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THE STUDY OF THE FAMILIES OF ONE-STEP METHODS

By

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ABSTRACT. Convergence results and error analysis are given for the families of one-step methods.

1. INTRODUCTION

It is well-known fact, that we have no "all-round" methods in the numerical solution of ordinary differential equations of the form

$$(1) \qquad \underline{y}' = f(t,\underline{y}) \; ; \quad \underline{y}(t_o) = \underline{y}_o \qquad (\underline{f} \in C([t_o,b] \times R^m,\ R^m)).$$

The effective solution of different groups of practical problems needs numerical methods with slightly different or contrasted structures. This situation also holds for one Cauchy-problem, if the exact solution quickly varies in character over a long computational interval.

In order to obtain more effective numerical processes, the families of numerical methods were introduced and proposed instead of single approximate methods. The most famous complex method and its FORTRAN program (DIFSUB) was developed by Gear in 1971 (see [3]), which have several variants, e.g. GEAR, EPISODE, DESOL (see [4]). Gear's process consists of several BDF's and Adams-methods and different decision functions for the choice of stepsize, the formula and the order. The convergence of such processes was proven by Gear, Tu and Watanabe in 1974.

There are also attempts to develop similar families from one-step methods. The studies in this direction are mainly experimental (see e.g. [5]-[6]). In this paper we report some results concerning the convergence and error analysis of the families of one-step methods.

2. RESULTS ON CONVERGENCE

We suppose the existence of a constant $L \geq 0$ such that

$$(2) \quad \|\underline{f}(t,\underline{y}) - \underline{f}(t,\underline{y}^*)\| \leq L \; \|\underline{y} - \underline{y}^*\| \quad (t \in [t_o,b]; \underline{y}; \underline{y}^* \in R^m).$$

Moreover it is assumed that for all $t^* \in [t_o,b]$ and for all $\underline{y}^* \in R^m$ the Cauchy-problem

$$(3) \qquad \underline{y}' = \underline{f}(t,\underline{y}) \; ; \quad \underline{y}(t^*) = \underline{y}^*$$

has exactly one solution with domain $[t_o,b]$. Let $t_o < x \leq b$ be an arbitrary but fixed point and let Δ_N be a grid over $[t_o,x]$ such that $\Delta_N: t_o < t_1 \; \ldots \; < t_N = x$. Denote by π_x the set of all grids Δ_N of the interval $[t_o,x]$. The norm of $\Delta_N \in \pi_x$ is defined by $\|\Delta_N\| = \max\limits_{1 \leq i \leq N-1} (t_{i+1} - t_i)$,

where $h_i = t_{i+1} - t_i$ is the ith steplength. At the point $t_n \in \Delta_N$ an approximate solution of the Cauchy-problem is denoted by $\underline{y}_n$.

Let $W = \{1,2,\ldots,w^*\}$ be finite and for each index $w \in W$ the one-step method defined by

$$(4) \qquad \underline{y}_{n+1} - \underline{y}_n = h_n \quad \Psi(w|t_n,\underline{y}_n,\underline{y}_{n+1},h_n) \qquad (t_{n+1} \in \Delta_N)$$

must be convergent in the sense of Henrici (see [2]). Thus we suppose that for all $w \in W$ the increment function $\Psi(w|.,.,.,.) \in C([t_o,b]\times R^m\times R^m\times[0,b-t_o],R^m)$,

$$(5) \qquad ||\Psi(w|t,\underline{y},\underline{z},h) - \Psi(w|t,\underline{y}^*,\underline{z}^*,h)|| \leq K_w(||\underline{y} - \underline{y}^*||+||\underline{z}-\underline{z}^*||$$

holds with a suitable constant $K_w \geq 0$ for every $t \in [t_o,b]$; $h \in [0,b-t_o]$; $\underline{y},\underline{y}^*,\underline{z},\underline{z}^* \in R^m$ as well as

$$(6) \qquad \Psi(w|t,\underline{y},\underline{y},0) = \underline{f}(t,\underline{y}) \qquad (t \in [t_o,b];\ \underline{y} \in R^m).$$

Definition 1. Let $I = I(\Delta_N):\{0,1,\ldots,N-1\} \to W$ be arbitrary indexfunction. Then the triple (Ψ,W,I) is said to be a family of one-step methods, if the approximate solution $\underline{y}_n$ $(n=0,1,\ldots,N)$ is computed by the recursion

$$(7) \qquad \underline{y}_{n+1} - \underline{y}_n = h_n \quad \Psi(I(n)|t_n,\underline{y}_{n+1},h_n) \qquad (t_{n+1} \in \Delta_N). \qquad ***$$

This definition means that in each step of the computation the indexfunction I choses the formula actually used. At the same time the stepsize h_n may change arbitrarily and independently of $I(n)$.

Using the works [1],[2] we can prove

Theorem 1. The family (Ψ, W, I) of one-step methods is convergent for all index set W and indexfunction I, i.e.

$$(8) \qquad \lim_{N \to +\infty} \max_{0 \leq n \leq N} \| \underline{y}_n - \underline{y}(t_n) \| = 0$$

is satisfied for every $\{\Delta_N\}_{N=1}^{\infty} \subset \pi_x$ $(\|\Delta_N\| \to 0)$. ***

For the estimation of the speed of convergence we need

Definition 2. Denote by $\underline{Y}_j : [t_o, b] \to R^m$ the exact solution of the perturbed Cauchy-problem

$$(9) \qquad \underline{y}' = \underline{f}(t, \underline{y}) \; ; \quad \underline{y}(t_j) = \underline{y}_j \quad (j=0,1,\ldots,N) \; .$$

The local truncation error of the family (Ψ, W, I) at the point $t_n \in \Delta_N$ with respect to the Cauchy-problem (9) is defined by

$$(10) \quad T_j(I(n) | t_n, h_n) = \underline{Y}_j(t_n) + h_n \Psi(I(n) | t_n, \underline{Y}_j(t_n), \underline{Y}_j(t_{n+1}), h_n) - \underline{Y}_j(t_{n+1}).$$

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In case $j=0$ we use simply the notation $T(I(n) | t_n, h_n)$ since $\underline{Y}_o(t) \equiv \underline{y}(t)$.

Using the discrete version of the Gronwall-Bellman lemma we can also prove the two-sided error bound

$$(11) \quad c_1 \max_{0 \leq k \leq N} \| \sum_{n=o}^{k} T(I(n) | t_n, h_n) \| \leq \max_{0 \leq n \leq N} \| \underline{y}_n - \underline{y}(t_n) \| \leq$$

$$\leq c_2 \max_{0 \leq n \leq N} \| \sum_{n=o}^{k} T(I(n) | t_n, h_n) \| ,$$

where $c_1, c_2 > 0$ are given constants depending on $max\{K_w | w \in W\}$. This inequality also implies the convergence and that the speed of convergence is determined by the method of minimum order among that are used in the computation over $\Delta_N \in \pi_x$. Thus the change of order (formula) is advantageous only if the additional error component decreases substantially or the structure of the exact solution strongly varies, e.g. in case of stiff differential systems.

3. ERROR ANALYSIS

In general the problem (1) is solved numerically, if for the sequence $\{\underline{y}_n\}_{n=o}^{N}$ the condition

(12) $$\|\underline{y}_n - \underline{y}(t_n)\| \leq \varepsilon^* \qquad (t_n \in \Delta_N)$$

holds, where $\varepsilon^* > 0$ is the requested accuracy.

The checking of this condition is usually made by the estimation of the local truncation errors

(13) $$T_n(I(n) | t_n, h_n) \qquad (n=0,1,\dots,N-1)$$

and the control of the relations

(14) $$\|T_n(I(n) | t_n, h_n)\| \leq c h_n \, \varepsilon^* \qquad [\|T_n(I(n) | t_n, h_n)\| \leq c \, \varepsilon^*],$$

where $c > 0$ $[c(\Delta_N) > 0]$ depends on the problem (1) and the family (Ψ, W, I). The hypothesis, that (12) follows from (14), is called the local error estimation principle (see [1],[2]).

It is noted that for explicit methods $T_n(I(n)|t_n,h_n)$ is identical with the local error $\underline{\ell}_n = \underline{y}_{n+1} - \underline{Y}_n(t_{n+1})$.

The theoretical base of the above principle is given in

Theorem 2. If for the local truncation error of the family (Ψ,W,I) and for the grid $\Delta_N \in \pi_x$, $(||\Delta_N|| \leq h^*)$ the condition

(15) $$||T_n(I(n)|t_n,h_n)|| \leq h_n\,\varepsilon \qquad [||T_n(I(n)|t_n,h_n)|| \leq \varepsilon]$$

$(n=0,1,\dots,N-1)$ is satisfied, then

(16) $$\max_{0\leq n\leq N} ||\underline{y}_n - \underline{y}(t_n)|| \leq c_3\,\varepsilon$$

holds with a suitable constant $c_3 = c_3(\underline{f}) > 0$ $[c_3 = c_3\ \underline{f},\Delta_N) > 0]$.

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In the first case of (15) the constant c_3 is independent of the grid Δ_N, in the other case c_3 is of order $O(N)$. If the stepsizes satisfy the relation $0 < Ah \leq h_n \leq Bh$ $(n=0,1,\dots,N-1)$ and $\varepsilon = h^p$ $(p > 1)$ then relation (16) changes to

(17) $$\max_{0\leq n\leq N} ||\underline{y}_n - \underline{y}(t_n)|| \leq c_4 h^{p-1}$$

in the second case of (15).

For a given class of Cauchy-problems of the form (1) and a given family (Ψ,W,I) the constant c_3 and the constant c in (14) can be estimated analitically. However the constant c is chosen experimentally in general. Practically, condition (14) is checked for the estimated value of $||T_n(I(n)|t_n,h_n)||$, but the study of this case can be reduced to the investigation of the applied error estimation processes. Thus one can find concrete effectivity theorems of the type due to T.E. Hull.

For a single one-step method ($W=\{1\}$) the step-halving (or step-doubling) error estimation is optimal in some sense (see [2]) and it can be also proven that the use of this error estimation process doesn't modify the previously proven form of the local error estimation principle ([2]). Latter result also holds for the families of one-step methods.

Assume that $\underline{y}_n$ has been computed and let $t_{n+1} = t_n + h$, $t_{n+2} = t_n + 2h$. We also suppose that $I(n) = I(n+1) = \xi$ in the computation of $\underline{y}_{n+1}$, $\underline{y}_{n+2}$. Denote $\overline{\overline{\underline{y}}}_{n+2}$ the approximated value of $\underline{y}(t_{n+2})$ computed by

$$(18) \qquad \overline{\overline{\underline{y}}}_{n+2} = \underline{y}_n + 2h\,\Psi(I(n)\,|\,t_n, \overline{\overline{\underline{y}}}_n, \underline{y}_{n+2}, 2h),$$

i.e. $\overline{\overline{\underline{y}}}_{n+2}$ is computed from $(t_n, \underline{y}_n)$, whith double steplength 2h. If $\underline{f}$ and the increment functions Ψ in (4) are sufficiently differentiable then we can prove

Theorem 3. If the indexfunction I of the family (Ψ, W, I) satisfies the order condition $p_{I(i)} \geq p_\xi$ $(i=0,1,\ldots,n-1)$ and $\Delta_N \in \pi_x$, $||\Delta_N|| \leq h^*$, then we have

$$(19) \qquad T_n(I(n)\,|\,t_n, h_n) = \frac{\overline{\overline{\underline{y}}}_{n+2} - \underline{y}_{n+2}}{2^{p_\xi+2} - 2} + O(||\Delta_N||^{p_\xi+2})$$

and

(20) $$T_{n+1}(I(n)|t_{n+1},h) = T_n(I(n)|t_n,h) + O(||\Delta_N||^{p_\xi+2}).$$

The proof of this result essentially is the same as in [2]. It is also noted that the accuracy of the error estimation determined by the minimum order p_ξ corresponds to the bound (11).

4. REMARKS

The main problem in the construction of any family (Ψ,W,I) of one-step methods is the choice of basic formulas (Ψ,W) and the indexfunction I. Concerning the choice of (Ψ,W) there are several interesting results (see e.g. [5],[6]). The structure of the indexfunction I may be similar to that used in DIFSUB, but its cost is more expensive for the usually applied one-step methods. In a comparison with the Gear-type processes (see [3], [4]) any family of one-step methods is more stable and more flexible with respect to the choice of stepsize and the formula.

At last we mention

Theorem 4. For the class of differential equations of the form

(21) $$\underline{y}' = \underline{\underline{A}}\,\underline{y}\ ;\quad \underline{y}(t_0) = \underline{y}_0 \qquad \underline{\underline{A}}\ (m \times m \text{ constant matrix}),$$

where $\underline{\underline{A}}$ is negative definite and hermitian, any infinite class of implicit Runge-Kutta methods related to the Padé-approximants $r_{k,s}(z)$ of e^z $(k \in \{s,s+1,s+2\}, s \geq 1)$ with arbitrary unbounded indexfunction I is convergent for every $\{\Delta_N\}_{N=1}^{\infty} \subset \pi_x$ $(||\Delta_N|| \to 0)$. ***

This result has an interesting contrast with the result of A.G. Werschulz on the optimal order of one-step methods ([7]).

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