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QUASI-NEWTON UPDATES IN ROW-METHODS FOR AVOIDING JACOBIANS

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1. Introduction

Numerical methods for solving stiff ordinary differential equations require high order of consistency as well as good stability properties. As a rule implicit methods only can treat stiff systems with acceptable step sizes. Replacing the nonlinear systems arising in implicit methods by some truncated Newton-method one obtains linearly implicit schemes. The ROW-methods form a quite arbitrary class of linearly implicit methods for solving stiff ODE's generalizing this idea. In this paper we report on some new approach jointly developed with Dr.W.Burmeister and Dr.S.Scholz which can be characterized by some truncated quasi-Newton method applied to implicit techniques. We use one quasi-Newton iteration only in each integration step of the ODE solver. Here, we sketch the main ideas only. For further details the interested reader is referred to [1], [2].

Let us consider the following initial value problem

$$y'(x) = f(y(x)) \;,\quad x \in (0,X), \qquad y(0) = y_0 \;. \tag{1}$$

We approximate the solution of this problem by a discretization technique with a fixed stepsize h>0. Steihaug/Wolfbrandt [6] proposed the following s stage W-method as a generalization of ROW-schemes:

$$y_{n+1} = y_n + h \sum_{i=1}^{s} w_i \; k_{i,n}$$

with $k_{i,n}$ as the solution of the linear systems

$$(I - h\gamma A_n)\, k_{i,n} = f(y_n + h \sum_{j=1}^{i-1} \alpha_{ij}\, k_{j,n}) + hA_n \sum_{j=1}^{i-1} \gamma_{ij}\, k_{j,n} \;. \tag{2}$$

Here w_i , α_{ij} , γ_{ij} , γ and A_n denote real parameters and matrices, respectively, defining the method. With the choice $A_n = f'(y_n)$ this method forms a ROW-method as considered in [4]. The order p of consistency of method (2) in the usual way can be derived from the the local truncation error

$$y(x+h) - y(x) - h \sum_{i=1}^{s} w_i \ k_i(y(x)) \tag{3}$$

with $k_i(.)$ defined analogously to (2). Expanding the functions in (3) according Taylor's formula we obtain powers of the stepsize h multiplied by some linear combinations of so called elementary differentials (e.d.). Using (2), we obtain the classical e.d.'s known from ROW-methods as well as additional e.d.'s. The following table summarizes these e.d.'s up to the order p=4.

p	classical e.d.'s	additional e.d.'s
1	f	
2	f'f	Af
3	f''ff, f'f'f	f'Af, Af'f, AAf
4	f'''fff, f'f''ff	f'AAf, f''fAf, AAAf, Af'Af, Af''ff
	f''ff'f, f'f'f'f	AAf'f, f'f'Af, f'Af'f, Af'f'f

Here the indices n are omitted to make the notation more simple. A stands for A_n and f' stands for $f'(y_n)$ e.g. We investigate the order of consistency of the proposed method by checking up to which order all of the occurring e.d.'s are vanishing. In the case of ROW-methods all e.d.'s containing the matrices A coincides with appropriate classical e.d.'s because of A=f'. In the general case if the matrices A are not related to the Jacobians f', however, the additional e.d.'s can't be canceled. As a consequence there does not exist any 3-stage method of order 3 as shown in [5]. However, the quasi-Newton update reduces the number of occurring condition significantly as shown later.

2. Elimination of some additional e.d.'s by quasi-Newton updates

In quasi-Newton methods the matrices A_n are updated such that some secant equation holds. We denote

$$s_n := y_n - y_{n-1} \ , \quad d_n := (f_n - f_{n-1})/h \tag{3}$$

Then the equations

$$A_n \ s_n = h \ d_n \tag{4}$$

are used as secant equation. Furthermore the generated matrices A_n are supposed to be uniformly bounded for any $h>0$ and for arbitrary indices n. We guarantee (4) to be satisfied by using the idea of Broyden's updating (see [5] e.g.). This leads to formulas of the type

$$A_n = B_n + \frac{(h\, d_n - B_n\, s_n)\, q_n^T}{q_n^T s_n} \tag{5}$$

with arbitrary matrices B_n and vectors q_n In [1], [2] we investigated especially the cases $q_n = s_n$ and $B_n = B$ or $B_n = A_{n-1}$ The later technique results in the updating formula

$$A_n = A_{n-1} + \frac{(h\, d_n - A_{n-1}\, s_n)\, s_n^T}{s_n^T s_n}$$

with some given starting matrix A_0. We obtain the approximation property

$$A_n f_n = f_n' f_n + O(h)$$

as an essential consequence of the proposed construction. This property will be used later to prove the order of consistency of the new method.

Next, we sketch the idea of deriving the expansion of the local truncation error. We restrict us to the order p up to 4 for the sake of simplicity of the representation. From the differential equation (1) and standard Taylor's expansion we obtain

$$y_{n-1} = y_n - hf_n + 1/2\, h^2 (f'f)_n - 1/6\, h^3 (f''ff + f'f'f)_n + O(h^p)$$

and

$$\begin{aligned} f_{n-1} = f_n &- h(f'f)_n + 1/2\, h^2 (f''ff + f'f'f)_n \\ &- 1/6\, h^3 (f'''fff + f'f''ff + 3f''ff'f + f'f'f'f)_n + O(h^p). \end{aligned}$$

Using (3), now, we can find expansions for s_n and d_n. Finally, with (4) this leads to the representation

$$\begin{aligned} A_n f_n = (f'f)_n &- 1/2\, h(f''ff + f'f'f)_n + 1/2 h A_n (f'f)_n \\ &+ 1/6\, h^2 (f'''fff + f'f''ff + 3f''ff'f + f'f'f'f)_n \\ &- 1/6\, h^2 A_n (f''ff + f'f'f)_n + O(h^{p-1}). \end{aligned}$$

This relation enables us to replace some of the additional e.d.'s occurring in the given table by classical ones. Thus, the number of order condition can be reduced significantly.

3. Convergence results for the new methods

We can show some efficient methods to exist by means of direct investigation of the resulting order conditions. The main results derived in [1] are:

Theorem 1: Let the initial matrix A_0 satisfy the condition $A_0 f_0 = f_0' f_0 + O(h)$ and the matrices A_n be constructed by (5) with fixed B_n. Then the proposed method (2) with 2 stages has the order $p=3$ if the parameters of the method are selected according

$$\gamma = 1/2(1+1/\sqrt{3}), \quad \alpha_{21} = 1.5773\ 5026, \quad \gamma_{21} = -2.9856\ 4060$$
$$w_1 = 0.7950\ 1732 \quad w_2 = 0.2049\ 8268.$$

For the parameters given above the related ROW-method is know to be strongly A-stable. The method considered here has the same stability behavior with respect to the linear test equation because the updating does not change the initial matrix $A_0 = f_0$ and the method forms a ROW-method for this special problem. The determination of the given parameters from the consistency conditions is rather technical. We refer the interested reader to [1], [2] for further details.

Furthermore in [1] a family of 4-stage methods of order $p=4$ has been constructed. Finally in [2] the variable stepsize case is investigated.

Numerical examples (see [1]) show a good coincidences of the theoretical results with the computer experiments.

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