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The Effect of Stopping Newton-Type Iterations in Implicit Linear Multistep Methods

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This talk deals with implicit linear multistep methods in the numerical solution of nonlinear initial value problems. The effect of stopping Newton-type iterations, in the actual application of linear multistep methods, is analysed and related to the stepsize of the methods. The accumulated effect of all local stopping errors is shown to be of an order which is greater (by one) than the order which one would expect in view of known estimates.

1. Linear multistep methods in the stiff situation

In this talk we deal with the numerical solution of the initial value problem

$$U'(t) = f(t, U(t)) \text{ for } 0 \le t \le T, \qquad U(0) = u_0. \tag{1}$$

Here $u_0 \in \mathbb{R}^s$ is given, and $U(t) \in \mathbb{R}^s$ is unknown. Further, $f : [0,T] \times D \to \mathbb{R}^s$ is a given nonlinear mapping, where $D \subset \mathbb{R}^s$.

Consider the *linear multistep method*

$$\alpha_0 v_n + \alpha_1 v_{n-1} + \cdots + \alpha_k v_{n-k} = h[\beta_0 f_n + \beta_1 f_{n-1} + \cdots + \beta_k f_{n-k}]. \tag{2}$$

Here $h > 0$ is the *stepsize*, and v_n approximates $U(t)$ at the *gridpoint* $t_n = nh$. We assume

$$k \ge 1, \quad \alpha_0 + \alpha_1 + \cdots + \alpha_k = 0, \quad \alpha_0 = 1, \quad \beta_0 > 0.$$

In the application of (2) one first calculates starting vectors $v_n \simeq U(t_n)$ $(0 \le n \le k-1)$. Next, for $n \ge k$, the approximations v_n are defined by (2), with $f_{n-i} = f(t_{n-i}, v_{n-i})$. Since $\beta_0 \neq 0$ and $f_n = f(t_n, v_n)$, one is faced with the problem of solving a nonlinear equation in order to determine v_n from (2).

In general this nonlinear equation cannot be solved exactly. Accordingly, in practice the linear multistep method only produces *approximations* to v_n, which will be denoted by u_n. These u_n are obtained as numerical approximations to the solution x^* of

$$F(x) = 0,$$

where

$$\begin{cases} F(x) & \equiv -x + h\beta_0 f(t_n, x) + y, \\ \quad y & = -(\alpha_1 u_{n-1} + \cdots + \alpha_k u_{n-k}) + h(\beta_1 f_{n-1} + \cdots + \beta_k f_{n-k}). \end{cases}$$

In the following we deal with the so-called *stiff* situation (i.e. the product of h and the Jacobian matrix $\frac{\partial}{\partial x} f(t, x)$ has entries some of which have very large absolute values – see e.g. SPIJKER (1996)). For obtaining approximations to x^*, in the stiff situation, one usually applies an appropriate version of *Newton's method*. We consider

$$F'(x_0)(x_j - x_{j-1}) = -F(x_{j-1}) \text{ for} j = 1, 2, 3, \ldots \tag{3}$$

Here $F'(x_0)$ denotes the Jacobian matrix of F at x_0, and x_j are approximations to x^*.

In the following the effect will be explored of the stopping of the iterations (3), after j steps. The errors $v_n - u_n$, which are due to this stopping, will be analysed in terms of the stepsize h. We shall measure these errors with an (arbitrary) norm $|\cdot|$ on $\mathbb{R}^s$.

2. THE NEWTON STOPPING ERROR

First we assess the norm $|x^* - x_j|$ of the *Newton stopping error* $x^* - x_j$. Assume that the initial guess x_0 satisfies

$$|x^* - x_0| = \mathcal{O}(h^q) \tag{4a}$$

(with an $\mathcal{O}$-constant of moderate size, and $q > 0$).

DORSSELAER & SPIJKER (1994) formulated conditions on f under which the Newton stopping error satisfies

$$|x^* - x_j| = \mathcal{O}(h^r), \text{ with } r = (j+1)q. \tag{4b}$$

Here $j \geq 1$, and the $\mathcal{O}$-constant is of moderate size, not affected by stiffness.

3. THE GLOBAL AND LOCAL STOPPING ERRORS

Let $Nh = T$, and consider the *global stopping error* $D_N = v_N - u_N$. In analysing this error it is convenient to introduce *local stopping errors* $d_n = x^* - x_j$. Here

d_n may be defined to be the Newton stopping error which would be present at t_n under the localizing assumption

$$u_{n-i} = U(t_{n-i}), \quad f_{n-i} = U'(t_{n-i}) \text{ for} 1 \le i \le k.$$

The global stopping error amounts to the accumulated effect of Newton stopping errors at the points $t_k, t_{k+1}, \dots, t_N$. For stable linear multistep methods the global stopping error D_N may thus be expected to satisfy

$$|D_N| = \mathcal{O}(|d_k| + |d_{k+1}| + \cdots + |d_N|).$$

Further, the local stopping errors can be estimated by (4b),

$$|d_n| = \mathcal{O}(h^r), \quad r = (j+1)q \quad (k \le n \le N). \tag{5}$$

Hence $|D_N| = \mathcal{O}(Nh^r) = \mathcal{O}(Th^{r-1})$, so that we expect

$$|D_N| = \mathcal{O}(h^{r-1}). \tag{6}$$

4. A NUMERICAL EXPERIMENT PERTINENT TO THE GLOBAL STOPPING ERROR

In order to check (6) we consider the problem

$$\begin{cases} U_1' = -10^8[U_1 - (U_2-2)^3] + 3(U_2-2)^2, \quad U_1(0) = -8, \\ U_2' \;\; = 10^8[U_1 - (U_2-2)^3] + 1, \quad U_2(0) = 0, \\ \qquad 0 \le t \le T = 1/2. \end{cases}$$

The true solution is

$$U_1(t) = (t-2)^3, \quad U_2(t) = t.$$

We consider the numerical solution of the above problem by the backward Euler method, that is

$$k = 1, \quad \alpha_0 = 1, \quad \alpha_1 = -1, \quad \beta_0 = 1, \quad \beta_1 = 0.$$

Further, we consider the situation where there is only 1 iteration step of (3), with

$$x_0 = u_{n-1}, \quad u_n = x_1 \text{ at } t = t_n \quad (n = 1, 2, \dots, N).$$

We deal with the sum-norm in $\mathbb{R}^2$. It is easily verified that the conditions of DORSSELAER & SPIJKER (1994), under which (4b), (5) hold, are fulfilled here. In fact, we have (5) with moderate $\mathcal{O}$-constant and

$$r = (j+1)q, \; j = 1, \; q = 1, \text{ so that } r = 2.$$

Hence (6) amounts to

$$|D_N| = \mathcal{O}(h^{r-1}) = \mathcal{O}(h).$$

Some actual ratios $|D_N|/h$ are listed in Table 1.

h	$\lvert D_N\rvert/h$	$\lvert D_N\rvert/h^2$
0.01	0.0183	1.83
0.005	0.00920	1.84
0.0025	0.00461	1.84

Table 1

From the table it is clear that (6) is too pessimistic in this example. The actual order is greater by 1 than the order in (6).

The question arises of whether the high order of D_N in this example is an exception just due to some coincidence. We shall see that it is no exception but an illustration of the interesting fact that

$$|D_N| = \mathcal{O}(h^r), \tag{7}$$

instead of (6), can be expected, in general situations.

5. Hundsdorfer's device

Relation (7) can be shown to be plausible by a general device used in Hundsdorfer (1992), Hundsdorfer & Steiniger (1991). Below we formulate this device for $k = 1$.

Theorem (*version of Hundsdorfer's device*). *Let y_n, $Y_n \in \mathbb{R}^s$ satisfy*

$$Y_n = S_n Y_{n-1} + y_n \quad (1 \le n \le N), \quad Y_0 = 0.$$

Here S_n are $s \times s$ matrices, with induced matrix norm $\|S_N \cdot \ldots \cdot S_j\| \le \sigma$ $(1 \le j \le N)$. Suppose the structure of y_n is as follows:

$$y_n = (S_n - I)h^r g(t_n),$$

$$|g(t)| \le c, \quad |g(t) - g(t-h)| \le c \cdot h \quad (\text{for } h \le t \le T).$$

Then

$$|Y_N| \le C \cdot h^r, \text{ with } C = (1 + \sigma + T\sigma) \cdot c.$$

In the applications of this device y_n, Y_n stand for local and global errors, respectively. It essentially states that local errors which are $\mathcal{O}(h^r)$ yield a global error which is of the same order – if the recurrence is stable and the local errors have the above structure.

It is possible to show that, if the linear multistep method is sufficiently stable,

$$Y_n = D_n \text{ and } y_n = d_n$$

satisfy relations which are essentially as required for applying the general device of Hundsdorfer, see Spijker (1995). This yields (7) in general situations, and explains the ratios we found in Table 1. Hence the reason for the high order of the global stopping error lies in the *special structure* of the local errors d_n.

6. Discretization errors

We stress that the high order in (7) is *not* due to a *strong damping* at the point $T = t_N$ of all preceeding local stopping errors d_n (with $n < N$). In this context it is instructive to consider the *discretization* errors in the application of the linear multistep method (2).

Let $E_N = U(t_N) - v_N$ denote the global discretization error, and e_n the local discretization error (i.e. the error $U(t_n) - v_n$ under the localizing assumption that $v_{n-i} = U(t_{n-i})$, $f_{n-i} = U'(t_{n-i})$ for $1 \le i \le k$). If a strong error damping mechanism would be present, we would expect the global error E_N to be of the same order as the local errors e_n.

In Table 2 we have listed actual ratios $|E_N|/h$ for our above example (Section 4).

h	$\lvert E_N\rvert/h$
0.01	1.99
0.005	2.00
0.0025	2.00

Table 2

We clearly see that actually $|E_N| = \mathcal{O}(h)$. Since in our example $|e_n| = \mathcal{O}(h^2)$, there is no strong damping – the global error is 1 order lower than the local error.

The phenomenon that D_N has the same order as d_n is not due to a damping mechanism pertinent to any local errors. It is due to the special structure of the local stopping errors.

7. Concluding remarks

1. Theoretical results similar to (7) are available for general linear multistep methods and variants to (3), see Spijker (1995).
2. Estimates of the form (7) are believed to be relevant to the question of how many Newton-type iterations should be carried out in order that the stopping error does not interfere with the intrinsic accuracy of the linear multistep method. In the above example, just 1 iteration step of (3), with $x_0 = u_{n-1}$, yields $|v_N - u_N| = \mathcal{O}(h^2)$, whereas $|U(t_N) - v_N| = \mathcal{O}(h)$. According to these estimates it certainly does not pay to perform more than 1 iteration step.
3. Many other numerical experiments were performed, supporting formula (7) in general situations ($k = 1, 2, 3$; $j = 1, 2, 3$).

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