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A NOTE ON TWO-STEP INTEGRATION FORMULAS OF THIRD ORDER ACCURACY WITH PRESCRIBED STABILITY FUNCTION

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A NOTE ON TWO-STEP INTEGRATION FORMULAS OF THIRD ORDER ACCURACY WITH PRESCRIBED STABILITY FUNCTION

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Abstract

A class of non-linear two-step integration formulas is given in third order accuracy. These formulas are characterized by the fact that the principal characteristic root (the stability function) can be adapted to the problem under consideration, while the parasitic root is zero. By choosing the stability function appropriately the integration formulas can be used for efficient integration of stiff equations. In a forthcoming paper we intend to publish numerical results.

1. Derivation of two-step formulas of third order accuracy.

Consider the autonomous vector differential equation

$$\frac{dy}{dx} = f(y). \tag{1.1}$$

We shall develop two-step formulas for the numerical integration of the initial value problem for this equation. The integration formulas are of the form

$$y_{n+1} = \alpha_1(h_nJ_n)\, y_n + \alpha_2(h_nJ_n)\, y_{n-1} + \tag{1.2}$$

$$+ h_n[\beta_1(h_nJ_n)\, f(y_n) + \beta_2(h_nJ_n)\, f(y_{n-1})],$$

where $h_n = x_{n+1}-x_n$ denotes the step length, y_n the numerical approximation to the solution $y(x)$ of (1.1) at $x = x_n$, J_n the Jacobian matrix of (1.1) at $y = y_n$, and α_1, α_2, β_1 and β_2 are polynomial or rational functions of h_nJ_n. In order to derive the consistency conditions for formula (1.2) we substitute a solution $y(x)$ of (1.1) into (1.2) and expand the left and right hand side in powers of h_n. For the sake of simplicity we restrict our considerations to a scalar differential equation although, for a vector differential equation the final consistency conditions are identical.

Let us define

$$q_n = \frac{h_{n-1}}{h_n}.$$

Then, by straightforward calculations we find that (1.2) can be written as

$$y'(x_n) = [1 + \alpha_2(0)q_n]^{-1}\, [h_n^{-1}(\alpha_1(0)+\alpha_2(0)-1)y(x_n) +$$

$$+ (\beta_1(0)+\beta_2(0))f(y(x_n)) + (\alpha_1'(0)+\alpha_2'(0))f_y(y(x_n))y(x_n) +$$

$$+ \frac{1}{2} h_n(\alpha_1''(0)+\alpha_2''(0)) f_y^2(y(x_n))y(x_n) +$$

$$+ \frac{1}{2} h_n(\alpha_2(0)q_n^2-2\alpha_2'(0)q_n+2\beta_1'(0)-2\beta_2(0)q_n+2\beta_2'(0)-1) y''(x_n) +$$

$$+ \frac{1}{6} h_n^2(\alpha_1'''(0)+\alpha_2'''(0)) f_y^3(y(x_n))y(x_n) +$$

$$- \frac{1}{6} h_n^2(\alpha_2(0)q_n^3+1) y'''(x_n) +$$

$$+ \frac{1}{2} h_n^2(\alpha_2'(0)q_n^2-\alpha_2''(0)q_n+\beta_1''(0)+\beta_2(0)q_n^2-2\beta_2'(0)q_n +$$

$$+ \beta_2''(0)) f_y(y(x_n)) y''(x_n) +$$

$$+ \frac{1}{2} \beta_2(0) q_n^2 h_n^3 f_{yy}(y(x_n))(y'(x_n))^2],$$

where $J(y(x_n))$ is replaced by $f_y(y(x_n))$.
By observing that

$$f_{yy}(y(x_n)) = y'''(x_n) - f_y(y(x_n)) y''(x_n)$$

we arrive at the consistency conditions for orders $p = 1$, 2 and 3 as listed in table 1.1.

2. Stability considerations

Formula (1.2) has the characteristic equation

$$R^2 - [\alpha_1(z) + z\beta_1(z)]R - [\alpha_2(z) + z\beta_2(z)] = 0, \tag{2.1}$$

where $z = h_n\delta$, δ being an eigenvalue of the Jacobian matrix J_n. This equation has two roots $R_1(z)$ and $R_2(z)$, one of them being the principal root the other being parasitic. The parasitic root is due to the fact that we solve a first order differential equation by a two-step formula. The corresponding solution component in the numerical approximation y_{n+1} is also parasitic and is not present in the analytical solution. This suggests to require that (2.1) has a root $R_1(z) = 0$, i.e.

Table 1.1. General consistency conditions for formula (1.2).

p	consistency conditions
$p \geq 1$	$1 + \alpha_2(0)q_n \neq 0$ $-\alpha_2(0)q_n + \beta_1(0) + \beta_2(0) = 1$ $\alpha_1(0) + \alpha_2(0) = 1$ $\alpha_1'(0) + \alpha_2'(0) = 0$
$p \geq 2$	$\alpha_1''(0) + \alpha_2''(0) = 0$ $\alpha_2(0)q^2 - 2\alpha_2'(0)q_n + 2\beta_1'(0) - 2\beta_2(0)q_n + 2\beta_2'(0) = 1$
$p \geq 3$	$\alpha'''(0) + \alpha_2'''(0) = 0$ $-\alpha_2(0)q_n^3 + 3\beta_2(0)q_n^2 = 1$ $-\alpha_2(0)q_n^3 + 3\alpha_2'(0)q_n^2 - 3\alpha_2'''(0)q_n + 3\beta_1''(0) +$ $+ 3\beta_2(0)q_n^2 - 6\beta_2'(0)q_n + 3\beta_2''(0) = 1$

(2.2) $\alpha_2(z) + z\beta_2(z) \equiv 0.$

The non-zero root is then given by

(2.3) $R(z) = \alpha_1(z) + z\beta_1(z).$

The root function R(z) governs the local stability of formula (1.2) and, therefore, is called the stability function. By identifying R(z) with a given appropriately chosen stability function we obtain conditions for the functions $\alpha_1(z)$ and $\beta_1(z)$. These conditions should be compatible with the consistency conditions listed in table 1.1. In order to find out which conditions a given stability function has to satisfy to be consistent with the consistency conditions, we substitute (2.2) into table 1.1. We then obtain

Table 2.1. Consistency conditions for formula (1.2) with a zero-characteristic root.

p		$R(z) = \alpha_1(z) + z\beta_1(z)$
	$\alpha_1(0) = 1$	$R(0) = 1$
$p \geq 1$	$\beta_1(0) - \alpha_2'(0) = 1$	$R'(0) = 1$
	$\alpha_1'(0) + \alpha_2'(0) = 0$	$\alpha_1'(0) + \alpha_2'(0) = 0$
$p \geq 2$	$2\beta_1'(0) - \alpha_2''(0) = 1$	$R''(0) = 1$
	$\alpha_1''(0) + \alpha_2''(0) = 0$	$\alpha_1''(0) + \alpha_2''(0) = 0$
	$3\beta_1''(0) - \alpha_2'''(0) = 1$	$R'''(0) = 1$
$p \geq 3$	$\alpha_1'''(0) + \alpha_2'''(0) = 0$	$\alpha_1'''(0) + \alpha_2'''(0) = 0$
	$-3\alpha_2'(0)q_n^2 = 1$	$\alpha_1'(0) = + 1/3q_n^2$

The second and third column contain equivalent conditions; the third column directly shows which conditions a given stability function has to satisfy in order to be consistent with the consistency conditions.

3. Construction of third order formulas with prescribed stability function.

Suppose that we are given a stability function $R(z)$ satisfying the derivative conditions as listed in table 2.1, i.e.

$$R^{(j)}(0) = 1, \qquad j = 0,1,2,3. \tag{3.1}$$

Then the construction of a third order formula of type (1.2) can be achieved in the following three steps:

Step 1: Select functions $\alpha_1(z)$ and $\beta_1(z)$ such that

$$\alpha_1'(0) = \frac{1}{3q_n^2}, \qquad \alpha_1(z) + z\beta_1(z) \equiv R(z). \tag{3.2}$$

Step 2: Select a function $\alpha_2(z)$ such that

$$\alpha_2(0) = 0, \qquad \alpha_2^{(j)}(0) = -\alpha_1^{(j)}(0), \qquad j = 1,2,3. \tag{3.3}$$

Step 3: Define the function $\beta_2(z)$ by

$$\beta_2(z) = -\frac{\alpha_2(z)}{z}. \tag{3.4}$$

One possibility to satisfy relations (3.2) - (3.4) is:

$$\begin{aligned} \alpha_1(z) &= 1 + \frac{1}{3q_n^2} z, \\ \beta_1(z) &= \frac{R(z) - 1}{z} - \frac{1}{3q_n^2}, \\ \alpha_2(z) &= -\frac{1}{3q_n^2} z, \\ \beta_2(z) &= \frac{1}{3q_n^2}. \end{aligned} \tag{3.5}$$

The corresponding integration formula becomes

$$(3.6) \qquad y_{n+1} = y_n + J_n^{-1} [R(h_n J_n)-1]\, f(y_n) + \frac{h_n^3}{3h_{n-1}^2} [J_n(y_n - y_{n-1}) - (f(y_n) - f(y_{n-1}))].$$

We observe that the order h_n^3 term vanishes for linear differential equations. Hence, in the linear case this term can be omitted without reducing the order of accuracy. In case of non-linear equations such a one-point formula is only second order exact. The order h_n term then presents a correction term which makes the formula third order exact. This means that this correction term may serve as an estimate of the non-linearity of the differential equation. Such an estimate is important when one uses a strategy in which the Jacobian matrix J_n is incidentally evaluated in order to save computing time. For instance, one may decide to reevaluate the Jacobian matrix when

$$(3.7) \qquad \frac{h_n^3}{3h_{n-1}^2} ||J(y_n - y_{n-1}) - (f(y_n) - f(y_{n-1}))|| > \eta ||y_{n+1}||,$$

where η is some given tolerance.

Formula (3.6) is one of the possibilities which fits into the class of formulas defined by (3.2) - (3.4). Further research might be done to find formulas in this class with a minimal truncation error.