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Two Classes of Numerical Methods for Stiff Problems

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Two classes of numerical methods for stiff problems are shown. Formulae contained in the second clase require to solve a system of only linear algebr. eqs. to obtain the solution of a nonlinear system of differential eqs. at each step. One such formula is tested on a very stiff problem and the comparison with other often used methods is given.

Let us consider the differential equation of the form:

$$y' = f(x, y) \quad y(x_0) = y_0 \quad x \in \langle x_0, x_d \rangle . \tag{1}$$

Under obvious conditions on f relations (1) are equivalent to:

$$y'' = f'(x, y) \quad y(x_0) = y_0 \quad y'(x_k) = f(x_k, y(x_k)) \quad x, x_k \in \langle x_0, x_d \rangle . \tag{2}$$

Defining the mesh $x_i = x_0 + ih$ on the interval $\langle x_0, x_k \rangle \subset \langle x_0, x_d \rangle$ and approximating the relations (2) by finite differences at mesh-points, we can derive different formulae having the following general form:

$$I \begin{bmatrix} y_{n+1} \\ \vdots \\ y_{n+k} \end{bmatrix} = \begin{bmatrix} y_n \\ \vdots \\ y_n \end{bmatrix} + h \begin{bmatrix} d_1 \\ \vdots \\ d_k \end{bmatrix} f(x_n, y_n) + h^2 \begin{bmatrix} e_1 \\ \vdots \\ e_k \end{bmatrix} f'(x_n, y_n) +$$

$$+ hB \begin{bmatrix} f(x_{n+1}, y_{n+1}) \\ \vdots \\ f(x_{n+k}, y_{n+k}) \end{bmatrix} + h^2 C \begin{bmatrix} f'(x_{n+1}, y_{n+1}) \\ \vdots \\ f'(x_{n+k}, y_{n+k}) \end{bmatrix} \tag{3}$$

where: I — unit $k \times k$ matrix, B, C — $k \times k$ matrices, d_i, e_i — real numbers, h — mesh size.

We assume y_n to be a known starting value. The unknown values $y_{n+1} \ldots, y_{n+k}$ are to be calculated from the formula (3) and y_{n+k} is used as a new starting value only.

We have shown for a sufficiently smooth right-hand side f the necessary and sufficient conditions for method (3) to be of order p. Further, we have proved that every formula (3) having order $p \geqslant 1$ is convergent and the rate of convergence is $O(h^p)$.

The class (3) contains as a subset the class of selfstarting overimplicit methods (*SOM*). It has been shown in [1] that there exist A-stable methods of arbitrarily high order in the class *SOM*. We have derived the A-stable formulae up to the order 6 which contain the second derivatives of the solution and therefore do not belong to the class *SOM*. We believe it is possible to show in a way similar to that referred in [1] that the formulae of class (3) (containing the second derivatives) can also yield A-stable methods of any arbitrary order. But we have not proved it yet.

By applying the formula (3) to a nonlinear system we have to solve a set of nonlinear eqs. at each step. We suggest to use a certain iterative procedure (resembling the Newton method) requiring an evaluation of the Jacobian (not Hessian) matrix of the right-hand side of original differential system only. This procedure is described in [2].

The main goal of this communication is to devise a way of avoiding any kind of iteration.

We shall illustrate our procedure on the simplest type of the class (3). The class (3) takes for $k = 1$ the form:

$$y_{n+1} = y_n + hdf(x_n, y_n) + h^2 ef'(x_n, y_n) + hbf(x_{n+1}, y_{n+1}) + h^2 cf'(x_{n+1}, y_{n+1}). \quad (4)$$

Let us now consider a system of diff. eqs. Then f and f' are vector functions and it holds: $f_i' = \frac{\partial f_i}{\partial x} + J_i f_i$, where J is the Jacobian matrix of f and the subscript i denotes that all values are taken at the point x_i, y_i. We replace in the formula (4) $f(x_{n+1}, y_{n+1})$ by $f_n + h\frac{\partial f_n}{\partial x} + J_n \Delta_n$ and $f'(x_{n+1}, y_{n+1})$ by $\frac{\partial f_n}{\partial x} + J_n f_n + {} + J_n \frac{\partial f_n}{\partial x} + J_n^2 \Delta_n$ where $\Delta_n = y_{n+1} - y_n$. Requiring the formula (4) to be of the order $p \geqslant 2$ we finally obtain:

$$[I - hbJ_n - h^2 cJ_n^2]\, \Delta_n = hf_n + h^2 \left[(0.5 - b)\, J_n f_n + 0.5 \frac{\partial f_n}{\partial x} + hcJ_n \frac{\partial f_n}{\partial x} \right] \quad (5)$$

This formula beeing applied to $y' = ay$ yields the same expression as the original formula (4). Therefore (5) is A-stable if and only if (4) is A-stable. We have proved that for a sufficiently smooth right-hand side f the formula (5) is convergent if (4) is convergent. If the order of (4) is $p \geqslant 2$, then the rate of convergence of (5) is $O(h^2)$. Referring to (5) a system of only linear algebraic Eqs. is to be solved at each step. For $b = 1$ and $c = -0.5$ the formula (5) is A-stable and of the second order.

We have tested this formula on a very stiff system arising in the reactor kinetics (taken from [3]).

$$y_1' = -0.04 y_1 + 10^4 y_2 y_3 \qquad y_2' = 0.04 y_1 - 10^4 y_2 y_3 - 3\,.\,10^7 y_2^2$$

$$y_3' = 3\,.\,10^7 y_2^2 \qquad y_1(0) = 1 \;\; y_2(0) = y_3(0) = 0$$

Results obtained for $x = 4$ are in following table:

h	y_1	$10^4 y_2$	$10 y_3$
0.4	0.98477	0.38157	0.35192
0.2	0.92398	0.24645	0.75995
0.05	0.90683	0.22557	0.93147
0.02	0.90561	0.22416	0.94361
0.01	0.90553	0.22406	0.94449
§	0.90552	0.22404	0.94458

§ – reference solution — Runge-Kutta method of 4-th order, $h = 0.001$

The comparison with several other methods has shown that our technique can very succesfully compete with all methods considered.

Method	$\lvert y_1 - \overset{*}{y}_1 \rvert$	$\lvert y_2 - \overset{*}{y}_2 \rvert$	$\lvert y_3 - \overset{*}{y}_3 \rvert$
BVT	2.2 E−4	3.8 E−8	2.2 E−4
Calahan	1.4 E+0	4.0 E−5	1.4 E+0
Allen	9.8 E−1	4.7 E−4	2.4 E+1
ISI3 (−100)	2.2 E−3	4.0 E−7	2.2 E−3
ISI3 (−∞)	2.2 E−3	3.9 E−7	2.2 E−3
LW1	1.6 E−4	2.4 E−4	3.2 E−3
LW2	5.9 E−4	2.9 E−3	4.0 E−2

$h = 0.02$ $x = 0.4$
BVT – method (5)
LW1, LW2 – derived in [2]
ISI3 (..) – derived in [4]

The one-step nature of our method allows to implement an automatic step-size control. Results calculated by a step-size control procedure are compared with those obtained using the constant step-size in the following table (for $x = 10$):

	h	$\lvert y_1 - \overset{*}{y}_1 \rvert$	$\lvert y_2 - \overset{*}{y}_2 \rvert . 10^4$	$\lvert y_3 - \overset{*}{y}_3 \rvert . 10$	*evaluation in RHS**
constant step	0.4	0.027	0.023	0.27	25
	0.05	0.001	0.001	0.01	200
	0.02	0.000	0.000	0.00	500
step-size control procedure		0.000	0.000	0.00	38

* RHS — right-hand side

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