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ON THE NUMERICAL SOLUTION OF VOLTERRA INTEGRAL EQUATIONS OF THE SECOND KIND. II. RUNGE-KUTTA METHODS

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On the numerical solution of Volterra integral equations of the second kind II Runge-Kutta methods

by

P.J. van der Houwen & J.G. Blom

ABSTRACT

The purpose of this paper is to present the stability regions of a number of Runge-Kutta methods for the integration of second kind Volterra integral equations. Unlike the usual stability analysis, the kernel function is allowed to vary linearly with the independent variable. A second aim of the paper is to show that the addition of certain terms in the numerical formula increases the stability regions considerably.

KEYWORDS & PHRASES: Integral equations, Volterra, stability regions, Runge-Kutta type formulas

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1. INTRODUCTION

In [4] stability conditions were derived for multistep and Runge-Kutta type methods when applied to second kind Volterra integral equations

(1.1)
$$f(x) = g(x) + \int_{x_0}^{x} K(x,\xi,f(\xi))d\xi,$$

with kernel functions K approximately satisfying the relations

(1.2)
$$\frac{\partial^2 K}{\partial f \partial \xi} = 0, \ \frac{\partial^2 K}{\partial f^2} = 0, \ \frac{\partial^2 K}{\partial f \partial x} = \text{constant}.$$

In addition, a modification of both multistep and Runge-Kutta methods was proposed of which it was claimed to have a stabilizing effect. In this paper, a number of Runge-Kutta methods are analyzed with respect to their stability regions. It turns out that in all cases the modified forms do have larger stability regions, sometimes to a considerable extent.

2. SINGLE-STEP METHODS

In this section we present integration formulas of the form (cf.[4])

(2.1)
$$f_{n+1}^{(0)} = f_{n};$$
$$f_{n+1}^{(j)} = \widetilde{F}_{n}(x_{n}+\mu_{j}h_{n}) + h_{n} \sum_{\ell=0}^{m} \lambda_{j\ell} K(x_{n}+\theta_{j\ell}h_{n}, x_{n}+\nu_{j\ell}h_{n}, f_{n+1}^{(\ell)}),$$
$$j = 1, 2, \dots, m;$$

$$f_{n+1} = f_{n+1}^{(m)}, \quad \mu_m = \theta_{m\ell} = 1, \quad \ell = 0(1)m,$$

where $\tilde{F}_{n}(x)$ is an approximation to the expression $g(x) + \int_{x_{0}}^{x_{n}} K(x,\xi,\tilde{f}(\xi))d\xi,$ $\tilde{f}(x)$ denoting an interpolation function through f_0, f_1, \ldots, f_n . In the following we assume that the weights w_{nj} define a quadrature rule of the form

(2.2) $\int_{x_0}^{n} \phi(x) dx = \sum_{j=0}^{n} w_{nj} \phi(x_j) + R_n.$

For each formula we will specify:

(1) The order of the quadrature error: $R_n = \tilde{F}_n(x) - g(x) - \int_{x_0}^{x_n} K(x,\xi,\tilde{f}(\xi))d\xi$ (2) The order of the truncation error: $T_n = f_{n+1}^* - f(x_{n+1})$, where f_{n+1}^* is the solution of (2.1) when $\tilde{F}_n(x)$ is replaced by $g(x) + \int_{x_0}^{x_n} K(x,\xi,f(\xi))d\xi$ and f_n by $f(x_n)$.

(3) The characteristic equation:

 $C(\zeta) = 0$, the roots of which are the amplification factors by which perturbations are amplified when the integrationformula is applied to the model problem (1.2).

(4) The stability region:

 $|\zeta| \leq 1$

2.1. Summary of the theory

To scheme (2.1) we may associate (internal) stability functions:

DEFINITION 2.1. The (internal) stability functions $Q_m(z,y)$, $R_m(z,y)$ and $S_m(z,y)$ of scheme (2.1) are defined by the recurrence relations

$$Q_{0}(z,y) = 1, \quad Q_{j}(z,y) = \sum_{\ell=0}^{m} \lambda_{j\ell}(z+\theta_{j\ell}y)Q_{\ell}(z,y)$$

$$(2.3) \quad R_{0}(z,y) = 0, \quad R_{j}(z,y) = 1 + \sum_{\ell=0}^{m} \lambda_{j\ell}(z+\theta_{j\ell}y)R_{\ell}(z,y), \quad j = 1(1)m.$$

$$S_{0}(z,y) = 0, \quad S_{j}(z,y) = \mu_{j} + \sum_{\ell=0}^{m} \lambda_{j\ell}(z+\theta_{j\ell}y)S_{\ell}(z,y)$$

THEOREM 2.1. Let $\tilde{F}_n(x)$ be defined by

(2.4)
$$\widetilde{F}_{n}(x) = g(x) + \sum_{j=0}^{n} w_{nj}K(x,x_{j},f_{j}),$$
$$\Delta w_{nj} = w_{n+1j} - w_{nj} = 0, \qquad j = 0(1)\overline{n} - 1,$$

then

(a)
$$f(x_{n+1}) - f_{n+1} = O(R_n) + O(T_n)$$
 as $h \to 0$.

When, in addition

(2.7) Δf_j are sufficiently small perturbations of f_j , j = 0(1)n, then (b) $A_n \Delta \vec{\nabla}_{n+1} = B_n \Delta \vec{\nabla}_n$,

where

(2.8)
$$\Delta \vec{V}_{n} = (\Delta f_{n}, \dots, \Delta f_{\overline{n}}, \Delta \widetilde{F}_{n}(x_{n}), \sum_{j=0}^{n} w_{nj} K_{xf}(x_{n}, x_{j}, f_{j}) \Delta f_{j})^{\mathsf{T}},$$

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and

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$$(2.10) \quad B_{n} = \begin{pmatrix} Q_{m} & 0 & R_{m} & h_{n}S_{m} \\ 1 & 0 & 0 & 0 \\ & \vdots & \vdots & \vdots \\ & & 1 & 0 & 0 & 0 \\ \Delta w_{nn}J_{n} & \ddots & \ddots & \Delta w_{nn}J_{n} & 1 & 0 \\ \Delta w_{nn}H_{n} & \ddots & \ddots & \Delta w_{nn}H_{n} & 0 & 1 \end{pmatrix}$$

$$Q_{m}, R_{m} \text{ and } S_{m} \text{ being evaluated at}$$

$$(z,y) = (h_{n}J_{n}, h_{n}^{2}H_{n}) = (h_{n}J(x_{n}, x_{n}, f_{n}), h_{n}^{2}H(x_{n}, x_{n}, f_{n})).$$

<u>PROOF</u>. See [4].

THEOREM 2.2. Let $\widetilde{F}_n(x)$ be defined by

(2.11)
$$\widetilde{F}_{n}(x) = g(x) + \sum_{j=0}^{n} w_{nj} K(x, x_{j}, f_{j}) + \left[f_{n} - g_{n} - \sum_{j=0}^{n} w_{nj} K(x_{n}, x_{j}, f_{j}) \right],$$
$$\Delta w_{nj} = w_{n+1j} - w_{nj} = 0, \quad j = 0(1)\overline{n} - 1,$$

then

(a)
$$f(x_{n+1}) - f_{n+1} = O(h^{-1}T_n) + O(R_n) \ as \ h \neq 0$$
,

when, in addition, conditions (2.5), (2.6) and (2.7) are satisfied, then

(b)
$$A_n \triangle \vec{V}_{n+1} = B_n \triangle \vec{V}_n$$
,

where

(2.13)
$$\Delta \vec{\Psi}_{n} = (\Delta f_{n}, \dots, \Delta f_{n}, \sum_{j=0}^{n} w_{nj} K_{xf}(x_{n}, x_{j}, f_{j}) \Delta f_{j})^{\mathsf{T}},$$
(2.14)
$$A_{n} = \begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & \ddots & & \\ & & & 1 & 0 \\ -w_{n+1n+1}H_{n} & 0 & \ddots & \ddots & 0 & 1 \end{pmatrix}$$

and

PROOF. See [4]

THEOREM 2.3. Let $\widetilde{F}_n(x)$ be defined by

(2.16)
$$\widetilde{F}_{n}(x) = g(x) + \sum_{j=0}^{n-1} \sum_{\ell=0}^{m} w_{nj}^{(\ell)} K(x, x_{j+1}^{(\ell)}, f_{j+1}^{(\ell)}), \\ \Delta w_{nj}^{(\ell)} = w_{n+1j}^{(\ell)} - w_{nj}^{(\ell)} = 0, \quad j = 0(1)n-1, \quad \ell = 0(1)m,$$

then

(a)
$$f(x_{n+1}) - f_{n+1} = O(T_n) + O(R_n) \text{ as } h \to 0.$$

When, in addition, conditions (2.5), (2,6) and (2.7) are satisfied then

(b)
$$A_n \triangle \vec{V}_{n+1} = B_n \triangle \vec{V}_n$$
,

where

(2.18) $\Delta \vec{V}_{n} = (\Delta f_{n}^{(1)}, \dots, \Delta f_{n}^{(m)}, \Delta \widetilde{F}_{n}(x_{n}), \\ \sum_{j=0}^{n-1} \sum_{\ell=0}^{m} w_{nj}^{(\ell)} K_{xf}(x_{n}, x_{j+1}^{(\ell)}, f_{j+1}^{(\ell)}) \Delta f_{j+1}^{(\ell)})^{T}.$



and

$$(2.20) B_{n} = \begin{pmatrix} 0 & \cdots & 0 & h_{n}^{\lambda} 10^{J} 10 & 1 & \mu_{1} h_{n} \\ \cdot & & \cdot & \cdot & \cdot \\ \cdot & & \cdot & \cdot & \cdot \\ 0 & \cdots & 0 & h_{n}^{\lambda} 0^{J} 0 & 1 & \mu_{m} h_{n} \\ 0 & \cdots & 0 & -w_{n+1n}^{(0)} J_{n} & -1 & 0 \\ 0 & \cdots & 0 & -w_{n+1n}^{(0)} H_{n} & 0 & -1 \end{pmatrix}$$

with $J_{j\ell} = J_n + \theta_{j\ell}h_nH_n$.

<u>PROOF</u>. (a) This statement was proved by *de Hoog and Weiss* [2]. (b) From the definition of $\tilde{F}_n(x)$ and conditions (2.5), (2.6) and (2.7) it follows that

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$$\begin{split} \Delta \widetilde{F}_{n}(\mathbf{x}) &\cong \sum_{\substack{j=0 \ \ell=0}}^{n-1} \sum_{\substack{w \ nj}}^{m} w_{nj}^{(\ell)} \frac{\partial K}{\partial f} (\mathbf{x}, \mathbf{x}_{j+1}^{(\ell)}, \mathbf{f}_{j+1}^{(\ell)}) \Delta \mathbf{f}_{j+1}^{(\ell)} \\ &\cong \sum_{\substack{j=0 \ \ell=0}}^{n-1} \sum_{\substack{w \ nj}}^{m} w_{nj}^{(\ell)} \left[\frac{\partial K}{\partial f} (\mathbf{x}_{n}, \mathbf{x}_{j+1}^{(\ell)}, \mathbf{f}_{j+1}^{(\ell)}) + (\mathbf{x}-\mathbf{x}_{n}) \frac{\partial^{2} K}{\partial \mathbf{x} \partial f} (\mathbf{x}_{n}, \mathbf{x}_{j+1}^{(\ell)}, \mathbf{f}_{j+1}^{(\ell)}) \right] \Delta \mathbf{f}_{j+1}^{(\ell)} \\ &= \Delta \widetilde{F}_{n}(\mathbf{x}_{n}) + (\mathbf{x}-\mathbf{x}_{n}) \Delta \mathbf{G}_{n}, \end{split}$$

where we have written

$$\Delta G_{n} = \sum_{j=0}^{n-1} \sum_{\ell=0}^{m} w_{nj}^{(\ell)} \frac{\partial^{2} K}{\partial x \partial f} (x_{n}, x_{j+1}^{(\ell)}, f_{j+1}^{(\ell)}) \Delta f_{j+1}^{(\ell)}.$$

Is is easily seen that the following relations hold:

$$\Delta f_{n+1}^{(j)} \cong \Delta \widetilde{F}_{n}(\mathbf{x}_{n}) + \mu_{j}h_{n}\Delta G_{n} + h_{n} \sum_{\ell=0}^{m} \lambda_{j\ell} \Big[J_{n} + \theta_{j\ell}h_{n}H_{n} \Big] \Delta f_{n+1}^{(\ell)},$$

$$\Delta \widetilde{F}_{n+1}(\mathbf{x}_{n+1}) \cong \Delta \widetilde{F}_{n}(\mathbf{x}_{n}) + h_{n}\Delta G_{n+1} + \sum_{\ell=0}^{m} w_{n+1n}^{(\ell)} J_{n}\Delta f_{n+1}^{(\ell)},$$

$$\Delta G_{n+1} \cong \Delta G_{n} + H_{n} \sum_{\ell=0}^{m} w_{n+1n}^{(\ell)} \Delta f_{n+1}^{(\ell)}.$$

These equations are easily verified to be identical to the vector equation $A_n \Delta \vec{\nabla}_{n+1} = B_n \Delta \vec{\nabla}_n$ of the theorem. \Box

DEFINITION 2.2. The characteristic equation of scheme (2.1) is defined by (2.21) det $(B_n - \zeta A_n) = 0$.

2.2. Simpson-Runge-Kutta formulas

Let $\tilde{F}_n(x)$ be defined by (2.4) using repeated Simpson rule for even values of n, and by repeated Simpson + $\frac{3}{8}$ rule for odd values of n > 1. The matrix W = (w_{nj}) , n = 2,3,..., j = 0(1)n is then defined by (constant step sizes)

$$(2.22) \quad W = \frac{h}{24} \begin{pmatrix} 8 & 32 & 8 \\ 9 & 27 & 27 & 9 \\ 8 & 32 & 16 & 32 & 8 \\ \cdot & \cdot & 17 & 27 & 27 & 9 \\ \cdot & \cdot & & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & 17 & 27 & 27 & 9 \\ \cdot & \cdot & & & \cdot & \cdot \\ \cdot & \cdot & \cdot & & 17 & 27 & 27 & 9 \\ 8 & 32 & 16 & 32 & \cdots & 16 & 32 & 16 & 32 & 8 \end{pmatrix}$$

For n = 1 we may define

(2.23)
$$\widetilde{F}_{1}(x) = g(x) + h \sum_{\ell=0}^{m} \lambda_{j\ell} K (x_{0}^{+\theta} j_{\ell} h, x_{0}^{+\nu} j_{\ell} h, f_{1}^{(\ell)}).$$

We shall call the class of formulas defined by (2.1), (2.4) and (2.22) Simpson-Runge-Kutta formulas.

The quadrature error ${\tt R}_{\tt n}$ of this class behaves as

(2.24)
$$R_n = O(h^4) \text{ as } h \to 0.$$

The characteristic equation (2.21) for the case where $h_n J_n$ and $h_n^2 H_n$ have a common set of eigenvectors with eigenvalues z and y, was derived in [4]. By working out the determinant we find for *odd* values of n the polynomial

$$\zeta^{6} - [2 + Q_{m} + \frac{1}{3} zR_{m} + \frac{1}{3} yR_{m} + \frac{1}{3} yS_{m}] \zeta^{5}$$

$$+ [1 + 2Q_{m} - \frac{23}{24} yR_{m} - \frac{5}{8} zR_{m} - \frac{5}{8} yS_{m}] \zeta^{4}$$

$$+ [- Q_{m} + \frac{17}{12} zR_{m} + \frac{11}{24} yR_{m} + \frac{17}{12} yS_{m}] \zeta^{3}$$

$$(2.25a) - [\frac{2}{3} zR_{m} + \frac{5}{24} yR_{m} + \frac{2}{3} yS_{m}] \zeta^{2}$$

$$+ [\frac{1}{4} zR_{m} + \frac{1}{24} yR_{m} + \frac{1}{4} yS_{m}] \zeta$$

$$- [\frac{1}{24} zR_{m} + \frac{1}{24} yR_{m} + \frac{1}{24} yS_{m}] = 0.$$

For even values we find

$$C(\zeta) = \zeta^{5} - [2 + Q_{m} + \frac{3}{8} zR_{m} + \frac{3}{8} yR_{m} + \frac{3}{8} yS_{m}] \zeta^{4}$$

$$+ [1 + 2Q_{m} - \frac{5}{12} zR_{m} - \frac{19}{24} yR_{m} - \frac{5}{12} yS_{m}] \zeta^{3}$$

$$(2.25b) + [-Q_{m} + zR_{m} + \frac{5}{24} yR_{m} + yS_{m}] \zeta^{2}$$

$$- [\frac{1}{4} zR_{m} + \frac{1}{24} yR_{m} + \frac{1}{4} yS_{m}] \zeta$$

$$+ [\frac{1}{24} zR_{m} + \frac{1}{24} yR_{m} + \frac{1}{24} yS_{m}] = 0.$$

When we use (2.11) instead of (2.4) for the calculation of $\tilde{F}_n(x)$, the same order relation (2.24) for the quadrature error is obtained. The characteristic equation (2.21) is obtained by application of theorem (2.2). Omitting the details we finally find for *odd* values of n

$$\zeta^{5} - [1 + Q_{m} + R_{m} + \frac{1}{3} yS_{m}] \zeta^{4}$$

$$(2.25a') + [Q_{m} + R_{m} - \frac{23}{24} yS_{m}] \zeta^{3}$$

$$+ \frac{11}{24} yS_{m}\zeta^{2} - \frac{5}{24} yS_{m}\zeta + \frac{1}{24} yS_{m} = 0,$$

and for even values of n

$$\zeta^{4} - [1 + Q_{m} + R_{m} + \frac{3}{8} yS_{m}] \zeta^{3}$$

$$(2.25b') + [Q_{m} + R_{m} - \frac{19}{24} yS_{m}] \zeta^{2}$$

$$+ \frac{5}{24} yS_{m}\zeta - \frac{1}{24} yS_{m} = 0.$$

In the following we only present the stability region $|\zeta(z,y)| \leq 1$ in the *third* quadrant of the (z,y)-plane since the integral equation itself is only stable in that area (cf. [4]).

2.2.1. Explicit formulas

When $\lambda_{jl} = 0$ for $l \ge j$ scheme (2.1) does not require the solution of implicit equations. From a computational point of view such formulas may be attractive when no instabilities are developed.

Third and fourth order Simpson-Beltjukov formulas

In [1] Beltjukov gives a formula in which $(j=1(1)3, \ell = 0(1)3)$

$$(\lambda_{j\ell}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/9 & 2/9 & 0 & 0 \\ 0 & 1/4 & 3/4 & 0 \end{pmatrix}, \quad (\theta_{j\ell}) = \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix},$$

$$(2.26) \qquad \qquad (\nu_{j\ell}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1/3 & 0 \end{pmatrix}, \quad (\mu_{j}) = \begin{pmatrix} 1 \\ 1/3 \\ 1 \end{pmatrix}.$$

The truncation error of this formula behaves as

(2.27)
$$T_n = O(h^4) \text{ as } h \to 0.$$

Thus, by virtue of (2.24), (2.27) and theorem 2.1 we may conclude that (2.4), (2.22), (2.23) and (2.26) generate a *fourth order* Simpson-Runge-Kutta formula. Its stability functions are easily found to be (apply (2.3))

(2.28)

$$Q_{3}(z,y) = \frac{1}{6} (z+y) (z+\frac{1}{2}y) (2+z+y),$$

$$R_{3}(z,y) = 1 + \frac{1}{6} (z+y) (6+z+y),$$

$$S_{3}(z,y) = 1 + \frac{1}{6} (z+y) (3+z+y).$$

In a similar way we conclude from theorem 2.2 that (2.11), (2.22), (2.23) and (2.26) generate a *third order* Simpson-Runge-Kutta formula.



Fig 2.1 Stability region of the Beltjukov-Simpson formula

The stability regions $|\zeta| \leq 1$, ζ being the roots of (2.25) and (2.25'), respectively, are the inside areas in the third quadrant bounded by the solid and broken lines, respectively. In the latter case the overall region of stability is given by the intersection of these two ares (n even and n odd). In the next figures the same conventions are used.

Fourth order Simpson-Pouzet formulas

Presumably the first Runge-Kutta type formula was given by *Pouzet* [3] in 1960. Its parameter matrices are

$$(\lambda_{j\ell}) = \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1/6 & 1/3 & 1/3 & 1/6 & 0 \end{pmatrix}, \quad (\theta_{j\ell}) = \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

$$(\nu_{j\ell}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 1/2 & 1 & 0 \end{pmatrix}, \quad (\mu_{j}) = \begin{pmatrix} 1/2 \\ 1/2 \\ 1 \\ 1 \end{pmatrix},$$

The truncation error is given by

(2.30)
$$T_n = O(h^5) \text{ as } h \to 0.$$

Hence, (2.4), (2.22), (2.23) and (2.29) generate a *fourth order* Simpson -Runge-Kutta formula. Replacing (2.4) by (2.11) again yields a *fourth order* formula.

The stability polynomials are given by

 $Q_{4}(z,y) = \frac{1}{6} (z+y) \{ 1 + (z+\frac{1}{2}y) [1+\frac{1}{2}(z+\frac{1}{2}y)(1+\frac{1}{2}z+\frac{1}{2}y)] \},$ $(2.31) \qquad R_{4}(z,y) = 1 + \frac{1}{6} (z+y) \{ 3 + (1+\frac{1}{2}z+\frac{1}{4}y)(2+z+y) \},$ $S_{4}(z,y) = 1 + \frac{1}{6} (z+y) \{ 2 + (1+\frac{1}{2}z+\frac{1}{4}y)(1+\frac{1}{2}z+\frac{1}{2}y) \}.$

The corresponding stability regions are shown in figure 2.2. by the solid and broken line, respectively.



Fig 2.2 Stability region of the Simpson-Pouzet formula

A fast third order formula and its stabilized second order modification

The formulas of Beltjukov and Pouzet both require two evaluations of the function $\widetilde{F}_n(x)$ in each integration step. Since these evaluations form the bulk of the computational effort, it is suggested to look for formulas which require only one evaluation of $\widetilde{F}_n(x)$ per integration step. This is achieved by choosing $\mu_j = 1$ for j = 1(1)m. Let us consider the class of explicit, two-stage formulas, i.e. m = 2, $\lambda_{jl} = 0$, for $l \ge j$. From [4, eq.(3.6)-(3.9)] we may derive that this class is *second order* consistent, i.e.

(2.32)
$$T_n = O(h^3)$$
 as $h \to 0$,

provided that

$$\begin{split} \lambda_{20} &+ \lambda_{21} = 1, \\ \nu_{20}\lambda_{20} &+ \nu_{21}\lambda_{21} = \frac{1}{2}, \\ \lambda_{10}\lambda_{21} &= \frac{1}{2}, \\ \lambda_{21} &= \frac{1}{2}. \end{split}$$

These equations lead to the following parameter matrices

(2.33)
$$\begin{aligned} &(\lambda_{j\ell}) = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} , \ (\mu_{j}) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \ (\theta_{j\ell}) = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix} \\ &(\nu_{j\ell}) = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix} . \end{aligned}$$

Thus, (2.4), (2.22), (2.23) and (2.29) generate a *third order* Simpson-Runge-Kutta formula which is roughly twice as cheap as the fourth order formulas of Beltjukov and Pouzet. Replacing (2.4) by (2.11) decreases the order by one but yields a larger stability region as may be derived by substituting the functions

(2.34)
$$Q_{2}(z,y) = \frac{1}{2}(z+y)(1+z+y),$$
$$R_{2}(z,y) = S_{2}(z,y) = 1 + \frac{1}{2}z + \frac{1}{2}y,$$

into the characteristic equations (2.25) and (2.25'). The stability regions are given in figure 2.3 by the solid and broken lines, respectively.



Fig 2.3 Stability region corresponding to (2.33)

An adaptive third order formula

The relatively small stability region of formula (2.33) leads us to consider higher point formulas (again with $\mu_j = 1$ for j = 1(1)m and to use the extra parameters to enlarge the stability region. For m = 3 the conditions for a third order truncation error T_n become [4]

$$\begin{split} &\lambda_{30} + \lambda_{31} + \lambda_{32} = 1, \\ &\nu_{30}\lambda_{30} + \nu_{31}\lambda_{31} + \nu_{32}\lambda_{32} = \frac{1}{2}, \\ &\lambda_{31} + \lambda_{32} = \frac{1}{2}, \\ &\lambda_{10}\lambda_{31} + (\lambda_{20}+\lambda_{21})\lambda_{32} = \frac{1}{2}. \end{split}$$

It is easily verified that the parameter matrices

satisfy the consistency conditions irrespective the values of λ_{10} and λ_{21} . The stability functions of scheme (2.35) read

(2.36)

$$Q_{3}(z,y) = \frac{1}{2}(z+y)[1 + (1-\lambda_{21})(z+y) + \lambda_{10}\lambda_{21}(z+y)^{2}]$$

$$R_{3}(z,y) = S_{3}(z,y) = 1 + \frac{1}{2}(z+y) + \frac{1}{2}\lambda_{21}(z+y)^{2}$$

Since λ_{10} and λ_{21} are free parameters we may use them to monitor the amplification factors corresponding to a particular eigenvector component in the perturbations Δf_i , i = 0(1)n. For instance, when the matrices $h_n J_n$ and $h_n^2 H_n$ has the eigenvalues z_0 and y_0 for this eigenvector, we may choose λ_{10} and λ_{21} such that

(2.37)
$$Q_3(z_0, y_0) = R_3(z_0, y_0) = S_3(z_0, y_0) = 0,$$

yielding the amplification factors $\zeta_1 = \zeta_2 = \zeta_3 = \zeta_4 = 0$, $\zeta_5 = \zeta_6 = 1$ for odd values of n (cf.(2.25a)) and $\zeta_1 = \zeta_2 = \zeta_3 = 0$, $\zeta_4 = \zeta_5 = 1$ for even

values of n (cf.(2.25b)). In the case of *scalar* integral equations where J_n and H_n have only one eigenvector, condition (2.37) would give *unconditional stability*. It is easily seen that (2.37) is solved by

(2.37')
$$\lambda_{10} = \frac{1 + (z_0 + y_0) + \frac{1}{2}(z_0 + y_0)^2}{(z_0 + y_0)(1 + \frac{1}{2}(z_0 + y_0))}, \lambda_{21} = -\frac{2 + z_0 + y_0}{(z_0 + y_0)^2}.$$



Fig 2.4 Parameters λ_{10} and λ_{21} as functions of $z_0 + y_0$

In figure 2.4 the behaviour of λ_{10} and λ_{21} as functions of $z_0 + y_0$ is shown revealing that λ_{10} becomes singular at $z_0 + y_0 = -2$ and $z_0 + y_0 = 0$, and λ_{21} becomes singular at $z_0 + y_0 = 0$. Let us choose

(2.38)
$$\begin{array}{l} \lambda_{21} = -1 \ \text{for } z_0 + y_0 \geq -1 \\ \lambda_{21} \ \text{according to} \ (2.37') \ \text{for } z_0 + y_0 \leq -1 \end{array} ,$$

and let λ_{10} be free for the moment. In the region $z_0 + y_0 \le -1$ the characteristic equations (2.25a) and (2.25b) then reduce to (at (z_0, y_0))

$$(2.25') \qquad \zeta^{3} - (2+Q_{3}(z_{0},y_{0}))\zeta^{2} + (1+2Q_{3}(z_{0},y_{0}))\zeta - Q_{3}(z_{0},y_{0}) = 0$$

which may be written in the form

$$(\zeta-1)(\zeta^2-(1+Q_3(z_0,y_0))\zeta + Q_3(z_0,y_0)) = 0.$$

The roots are within or on the unit circle when

$$|Q_3(z_0,y_0)| \le 1, \quad z_0 + y_0 \le -1$$

where

$$Q_{3}(z_{0}, y_{0}) = \frac{1}{2} [(1 - \lambda_{10})(z_{0} + y_{0})^{2} + 2(1 - \lambda_{10})(z_{0} + y_{0}) + 2],$$

$$z_{0} + y_{0} \leq -1$$

Let us choose

(2.39)
$$\lambda_{10} = 2 \quad \text{for } z_0 + y_0 \ge -1 - \sqrt{3}$$
$$\lambda_{10} \text{ according to } (2.37') \quad \text{for } z_0 + y_0 \le -1 - \sqrt{3}$$

Then the amplification factors corresponding to all points (z_0, y_0) with $z_0 + y_0 \leq -2$ (in figure 2.5 indicated by the dotted area) are less than or equal to unity in absolute value. When the point (z_0, y_0) to which the scheme is to be adapted is such that $z_0 + y_0 \geq -1$ we have $\lambda_{10} = 2$ and $\lambda_{21} = -1$ the stability region of which is shown in figure 2.5 by the shaded area. Thus, the formula defined by (2.35), (2.38) and (2.39) is unstable when (z_0, y_0) lies in the blanc region in figure 2.5, which is approximately given by

$$z_0 + y_0 \le -2$$
, $6y_0 + 4z_0 \ge -3$.

This leads to a small region of "forbidden" values for the integration step h.



Fig 2.5 Stability region corresponding to (2.35) with λ_{10} and λ_{21} defined by (2.38) and (2.39).

2.2.2. Weakly implicit formulas

When $\lambda_{jl} = 0$ for l > j scheme (2.1) requires the successive solution of at most m equations. Whe shall call such schemes *weakly implicit* to distinguish them from *fully implicit* schemes which require the solution of m simultaneous equations.

A third order one-point formula and its stabilized second order modification

For m = 1 the conditions for second order consistency, i.e.

(2.40) $T_n = 0(h^3)$ as $h \to 0$, read (cf.[4])

$$\lambda_{10} + \lambda_{11} = 1 \nu_{10}\lambda_{10} + \nu_{11}\lambda_{11} = \frac{1}{2}, \lambda_{11} = \frac{1}{2}$$

which lead to the parameter matrices

(2.41)
$$\begin{aligned} & (\lambda_{j\ell}) = (\frac{1}{2}, \frac{1}{2}), \quad (\mu_j) = (1), \quad (\theta_{j\ell}) = (1, 1), \\ & (\nu_{j\ell}) = (\nu_{10}, 1 - \nu_{10}) \end{aligned}$$

with stability functions

(2.42)
$$Q_{1}(z,y) = \frac{z+y}{2-(z+y)},$$
$$R_{1}(z,y) = S_{1}(z,y) = \frac{2}{2-(z+y)}.$$

The stability regions corresponding to (2.4) (solid lines) and (2.11) (broken lines) are presented in figures 2.6 and 2.6'.



Fig 2.6 Stability region corresponding to (2.41)



Fig 2.6' Stability region corresponding to (2.41)

"Two point" formulas of fourth order and their stabilized third order modifications

First of all we remark that fourth order formulas require at least two \tilde{F}_n -evaluations. This may be concluded from the following three consistency conditions (cf.[4]

$$\mu_{m} = 1,$$

$$\sum_{\ell=1}^{m} \lambda_{m\ell} \mu_{\ell} = \frac{1}{2},$$

$$\sum_{\ell=1}^{m} \lambda_{m\ell} \mu_{\ell}^{2} = \frac{1}{3}.$$

Since μ_m is already fixed at the value 1, at least one μ_{ℓ} should differ from 0 or 1 in order to satisfy these conditions.

Secondly, for m = 1 no third order formulas exist. This follows from the following two consistency conditions (follow from the fourth and eighth condition of equations (3.6) - (3.9) in [4])

$$\begin{array}{rl} \lambda_{11} &= \frac{1}{2} \\ \frac{1}{2} \lambda_{11} &= \frac{1}{6} \end{array},$$

$$\begin{split} \lambda_{20} + \lambda_{21} + \lambda_{22} &= 1, \\ \nu_{20}\lambda_{20} + \nu_{21}\lambda_{21} + \nu_{22}\lambda_{22} &= \frac{1}{2}, \\ \mu_{1}\lambda_{21} + \lambda_{22} &= \frac{1}{2}, \\ (\lambda_{10}+\lambda_{11})\lambda_{21} + \lambda_{22} &= \frac{1}{2}, \\ \mu_{1}^{2}\lambda_{21} + \lambda_{22} &= \frac{1}{3}, \\ (\lambda_{10}\nu_{10}+\lambda_{11}\nu_{11})\lambda_{21} + \frac{1}{2}\lambda_{22} &= \frac{1}{6}, \\ \lambda_{11}\mu_{1}\lambda_{21} + \frac{1}{2}\lambda_{22} &= \frac{1}{6}, \\ \lambda_{11}(\lambda_{10}+\lambda_{11})\lambda_{21} + \frac{1}{2}\lambda_{22} &= \frac{1}{6}, \\ \nu_{20}^{2}\lambda_{20} + \nu_{21}^{2}\lambda_{21} + \nu_{22}^{2}\lambda_{22} &= \frac{1}{3}, \\ \nu_{21}\mu_{1}\lambda_{21} + \nu_{22}\lambda_{22} &= \frac{1}{3}, \\ \nu_{21}(\lambda_{10}+\lambda_{11})\lambda_{21} + \nu_{22}\lambda_{22} &= \frac{1}{3}, \\ \lambda_{21}(\lambda_{10}+\lambda_{11})\lambda_{21} + \lambda_{22} &= \frac{1}{3}, \\ \mu_{1}(\lambda_{10}+\lambda_{11})\lambda_{21} + \lambda_{22} &= \frac{1}{3}, \\ \nu_{21}\lambda_{21} + \nu_{22}\lambda_{22} &= \frac{1}{3}, \\ \nu_{21}\lambda_{21} + \nu_{22}\lambda_{22} &= \frac{1}{2}. \end{split}$$

These equations are greatly simplified when we put (2.43) $\lambda_{20} = 0$, $\mu_1 = \lambda_{10} + \lambda_{11}$. This immediately yields

(2.44) $\mu_2 = 1$, $\mu_1 = \frac{1}{3}$, $\lambda_{21} = \frac{3}{4}$, $\lambda_{22} = \frac{1}{4}$.

Substitution into the remaining equations leads to the conditions

 $3v_{21} + v_{22} = 2$, $v_{21} + v_{22} = \frac{4}{3}$, $\lambda_{10} + \lambda_{11} = \frac{1}{3}$, $\lambda_{10} v_{10} + \lambda_{11} v_{11} = \frac{1}{18}$, $\lambda_{11} = \frac{1}{6}$, $3v_{21}^2 + v_{22}^2 = \frac{4}{3}$, $\lambda_{10}^{\theta}_{10} + \lambda_{11}^{\theta}_{11} = \frac{1}{9}$,

which finally result in the parameter matrices

$$(\lambda_{j\ell}) = \begin{pmatrix} \frac{1}{6} & \frac{1}{6} & 0 \\ 0 & \frac{3}{4} & \frac{1}{4} \end{pmatrix}, \quad (\mu_j) = \begin{pmatrix} \frac{1}{3} \\ 1 \end{pmatrix}, \quad (\theta_{j\ell}) = \begin{pmatrix} \theta_{10} & \frac{2}{3} - \theta_{10} & 0 \\ 0 & 1 & 1 \end{pmatrix},$$

$$(2.45) \qquad (\nu_{j\ell}) = \begin{pmatrix} \nu_{10} & \frac{1}{3} - \nu_{10} & 0 \\ 0 & \frac{1}{3} & 1 \end{pmatrix}.$$

,

Together with the approximations (2.4) and (2.11), respectively, these parameters generate a family of fourth order and third order Simpson-Runge-Kutta formulas with stability functions

$$Q_{2}(z,y) = \frac{3(z+y)}{4 - (z+y)} \frac{z + \theta_{10}y}{6 - z - (\frac{2}{3} - \theta_{10})y},$$

$$(2.46) \qquad R_{2}(z,y) = \frac{1}{4 - (z+y)} \left[4 + \frac{18(z+y)}{6 - z - (\frac{2}{3} - \theta_{10})y} \right],$$

$$S_{2}(z,y) = \frac{1}{4 - (z+y)} \left[4 + \frac{6(z+y)}{6 - z - (\frac{2}{3} - \theta_{10})y} \right].$$

In figure 2.7 the stability regions are shown for $\theta_{10} = \frac{1}{3}$.



Fig.2.7 Stability region corresponding to (2.45) with $\theta_{10} = \frac{1}{3}$.

The formulas (2.45) require the solution of two equations in one variable. It was pointed out by Schilder [5] that it is possible to construct formulas, which require the solution of only one equation in a single variable. It is easily verified that the matrices

$$(2.47) \qquad (\lambda_{j\ell}) = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0\\ \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}, \qquad (\mu_j) = \begin{pmatrix} \frac{2}{3}\\ 1 \end{pmatrix}, \qquad (\theta_{j\ell}) = \begin{pmatrix} \theta_{10} & \frac{4}{3} - \theta_{10} & 0\\ 1 & 1 & 1 \end{pmatrix}, (\nu_{j\ell}) = \begin{pmatrix} \nu_{10} & \frac{2}{3} - \nu_{10} & 0\\ 0 & \frac{2}{3} & 0 \end{pmatrix}$$

together with respectively (2.4) and (2.11), generate a *fourth* and *third* order formula with stability functions

$$Q_{2}(z,y) = \frac{1}{4} (z+y) \left[1 + \frac{3(z+\theta_{10}y)}{3-z-(\frac{4}{3}-\theta_{10})y} \right],$$

$$(2.48) \qquad R_{2}(z,y) = 1 + \frac{9(z+y)}{4(3-z-(\frac{4}{3}-\theta_{10})y)},$$

$$S_{2}(z,y) = 1 + \frac{3(z+y)}{2(3-z-(\frac{4}{3}-\theta_{10})y)}.$$

In figure 2.8 the stability regions are given for $\theta_{10} = \frac{2}{3}$.



Fig 2.8 Stability region corresponding to (2.47) with $\theta_{10} = \frac{2}{3}$

Fourth order Simpson-Newton-Cotes formula and its third order stabilization

Instead of solving consistency conditions, one may construct formulas by using quadrature rules. Let us consider formulas where (j=1(1)m)x +u.h

(2.49)
$$f_{n+1}^{(j)} \stackrel{\sim}{=} \widetilde{F}_n^{(x_n+\mu_jh_n)} + \int_{x_n}^{n+j} K(x_n + \mu_jh_n, x, \widetilde{f}(x)) dx,$$

where $\mu_m = 1$ and $\tilde{f}(x)$ denotes an interpolation function through $f_{n+1}^{(j)}$. The Runge-Kutta scheme is then obtained by replacing the integral by a quadrature rule. The most simple application of this approach is the use of the trapezoidal rule for $f_{n+1}^{(1)}$ and the Simpson rule for $f_{n+1} = f_{n+1}^{(2)}$. This immediately leads to the parameter matrices

$$(2.50) \qquad (\lambda_{j\bar{\ell}}) = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0\\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{pmatrix}, \quad (\mu_{j}) = \begin{pmatrix} \frac{1}{2}\\ 1 \end{pmatrix}, \quad (\theta_{j\ell}) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0\\ 1 & 1 & 1 \end{pmatrix}, \\ (\nu_{j\ell}) = \begin{pmatrix} 0 & \frac{1}{2} & 0\\ 0 & \frac{1}{2} & 1 \end{pmatrix}, \quad (\mu_{j\ell}) = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} & 0\\ 1 & 1 & 1 \end{pmatrix},$$

The truncation error is obviously of fourth order as $h \rightarrow 0.$ The stability functions become

$$Q_{2}(z,y) = \frac{z+y}{6-(z+y)} \left[1 + \frac{4(z+\frac{1}{2}y)}{4-(z+\frac{1}{2}y)} \right],$$

$$(2.51) \qquad R_{2}(z,y) = \frac{6}{6-(z+y)} \left[1 + \frac{8(z+y)}{3(4-(z+\frac{1}{2}y))} \right],$$

$$S_{2}(z,y) = \frac{6}{6-(z+y)} \left[1 + \frac{4(z+y)}{3(4-(z+\frac{1}{2}y))} \right],$$

from which the stability region in figure 2.9 result.



Fig 2.9 Stability region correponding to (2.50)

Fourth order Simpson-Newton-Cotes formulas

Choosing the reference points $x_n + \mu_j h_n$ at x_n , $x_n + h_n/4$, $x_n + h_n/2$ and at x_{n+1} , and defining $f_{n+1}^{(1)}$ by the trapezoidal rule, $f_{n+1}^{(2)}$ by Simpson's rule at the points $(x_n, x_n + h_n/4, x_n + h_n/2)$, and f_{n+1} by Simpson's rule at the points $(x_n, x_n + h_n/4, x_n + h_n/2)$, we arrive at the parameter matrices

$$(\lambda_{j\ell}) = \begin{pmatrix} \frac{1}{8} & \frac{1}{8} & 0 & 0 \\ \frac{1}{12} & \frac{1}{3} & \frac{1}{12} & 0 \\ \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} \end{pmatrix}, \quad (\mu_{j}) = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 1 \end{pmatrix},$$

$$(2.52)$$

$$(\theta_{j\ell}) = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad (\nu_{j\ell}) = \begin{pmatrix} 0 & \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & 1 \end{pmatrix}$$

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It is easily seen that this formula has a fifth order truncation error so that both combinations (2.4) - (2.52) and (2.11) - (2.52) yield a *fourth* order formula. The stability functions are given by

$$Q_{4}(z,y) = \frac{z+y}{6-z-y} \left[1 + .4 \frac{(2z+y)(32+12z+3y)}{(24-2z-y)(32-4z-y)} \right],$$

$$(2.53) \qquad R_{4}(z,y) = \frac{2}{6-z-y} \left[3 + 16 \frac{(z+y)(96+20z+13y)}{(24-2z-y)(32-4z-y)} \right],$$

$$S_{4}(z,y) = \frac{2}{6-z-y} \left[3 + 8 \frac{(z+y)(96+4z+5y)}{(24-2z-y)(32-4z-y)} \right].$$



Fig 2.10 Stability region corresponding to (2.52)

2.2.3. Fully implicit formulas

Although weakly implicit formulas possess larger stability regions than explicit formulas, provided that the modified form (2.11) of the function $\tilde{F}_n(x)$ is used, we still have no unconditional stability in the region z < 0, y < 0. Therefore, we now consider a few fully implicit formulas.

A fourth order two-point formula and its third order stabilization

By putting $\lambda_{10} = \lambda_{20} = 0$, $\lambda_{11} + \lambda_{12} = \mu_1$ and $\lambda_{22} = \frac{1}{4}$ in the consistency conditions (cf.[4]) the order equations considerably simplify and easily lead to the solution

$$(\lambda_{j\ell}) = \begin{pmatrix} 0 & \frac{5}{12} & -\frac{1}{12} \\ 0 & \frac{3}{4} & \frac{1}{4} \end{pmatrix}, \quad (\mu_j) = \begin{pmatrix} \frac{1}{3} \\ 1 \end{pmatrix}, \quad (\theta_{j\ell}) = \begin{pmatrix} 0 & \theta & 5\theta - \frac{4}{3} \\ 0 & 1 & 1 \end{pmatrix},$$

$$(2.54) \qquad (\nu_{j\ell}) = \begin{pmatrix} 0 & \nu & 5\nu - \frac{2}{3} \\ 0 & \frac{1}{3} & 1 \end{pmatrix},$$

where θ and ν are free parameters. The truncation error behaves as

(2.55)
$$T_n = O(h^4) \text{ as } h \neq 0$$

and, setting $\theta = \frac{1}{3}$, the stability functions become

$$Q_{2}(z,y) = 0$$

(2.56)
$$R_{2}(z,y) = 4 \frac{27(z+y) + (36-15z-5y)}{3(z+y)(3z+y) + (36-15z-5y)(4-z-y)}$$

$$S_{2}(z,y) = 4 \frac{9(z+y) + (36-15z-5y)}{3(z+y)(3z+y) + (36-15z-5y)(4-z-y)}$$

The stability regions are given in figure 2.11.



Fig 2.11 Stability region corresponding to (2.54) with $\theta = \frac{1}{3}$

Fourth order Simpson-Newton-Cotes formulas

Fifth order and higher order truncation errors can be obtained by using quadrature rules and basing the method on formula (2.49). Let us choose the reference points at x_n , $x_n + h_n/2$ and x_{n+1} and define $f_{n+1}^{(1)}$ by a formula with "external" point x_{n+1} and f_{n+1} by Simpson's rule. This leads to a Runge-Kutta method with the parameter matrices

$$(2.57) \qquad (\lambda_{j\ell}) = \begin{pmatrix} \frac{5}{24} & \frac{8}{24} & -\frac{1}{24} \\ \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \end{pmatrix}, \quad (\mu_{j}) = \begin{pmatrix} \frac{1}{2} \\ 1 \end{pmatrix}, \\ (\theta_{j\ell}) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 1 & 1 & 1 \end{pmatrix}, \quad (\nu_{j\ell}) = \begin{pmatrix} 0 & \frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix}.$$

The truncation error is evidently given by

(2.58)
$$T_n = O(h^5)$$
 as $h \to 0$,

so that both (2.4) and (2.11) yield fourth order methods. The stability functions are given by

$$Q_{2}(z,y) = \frac{3(z+y)(4+2z+y)}{2(6-2z-y)(6-z-y) + (z+y)(2z+y)} ,$$

$$(2.59) \qquad R_{2}(z,y) = \frac{12(6-2z-y) + 48(z+y)}{2(6-2z-y)(6-z-y) + (z+y)(2z+y)} ,$$

$$S_{2}(z,y) = \frac{12(6-2z-y) + 24(z+y)}{2(6-2z-y)(6-z-y) + (z+y)(2z+y)} ,$$



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