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ON GENERALIZED RUNGE-KUTTA METHODS USING AN EXACT JACOBIAN AT A NON-STEP POINT

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On generalized Runge-Kutta methods using an exact Jacobian at a non-step point *)

by

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ABSTRACT

In this note we investigate a two-stage generalized Runge-Kutta formula which can be used for the numerical integration of stiff systems of ordinary differential equations. Attention is focussed to formulas which evaluate the Jacobian at non-step points.

KEY WORDS & PHRASES: *numerical integration, stiff equations, generalized Runge-Kutta methods*

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*) This report will be submitted for publication elsewhere.

1. Introduction

Let

$$y' = f(y), \qquad y(x_0) = y_0 \tag{1}$$

represent the initial value problem for a *stiff system* of ordinary differential equations, written in autonomous form, of which the real vector function $f(y)$ is sufficiently differentiable. An important class of numerical integration methods for this problem are formed by the so-called Rosenbrock formulas [7]. A Rosenbrock formula may be characterized as an explicit, one-step Runge-Kutta formula of which the scalar parameters have been replaced by particular rational functions of the stepsize h and the Jacobian matrix $J(y) = \partial f(y)/\partial y$. The aim of this replacement is to obtain attractive stability properties, such as A-stability. In the original Rosenbrock method the treatment of each new Runge-Kutta stage, which means a new f-evaluation, may require a new J-evaluation. As each J-evaluation also involves an LU-decomposition, this is not recommended. Consequently, most authors discussing Rosenbrock type methods consider schemes which evaluate J once per integration step, viz. at the *step point* $y = y_n$ [1,2,4,6,7,10,11,12]. However, if we allow *one J-evaluation per integration step,* it is also possible to investigate schemes which evaluate J at some *non-step point,* rather than at $y = y_n$. The aim is, e.g., the development of schemes giving more accuracy at the cost of the same number of operations, or the development of schemes which are more flexible with respect to the implementation of some error control mechanism.

Two first investigations in this direction have been reported by Scholz, Bräuer and Thomas [8] and Scholz [9], respectively. Scholz [9] investigates a modification of the original Rosenbrock method. He constructs a one-stage formula and several two-stage formulas, all evaluating J at a non-step point. In addition, he is able to show that his formulas satisfy the S-*stability requirements* [12].

In this note we apply the idea of Scholz, of evaluating the Jacobian once per integration step at a non-step point, to the two-stage formula

$$y_{n+1} = y_n + \Theta_0(hJ_{n+\eta})hf(y_n) \qquad (2)$$

$$+ \Theta_1(hJ_{n+\eta})hf(y_n+\Lambda(hJ_{n+\eta})hf(y_n)).$$

Here $J_{n+\eta} = J(y_n+\eta hf(y_n))$, η a scalar, and Θ_0, Θ_1 and Λ are rational functions with real coefficients. Following van der Houwen [10], we do not specify these functions beforehand and call (2) a generalized Runge-Kutta formula. Class (2) contains the modified Rosenbrock formulas constructed by Scholz.

2. The local truncation error and the stability function

Let the operator equation $y_{n+1} = E_n(y_n)$ represent (2). Let y be an exact and sufficiently differentiable solution for (1). Denote

$$\theta_i = \Theta_i(0), \theta_i' = \frac{d}{dz}\,\Theta(z)\Big|_{z=0}, \quad \lambda = \Lambda(0),\ \lambda' = \frac{d}{dz}\,\Lambda(z)\Big|_{z=0}, \ldots .$$

By means of Taylor's theorem for functions of several variables, and using tensor notation [3], the *local truncation error* $y(x_{n+1}) - E_n(y(x_n))$ can be expanded as

$$y(x_{n+1}) - E_n(y(x_n)) = \qquad (3)$$

$$h[1-(\theta_0+\theta_1)]f +$$

$$h^2[\tfrac{1}{2}-(\theta_0'+\theta_1'+\theta_1\lambda)]f_j f^j +$$

$$h^3[\frac{1}{6} - (\frac{1}{2}\theta_0'' + \theta_1\lambda' + \theta_1'\lambda + \frac{1}{2}\theta_1'')]f_j f_k^j f^k +$$

$$h^3[\frac{1}{6} - (\eta\theta_0' + \frac{1}{2}\theta_1\lambda^2 + \theta_1'\eta)]f_{jk} f^j f^k +$$

$$h^4[\frac{1}{24} - (\frac{1}{6}\theta_0''' + \frac{1}{2}\theta_1\lambda'' + \theta_1'\lambda' + \frac{1}{2}\theta_1''\lambda + \frac{1}{6}\theta_1''')]f_j f_k^j f_\ell^k f^\ell +$$

$$h^4[\frac{1}{24} - (\frac{1}{2}\theta_0''\eta + \eta\theta_1\lambda' + \frac{1}{2}\theta_1'\lambda^2 + \frac{1}{2}\theta_1''\eta)]f_j f_{k\ell}^j f^k f^\ell +$$

$$h^4[\frac{3}{24} - (\frac{1}{2}\theta_0''\eta + \lambda\lambda'\theta_1 + \lambda\eta\theta_1' + \frac{1}{2}\theta_1''\eta)]f_{jk} f_\ell^j f^k f^\ell +$$

$$h^4[\frac{1}{24} - (\frac{1}{2}\theta_0'\eta^2 + \frac{1}{6}\theta_1\lambda^3 + \frac{1}{2}\theta_1'\eta^2)]f_{jk\ell} f^j f^k f^\ell +$$

$$h^5[\frac{1}{120} - (\frac{1}{24}\theta_0'''' + \frac{1}{6}\theta_1\lambda''' + \frac{1}{2}\theta_1'\lambda'' + \frac{1}{2}\theta_1''\lambda' + \frac{1}{6}\theta_1'''\lambda + \frac{1}{24}\theta_1'''')]f_j f_k^j f_\ell^k f_m^\ell f^m +$$

$$h^5[\frac{3}{120} - (\frac{1}{6}\theta_0'''\eta + \frac{1}{2}\theta_1\lambda''\eta + \theta_1'\lambda\lambda' + \frac{1}{2}\theta_1''\eta\lambda + \frac{1}{6}\theta_1'''\eta)]f_j f_{k\ell}^j f_m^k f^\ell f^m +$$

$$h^5[\frac{1}{120} - (\frac{1}{6}\theta_0'''\eta + \frac{1}{2}\theta_1\lambda''\eta + \theta_1'\eta\lambda' + \frac{1}{4}\theta_1''\lambda^2 + \frac{1}{6}\theta_1'''\eta)]f_j f_k^j f_{\ell m}^k f^\ell f^m +$$

$$h^5[\frac{1}{120} - (\frac{1}{4}\theta_0''\eta^2 + \frac{1}{2}\theta_1\lambda'\eta^2 + \frac{1}{6}\theta_1'\lambda^3 + \frac{1}{4}\theta_1''\eta^2)]f_j f_{k\ell m}^j f^k f^\ell f^m +$$

$$h^5[\frac{3}{120} - \frac{1}{2}\theta_1\lambda'^2]f_{jk} f_\ell^j f_m^k f^\ell f^m +$$

$$h^5[\frac{4}{120} - (\frac{1}{6}\theta_0'''\eta + \frac{1}{2}\theta_1\lambda\lambda'' + \theta_1'\lambda'\eta + \frac{1}{2}\theta_1''\eta\lambda + \frac{1}{6}\theta_1'''\eta)]f_{jk} f_\ell^j f_m^\ell f^k f^m +$$

$$h^5[\frac{4}{120} - (\frac{1}{2}\theta_0''\eta^2 + \lambda\lambda'\eta\theta_1 + \frac{1}{2}\theta_1'\eta\lambda^2 + \frac{1}{2}\theta_1''\eta^2)]f_{jk} f_{\ell m}^j f^k f^\ell f^m +$$

$$h^5[\frac{6}{120} - (\frac{1}{4}\theta_0''\eta^2 + \frac{1}{2}\theta_1\lambda^2\lambda' + \frac{1}{2}\theta_1'\lambda\eta^2 + \frac{1}{4}\theta_1''\eta^2)]f_{jk\ell} f_m^j f^k f^\ell f^m +$$

$$h^5[\frac{1}{120} - (\frac{1}{6}\theta_0'\eta^3 + \frac{1}{24}\theta_1\lambda^4 + \frac{1}{6}\theta_1'\eta^3)]f_{jk\ell m} f^j f^k f^\ell f^m + O(h^6).$$

In the sequel, the integer p will stand for *the order of consistency,* i.e. p is the largest integer satisfying $y(x_{n+1}) - E_n(y(x_n)) = O(h^{p+1}),\ h \to 0$.

Using the theory of Butcher series, van Kampen [11] has shown that for an m-stage method of type (2), with $\eta = 0$, the order p cannot exceed 2m. For the case $m \le 2$ this result can be verified by inspection of (3). If $\eta = 0$ and $m = 1$, i.e. $\Theta_1 = 0$, the differential $f_{jk}f^jf^k$ is not present and if $\eta = 0$ and $m = 2$, we see that $f_{jk}f^j_{\ell m}f^kf^\ell f^m$ is missing. An interesting question is now, whether by the introduction of the parameter η an increase of the order can be realized. It turns out that for the one-stage formula $p = 3$ can be obtained (see [9] and section 3), whereas for the two-stage formula we always have $p \le 4$ (see section 4).

When applied to the *stability test-model* $y' = \delta y$, $\delta \in \mathbb{C}$, (2) will result into the scalar relation $y_{n+1} = R(z)y_n$, $z = h\delta$, where

$$R(z) = 1 + z\Theta_0(z) + z\Theta_1(z) + z^2\Theta_1(z)\Lambda(z). \tag{4}$$

The stability properties of (2), such as A-stability, are determined by the so-called *stability function* R (see e.g. [5]). In the remaining part of the note we shall make frequent use of the concept of stability function. Here - with we use the following definitions (cf. [5]): R is said to be (a) *A-acceptable,* if $|R(z)| < 1$ whenever $Re(z) < 0$; (b) *strongly A-acceptable,* if it is A-acceptable and satisfies $\lim |Re(z)| < 1$ as $Re(z) \to -\infty$; (c) *L-acceptable,* if it is A-acceptable and satisfies $\lim R(z) = 0$ as $Re(z) \to -\infty$. Further, we let q denote *the order of consistency of R,* i.e. q is the largest integer satisfying $R(z) - e^z = O(z^{q+1})$, $z \to 0$.

3. One-stage formulas of order three

In this section we concentrate on the class of formulas ($\Theta_1 = 0$ in (2))

$$y_{n+1} = y_n + \Theta_0(hJ_{n+\eta})hf(y_n). \tag{5}$$

THEOREM 1. *Let* I *denote the unit matrix. Let* R *represent some adaptive stability function of order* q. *The formula*

$$y_{n+1} = y_n + (hJ_{n+\eta})^{-1}(R(hJ_{n+\eta})-I)hf(y_n) \tag{6}$$

is of order $p = 3$ *if* $\eta = \frac{1}{3}$ *and* $q \geq 3$. *If* η *is arbitrary and* $q \geq 2$, *we always have* $p = 2$. □

The proof follows from a simple calculation with (3). By pursuing this calculation somewhat further, it is also easy to see that we always have $p \leq 3$. The applicability of this theorem lies in the *adaptivity* of the stability function R. In fact, (6), where $\eta = \frac{1}{3}$ and $q \geq 3$, represents a large class of third order integration formulas of which, to a certain extent, the stability behaviour can be adapted to the problem under consideration (cf. [10]). For example, we can choose the third order stability function

$$R(z) = \frac{1+(1+\alpha)z+(\frac{1}{3}+\frac{1}{2}\alpha)z^2}{1+\alpha z-(\frac{1}{6}+\frac{1}{2}\alpha)z^2} \tag{7}$$

of Liniger and Willoughby (see [10], p.79), where the free parameter α can be used for exponential fitting. Function (7) is A-acceptable if $\alpha \leq -\frac{1}{2}$ and L-acceptable if $\alpha = -\frac{2}{3}$. Observe that if the stability function R in (6) is strongly A-acceptable, the method is also S-stable [12]. Another member of class (6) is defined by the third order function given by Scholz [9], viz.

$$R(z) = \frac{1-\frac{1}{3}\sqrt{3}\,z-(\frac{1}{6}+\frac{1}{6}\sqrt{3})z^2}{(1-(\frac{1}{2}+\frac{1}{6}\sqrt{3})z)^2}, \tag{8}$$

which is strongly A-acceptable. An attractive property of (8), with respect to the aspect of computer implementation (see [9]), is that the denominator is factorized into two equal linear terms.

4. Two-stage formulas of order four

Following [10, section 2.7.8], we express the derivatives of Θ_0, at $z = 0$, into the derivatives of Θ_1, Λ and R:

$$\theta_0 = R'(0) - \theta_1,\ \theta_0' = \frac{1}{2}R''(0) - \theta_1' - \theta_1\lambda,\ \theta_0'' = \frac{1}{3}R'''(0) - \theta_1'' - 2\theta_1'\lambda - 2\theta_1\lambda',$$

$$\theta_0''' = \frac{1}{4}R''''(0) - \theta_1''' - 3\theta_1''\lambda - 6\theta_1'\lambda' - 3\theta_1\lambda''. \tag{9}$$

Assuming that R is a 4-th order consistent approximation to e^z and substitution of (9) into the ($p \le 4$)-expressions of expansion (3), yields the remaining conditions for 4-th order accuracy:

$$\eta(\tfrac{1}{2}-\theta_1\lambda) = \tfrac{1}{6}-\tfrac{1}{2}\theta_1\lambda^2, \qquad \eta^2(\tfrac{1}{2}-\theta_1\lambda) = \tfrac{1}{12}-\tfrac{1}{3}\theta_1\lambda^3,$$
$$\eta(\tfrac{1}{6}-\theta_1'\lambda) = \tfrac{1}{24}-\tfrac{1}{2}\theta_1'\lambda^2, \qquad \eta(\tfrac{1}{6}-\theta_1\lambda') = \tfrac{3}{24}-\lambda\lambda'\theta_1. \tag{10}$$

If the new parameter $\eta = 0$, the remaining parameters are: $\theta_1 = \frac{16}{27}$, $\lambda = \frac{3}{4}$, $\theta_1' = \frac{4}{27}$, $\lambda' = \frac{9}{32}$. First we prove the following negative result:

<u>THEOREM 2</u>. *The introduction of the parameter η into the 2-stage generalized Runge-Kutta method does not result into an increase of the order of consistency. The maximal order remains* $p = 4$.

<u>PROOF</u>. We only need to show that $p = 5$ is impossible. Let $\xi = \theta_1\lambda$. The elimination of η between the first two equations of (10) yields

$$(6\lambda^2)\xi^2 + (12\lambda-12\lambda^2-6)\xi + 1 = 0. \tag{11}$$

The last term in (3) yields the order relation $\eta^3(\frac{1}{2}-\xi) = \frac{1}{20}-\frac{1}{4}\xi\lambda^3$. By again eliminating η, we then find

$$(30\lambda^3)\xi^2 + (15\lambda+20\lambda^2-45\lambda^3-18)\xi + 4 = 0. \tag{12}$$

A simple calculation reveals that (11) and (12) are incompatible. □

The solution of system (10) can be written as the one-parameter solution

$$\theta_1 = (1-2\lambda+2\lambda^2+\sqrt{(1-2\lambda+2\lambda^2)^2-\tfrac{2}{3}\lambda^2})/\zeta, \qquad \eta = (\tfrac{1}{6}-\tfrac{1}{2}\theta_1\lambda^2)/(\tfrac{1}{2}-\theta_1\lambda),$$
$$\theta_1' = (\tfrac{1}{24}-\tfrac{1}{6}\eta)/(\tfrac{1}{2}\lambda^2-\eta\lambda), \qquad \lambda' = (\tfrac{3}{24}-\tfrac{1}{6}\eta)/(\lambda\theta_1-\eta\theta_1), \tag{13}$$

where $\zeta = \frac{81}{64}$ if $\lambda = \frac{3}{4}$ and $\xi = 2\lambda^3$ if $\lambda \ne \frac{3}{4}$. The free parameter λ can take all values except zero. We are thus led to the following theorem:

THEOREM 3. *Let* R *be an adaptive stability function of order* $q \geq 4$. *Equations* (9) *and* (13) *then define a four-parameter class of generalized Runge-Kutta formulas of order* $p = 4$. The free parameters are θ_1'', θ_1''', λ'' *and* λ $(\lambda \neq 0)$.

Of interest, with respect to the stability behaviour, is the freedom which is left in the choice of R and the functions Θ_0, Θ_1 and Λ. A nice example is the fourth order modified Rosenbrock formula given by Scholz [9]. The stability function of that formula, which also appears in another type of Rosenbrock formula developed by Kaps [4], is L-acceptable and factorized. Further, the functions Θ_0, Θ_1 and Λ are such that the formula is also internally S-stable (cf. [12]). Another example of a formula belonging to class (9), (13) is the L-stable formula discussed by van Kampen [11]. Here the parameter $\eta = 0$.

5. Some final remarks

From the foregoing it shall be clear that if we consider 2-stage formulas of order $p = 3$, we have a considerable degree of freedom with respect to the parameter choice. One possibility is to construct a scheme with a build in error control. It is an easy task to show that, thanks to the introduction of the parameter η, one can construct 2-stage formulas of order $p = 3$ such that $y_{n+1} - [y_n + \Lambda(hJ_{n+\eta})f(y_n)]$ provides an estimate of $y'''(x_n)$. Another conservative error estimator, which can be used for every 1-stage formula (6), is provided by the expression $J_{n+1+\eta}f(y_{n+1}) - J_{n+\eta}f(y_n)$, where $\eta = \frac{1}{3}$. This expression also estimates $y'''(x_n)$.

For a 2-stage formula order 4 can already be achieved with four degrees of freedom. Therefore it is likely that $p = 5$ can be obtained if we perform a third f-evaluation. Along the lines of section 4 it is then possible to develop a family of 5-th order , 3-stage formulas with an adaptive stability function. In this connection, the stability functions discussed by Kaps [4] are of interest.

One might also think of generalized Runge-Kutta schemes which evaluate the Jacobian at some weighted sum $\alpha y_n + \beta y_{n-1} + \ldots$. Here we avoid the occurrence of the *explicit* expression $y_n + \eta h f(y_n)$ in the J-evaluation. For stiff, highly non-linear problems, that is problems with a strongly varying Jacobian J(y), we then expect a somewhat better stability-accuracy behaviour.

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