$$

where E_j are projectors and the spectral radius $\rho(R)<1$. If the local error of method (3.1) has an expansion (3.7), we define *consistency of order p* by (3.8) with $E=E_1$.

For a multi-index $m=(m_1, \ldots, m_l)$ with $m_j \geqq 0$ we denote

$$\zeta^m=\zeta_1^{m_1}\cdot\ldots\cdot\zeta_l^{m_l}, \qquad |m|=m_1+\ldots+m_l.$$

Theorem 3. *Let the method* (3.1) *with $\Phi_n = \Phi$ independent of n be stable and consistent of order $p (p \geqq 1)$. Then the global error has an asymptotic expansion of the form*

$$u_n - z_n = h^p \sum_{|m|=1} \zeta^{nm} e_{pm}(x_n) + \ldots + h^N \sum_{1 \leqq |m| \leqq N-p+1} \zeta^{nm} e_{Nm}(x_n) + E(n,h)\, h^{N+1} \tag{4.2}$$

where $e_{jm}(x)$ are smooth functions and $E(n,h)$ is uniformly bounded for $0 < \delta \leqq nh \leqq$ const.

This theorem can be proved by extending the proof of Theorem 2. Details are shown in the appendix. For the most important special case, where all $\zeta_j (j=1, \ldots, l)$ are roots of unity, a simple proof is given below.

Corollary 4. *Let the method* (3.1) *satisfy the assumptions of Theorem* 3 *and assume that $\zeta_j^q = 1$ for $j = 1, \ldots, l$. Then we have with $w = e^{2\pi i/q}$*

$$u_n - z_n = \sum_{s=0}^{q-1} w^{ns} \{e_{ps}(x_n)\, h^p + \ldots + e_{Ns}(x_n)\, h^N\} + E(n,h)\, h^{N+1} \tag{4.3}$$

where $e_{js}(x)$ and $E(n,h)$ are as in Theorem 3.

Proof. We study the method, which is obtained by considering q consecutive steps of method (3.1) as one large step. Putting $\tilde{u}_n = u_{nq+i} (0 \leqq i \leqq q-1$ fixed), $\tilde{h} = qh$ and $\tilde{x}_n = x_i + n\tilde{h}$, this method becomes

$$\tilde{u}_{n+1} = S^q \tilde{u}_n + \tilde{h} \tilde{\Phi}(\tilde{x}_n, \tilde{u}_n, \tilde{h}) \tag{4.4}$$

with a suitably chosen $\tilde{\Phi}$. Method (4.4) is strictly stable, since by assumption

$$\lim_{n \to \infty} (S^q)^n = \tilde{E} = E_1 + \ldots + E_l$$

exists. A straight-forward calculation shows that the local error of (4.4) satisfies

$$\tilde{d}_0 = O(h^p)$$
$$\tilde{d}_{n+1} = (I + S + \ldots + S^{q-1})\, d_p(\tilde{x}_n)\, \tilde{h}^p + O(h^{p+1}).$$

Inserting (4.1) and using $\zeta_j^q = 1$ we obtain

$$\tilde{E}(I + S + \ldots + S^{q-1})\, d_p(x)$$
$$= \tilde{E}\Big(I - \tilde{E} + qE + \sum_{j=2}^{l} \frac{1-\zeta_j^q}{1-\zeta_j} E_j + \sum_{j=1}^{q-1} R^j\Big)\, d_p(x) = qE d_p(x),$$

which vanishes by (3.8). Hence, also method (4.4) is consistent of order p. Applying Theorem 2 to method (4.4) yields

$$u_{nq+i} - z_{nq+i} = \tilde{e}_{pi}(x_{nq+i})\, h^p + \ldots + \tilde{e}_{Ni}(x_{nq+i})\, h^N + E_i(n,h)\, h^{N+1}$$

where $E_i(n,h)$ has the desired boundedness-properties. If we define $e_{js}(x)$ as solution of the Vandermonde-type system

$$\sum_{s=0}^{q-1} w^{is} e_{js}(x) = \tilde{e}_{ji}(x)$$

we obtain (4.2). This proves the corollary. □

5. Symmetric Fixed-Stepsize Methods and h^2-Expansions

For fixed-stepsize methods the correct value function $z(x, h)$, the starting procedure $\phi(h)$ and the increment function $\Phi(x, u, h)$ are usually defined also for negative h (cf. (3.3)). We shall give here a precise meaning to the numerical solution $u(x, h)$ for negative h and show that the results of the previous sections hold independent of the sign of h. This then leads in a natural way to asymptotic expansions in even powers of h.

We consider the method

$$\begin{aligned} u(x_0, h) &= \phi(h) \\ u(x+h, h) &= S u(x, h) + h\Phi(x, u(x, h), h) \qquad \text{for } x = x_0 + nh. \end{aligned} \tag{5.1}$$

For positive h and $n \geqq 0$ this is just the fixed-stepsize method (3.1) with an increment function independent of n. If we replace h by $-h$ in (5.1) we obtain

$$u(x-h, -h) = S u(x, -h) - h\Phi(x, u(x, -h), -h).$$

For small h and nonsingular S this equation can be solved for $u(x, -h)$ and yields

$$\begin{aligned} u(x_0, -h) &= \phi(-h) \\ u(x, -h) &= S^{-1} u(x-h, -h) + h\hat{\Phi}(x, u(x-h, -h), h). \end{aligned} \tag{5.2}$$

$u(x, -h)$ can thus be interpreted as the numerical solution of the *inverse fixed-stepsize method* (5.2), whose correct value function is $z(x, -h)$.

Our next aim is to show that the expansion (4.2) holds also for negative h with the same coefficients $e_{jm}(x)$. For this it is necessary that also the inverse method (5.2) is convergent and hence stable. Therefore all eigenvalues of S must lie on the unit circle. With the notation of Theorem 3 we have

Theorem 5. *Assume* (5.1) *and* (5.2) *to be stable and the following consistency condition to hold for* $h \in [-h_0, h_0]$

$$\begin{aligned} & z(x+h, h) - S z(x, h) - h\Phi(x, z(x, h), h) \\ & \quad = d_p(x) h^p + d_{p+1}(x) h^{p+1} + \dots + d_{N+1}(x) h^{N+1} + O(h^{N+2}) \\ & E_1 d_p(x) = 0 \end{aligned} \tag{5.3}$$

with $p \geqq 1$. *Then the global error has an asymptotic expansion of the form*

$$\begin{aligned} u(x_n, h) - z(x_n, h) = h^p \sum_{|m|=1} \zeta^{nm} e_{pm}(x_n) + \dots \\ + h^N \sum_{1 \leqq |m| \leqq N-p+1} \zeta^{nm} e_{Nm}(x_n) + E(x_n, h) h^{N+1} \end{aligned} \tag{5.4}$$

where $e_{jm}(x)$ are smooth functions and $E(x,h)$ is uniformly bounded for $x=x_0+nh$ with $x_0 \leqq x \leqq \bar{x}$ and $-h_0 \leqq h \leqq h_0$.

Proof. a) If we replace h by $-h$ in (5.3) and then solve for $z(x,-h)$ we obtain as in (5.2)

$$z(x,-h)=S^{-1}z(x-h,-h)+h\hat{\Phi}(x,z(x-h,-h),h)+S^{-1}d_p(x-h)h^p+O(h^{p+1}).$$

Since $E_1S^{-1}=E_1$, this shows that the inverse method (5.2) is again consistent of order p. As it is stable by assumption, it is convergent.

b) We now restrict ourselves to the case where all eigenvalues of S are roots of unity. Because of a), the verification of (5.4) is exactly the same as in Corollary 4 and Theorem 2, independent of the sign of h. It becomes even simpler, since $S^q=I$ and $\delta_n^j=0$. This implies that ε_n can be omitted in (3.11), and so the increment function of method (3.12) is again independent of n. For method (4.4) we thus arrive at an expansion of the form (3.10) with $\varepsilon_n^j=0$. The statement now follows as at the end of the proof of Corollary 4.

In the general case (where some eigenvalue of S is not a root of unity) one has to apply Theorem 7 instead of Corollary 4. □

For many methods of practical interest the above result leads to expansions in even powers of h. The correct value function $z(x,h)$ usually satisfies a *symmetry relation*

$$z(x,h)=Qz(x+qh,-h) \tag{5.5}$$

where Q is a square matrix and q an integer.

Method (5.1) is called a *symmetric fixed-stepsize method*, if the numerical solution $u(x,h)$ satisfies the analogue of (5.5):

$$u(x,h)=Qu(x+qh,-h). \tag{5.6}$$

In the following examples we denote the global error by

$$\varepsilon(x,h)=u(x,h)-z(x,h)$$

and its j-th component by $\varepsilon_j(x,h)$.

Examples. a) One-step methods satisfy (5.5) with

$$Q=\text{identity} \quad \text{and} \quad q=0.$$

If the method is symmetric (see e.g. [7, 9]) then

$$\varepsilon(x,h)=\varepsilon(x,-h),$$

which, by Theorem 5, leads to an asymptotic expansion in even powers of h.

b) For linear multistep methods (5.5) holds with (cf. (3.3))

$$Q=\begin{pmatrix} 0 & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & 0 \end{pmatrix} \quad \text{and} \quad q=k-1.$$

If the coefficients of the method satisfy

$$\alpha_{k-j}=-\alpha_j, \qquad \beta_{k-j}=\beta_j$$

(such methods are commonly called symmetric [3, 7]), then a straight-forward calculation shows that the symmetry relation (5.6) holds for all $x=x_0+nh$, whenever it is satisfied for $x=x_0$. This imposes a condition on the starting procedure $\phi(h)$. The relation (5.6) implies

$$\varepsilon_k(x, -h)=\varepsilon_1(x-(k-1)h, h).$$

Furthermore, for any multistep method we have

$$\varepsilon_k(x, h)=\varepsilon_1(x-(k-1)h, h)$$

so that

$$\varepsilon_k(x, h)=\varepsilon_k(x, -h)$$

for symmetric methods. Therefore, Theorem 5 implies the existence of an asymptotic expansion in even powers of h.

The best known example is the explicit midpoint rule

$$y_{n+1}-y_{n-1}=2hf(x_n, y_n)$$

with the starting procedure of Gragg

$$\phi(h)=(y_0+hf(x_0, y_0), y_0)^T.$$

c) For Nordsieck methods (see e.g. Sect. 6.2 of [7]) the correct value function is given by

$$z(x, h)=\left(y(x), hy'(x), \ldots, \frac{h^k}{k!}y^{(k)}(x)\right)^T$$

and satisfies the relation (5.5) with

$$Q=\operatorname{diag}(1, -1, \ldots, (-1)^k) \quad \text{and} \quad q=0.$$

If such a method is symmetric, the j-th component of the global error satisfies

$$\varepsilon_j(x, h)=(-1)^j\varepsilon_j(x, -h).$$

Again, by Theorem 5, this leads to asymptotic expansions in even (or odd) powers of h.

Remark. For linear multistep methods the above results are due to Gragg [3] and Stetter [7]. The idea to work with $u(x, -h)$ can be found in Bulirsch-Stoer [8].

6. Appendix: Proof of Theorem 3

We consider methods (3.1) with increment functions

$$\Phi_n(x, u, h)=\Phi(x, u+h\alpha_n(x, h), h)+\beta_n(x, h), \tag{6.1}$$

where α_n and β_n are polynomials in h, whose coefficients are of the form

$$\alpha_n^j(x)=\sum_m \zeta^{nm} a_{mj}(x)+a_n^j, \qquad \beta_n^j(x)=\sum_m \zeta^{nm} b_{mj}(x)+b_n^j.$$

Here the summation is over a finite number of equivalence classes of multi-indices, where m and m' are identified, if $\zeta^m=\zeta^{m'}$. Furthermore we assume a_n^j, $b_n=O(\rho^n)$ with $\rho(R)<\rho<1$ (cf. (4.1)). The local error of such a method has a unique expansion of the form

$$\begin{aligned} d_0 &= \gamma_0+\gamma_1 h+\ldots+\gamma_N h^N+O(h^{N+1}) \\ d_{n+1} &= \Big(\sum_m \zeta^{nm} d_{0m}(x_n)+\delta_n^0\Big)+\ldots+\Big(\sum_m \zeta^{nm} d_{N+1,m}(x_n)+\delta_n^{N+1}\Big) h^{N+1}+O(h^{N+1}) \end{aligned} \tag{6.2}$$

with $\delta_n^j=O(\rho^n)$. For the multi-index $m=e^i=(0,\ldots,1,\ldots,0)$ we also use the notation $d_{ji}(x)$ instead of $d_{jm}(x)$.

A method (3.1) with increment function (6.1) is called *consistent of order p*, if

$$\begin{aligned} d_n &= O(h^p) && \text{for } nh \leqq \text{const.} \\ E_i d_{pi}(x) &= 0 && \text{for } i=1,\ldots,l. \end{aligned} \tag{6.3}$$

If $d_{pm}(x)=0$ for $m \neq e^1=(1,0,\ldots,0)$ (cf. (3.6)), this definition coincides with (3.8), since $E=E_1$. We have

Theorem 6. *A method* (3.1) *with increment function* (6.1), *which is stable and consistent of order p, is also convergent of order p.*

Proof. By Lemma 3.5 of (6) it suffices to prove that

$$\sum_{j=0}^{n} S^{n-j} d_{j+1}=O(h^p) \qquad \text{for } nh \leqq \text{const.}$$

Using (4.1) and (6.3) this is satisfied, if

$$\sum_{j=0}^{n} (\zeta_1^{n-j} E_1+\ldots+\zeta_l^{n-j} E_l) \sum_m \zeta^{jm} d_{pm}(x_j) \tag{6.4}$$

is uniformly bounded in n. The expression (6.4) can be written as

$$\sum_{i=1}^{l} \zeta_i^n E_i \sum_m D_n^{im} \quad \text{with} \quad D_n^{im}=\sum_{j=0}^{n} (\zeta^m/\zeta_i)^j d_{pm}(x_j).$$

If $m=e^i$, we have $E_i D_n^{im}=0$ by (6.3). If $m \neq e^i$, then $\eta=\zeta^m/\zeta_i \neq 1$, and D_n^{im} is uniformly bounded in n, since by "Abel summation"

$$D_n^{im}=\frac{1-\eta^{n+1}}{1-\eta} d_{pm}(x_n)-\sum_{j=0}^{n-1} \frac{1-\eta^{j+1}}{1-\eta}(d_{pm}(x_{j+1})-d_{pm}(x_j)).$$

and $d_{pm}(x)$ is a smooth function. □

In order to extend the proof of Theorem 2, it is convenient to formulate the following generalization of Theorem 3:

Theorem 7. *Let the method* (3.1) *with* Φ_n *given by* (6.1) *be stable and consistent of order* $p(p \geqq 1)$. *Then the global error has an asymptotic expansion of the form*

$$u_n - z_n = h^p \sum_m \zeta^{nm} e_{pm}(x_n) + \ldots + h^N \sum_m \zeta^{nm} e_{Nm}(x_n) + E(n,h)\, h^{N+1}$$

where $e_{jm}(x)$ *and* $E(n,h)$ *are as in Theorem* 3.

Proof. The proof is along the lines of that of Theorem 2. a) We consider a method (3.12) with increment function

$$\Phi_n^*(x,u,h) = \Phi_n(x, u + (\sum_m \zeta^{nm} e_m(x) + \varepsilon_n)\, h^p, h)$$
$$- \sum_m \zeta^{nm}(\zeta^m e_m(x+h) - S e_m(x))\, h^{p-1} - (\varepsilon_{n+1} - S\varepsilon_n)\, h^{p-1},$$

which has as numerical solution

$$u_n^* = u_n - (\sum_m \zeta^{nm} e_m(x_n) + \varepsilon_n)\, h^p.$$

b) The local error d_n^* of this method is given by

$$d_0^* = (\gamma_p + \sum_m e_m(x_0) + \varepsilon_0)\, h^p + O(h^{p+1})$$
$$d_{n+1}^* = d_{n+1} + [\sum_m \zeta^{nm}(\zeta^m I - S)\, e_m(x_n) + (\varepsilon_{n+1} - S\varepsilon_n)]\, h^p$$
$$+ [-G(x_n)(\sum_m \zeta^{nm} e_m(x_n) + \varepsilon_n) + \sum_m \zeta^{nm} \zeta^m e_m'(x_n)]\, h^{p+1} + O(h^{p+2}).$$

It is thus consistent of order $p+1$, if

(i) $\varepsilon_0 = -\gamma_p - \sum_m e_m(x_0)$

(iia) $d_{p1}(x) = (S-I)(e_1(x)+c)$

(iib) $\varepsilon_{n+1} - c = S(\varepsilon_n - c) - \delta_n^p$

(iic) $d_{pm}(x) + (\zeta^m I - S)\, e_m(x) = 0 \quad$ for $m \neq e^1 = (1,0,\ldots,0)$

(iii) $\zeta_i E e_i'(x) = E_i G(x)\, e_i(x) - E_i d_{p+1,i}(x) \quad$ for $i = 1, \ldots, l$.

In part d) of the proof we shall show that (i)-(iii) has a solution. With the $e_m(x)$ and ε_n, obtained in this way, the above method is convergent of order $p+1$ by Theorem 6.

c) The same induction argument as in Theorem 2 yields the result.

d) For $m \neq e^i = (0, \ldots, 1, \ldots, 0)$ the matrix $(\zeta^m I - S)$ is nonsingular, and $e_m(x)$ can be computed from (iic).

Using the identity

$$(\zeta_i I - S) = \zeta_i (I - E_i)(I - \zeta_i^{-1} S + E_i),$$

formulas (iia) and (iic) yield

$$(I-E)(e_1(x)+c) = -(I-S+E)^{-1} d_{p1}(x)$$
$$\zeta_i (I-E_i)\, e_i(x) \quad = -(I - \zeta_i^{-1} S + E_i)^{-1} d_{pi}(x), \qquad i = 2, \ldots, l. \tag{6.5}$$

From (i) we obtain $\varepsilon_0 - c = -\gamma_p - (e_1(x_0) + c) - \sum_{m \neq e^1} e_m(x_0)$, so that by (6.5)

$$(I-E)(\varepsilon_0 - c) = -(I-E)\gamma_p + (I-S+E)^{-1} d_{p1}(x_0) - (I-E) \sum_{m \neq e^1} e_m(x_0).$$

Because of $E d_{p1}(x_0) = 0$, this relation is satisfied, if in particular

$$\varepsilon_0 - c = -(I-E)\gamma_p + (I-S+E)^{-1} d_{p1}(x_0) - (I-E) \sum_{m \neq e^1} e_m(x_0). \tag{6.6}$$

By (ii b)

$$\begin{aligned} \varepsilon_n - c &= S^n(\varepsilon_0 - c) - \sum_{j=1}^{n} S^{n-j} \delta_{j-1}^p \\ &= \sum_{i=1}^{l} \zeta_i^n E_i(\varepsilon_0 - c) - \sum_{i=1}^{l} \zeta_i^n E_i \sum_{j=0}^{\infty} \zeta_i^{-j-1} \delta_j^p + R^n(\varepsilon_0 - c) \\ &\quad - \sum_{j=1}^{n} R^{n-j} \delta_{j-1}^p + \sum_{i=1}^{l} \zeta_i^n E_i \sum_{j=n}^{\infty} \zeta_i^{-j-1} \delta_j^p. \end{aligned}$$

Since $E(\varepsilon_0 - c) = 0$, the sequence (ε_n) satisfies $\varepsilon_n = O(\rho^n)$, if $c = E \sum_{j=0}^{\infty} \delta_j^p$ and

$$E_i(\varepsilon_0 - c) = E_i \sum_{j=0}^{\infty} \zeta_i^{-j-1} \delta_j^p. \tag{6.7}$$

Inserting (6.6) into (6.7) yields

$$E_i \sum_{m \neq e^1} e_m(x_0) = -E_i \gamma_p + (I-S+E)^{-1} E_i d_{p1}(x_0) - E_i \sum_{j=0}^{\infty} \zeta_i^{-j-1} \delta_j^p. \tag{6.8}$$

We now multiply the second relation of (6.5) with E_k and obtain

$$\zeta_i E_k e_i(x_0) = -(I - \zeta_i^{-1} S + E_i)^{-1} E_k d_{pi}(x_0), \qquad k \neq i, \quad i \neq 1. \tag{6.9}$$

Using this relation, $E_i e_i(x_0)$ can be computed from (6.8). Together with (6.5) we have thus obtained $e_i(x_0)$ for $i = 2, \ldots, l$. $e_1(x_0)$ is then given by (i).

In order to find $e_i(x)$ we define

$$v_i(x) = \zeta_i E_i e_i(x).$$

With the help of (6.5) and observing that $(I-E)c = 0$ we have

$$\zeta_i e_i(x) = v_i(x) - (I - \zeta_i^{-1} S + E_i)^{-1} d_{pi}(x), \qquad i = 1, \ldots, l. \tag{6.10}$$

Equation (iii) is now equivalent to

$$v_i'(x) = \zeta_i^{-1} E_i G(x) \{ v_i(x) - (I - \zeta_i^{-1} S + E_i)^{-1} d_{pi}(x) \} - E_i d_{p+1,i}(x).$$

This differential equation together with the initial value $v_i(x_0) = \zeta_i E_i e_i(x_0)$ can be solved for $v_i(x)$ and we obtain $e_i(x)$ by (6.10). These functions $e_i(x)$ and the above defined ε_n represent a solution of (i)–(iii). □

Acknowledgement. We are greatful to Gerhard Wanner and Peter Deuflhard for many helpful discussions and for their interest in this work. We thank the anonymous referee, who encouraged us to add the section on symmetric methods and h^2-expansions.

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Received October 27, 1983/July 30, 1984