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P.J. VAN DER HOUWEN

STABILIZED RUNGE-KUTTA METHODS FOR SECOND ORDER DIFFERENTIAL EQUATIONS WITHOUT FIRST DERIVATIVES

2e boerhaavestraat 49 amsterdam

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Stabilized Runge-Kutta methods for second order differential equations without first derivatives

by

P.J. Van Der Houwen

ABSTRACT

Second and third order Runge-Kutta formulas are presented for the integration of systems of second order differential equations without first derivatives. These methods are characterized by their low storage requirements and their relatively large real stability interval which make them suitable for the integration of second order partial differential equations of hyperbolic type. The new methods are compared with the methods which arise when the second order equations are transformed to first order form and treated by stabilized Runge-Kutta methods for first order equations. It turns out that a gain factor larger than 2 and in some formulas up to 4 is obtained.

KEY WORDS & PHRASES: *Runge-Kutta formulas, difference schemes, second order differential equations, hyperbolic equations, extended stability region.*

CONTENTS

1. INTRODUCTION

Runge-Kutta methods for second order differential equations with prescribed initial values are well known in the literature (e.g. ZONNEVELD [1964], FEHLBERG [1972]). So far the investigations of these methods have been mainly concentrated on improvement of the *order of accuracy;* we do not know of any work on the improvement of the *stability region* of Runge-Kutta methods for second order equations. In this paper we start with an investigation of how the stability region can be extended by increasing the number of stages (function evaluations) of the formula. In particular, the maximization of the *negative stability interval* will be considered. This means that the formulas developed in this paper are only relevant for equations where the Jacobian matrix of the right-hand side has negative eigenvalues. The results presented here are only partial. For instance, we did not succeed in analyzing the general case *with* first derivative but had to restrict our considerations to problems of the type

$$\frac{d^2\vec{y}}{dx^2} = \vec{f}(\vec{y}), \tag{1.1}$$

$\vec{y}$ and $d\vec{y}/dx$ being prescribed at $x = x_0$. The conditions for optimally stabilized formulas of second and third order are derived. In the second order case we satisfied these conditions for the general m-point formula; in the third order case we only satisfied the conditions for two-point formulas. The resulting stability conditions are, respectively,

$$h_n \leq \frac{2m}{\sqrt{\sigma(J_1)}} \qquad \text{for } p = 2 \tag{1.2}$$

and

$$h_n \leq \frac{2.66}{\sqrt{\sigma(J_1)}} \qquad \text{for } p = 3,\ m = 2. \tag{1.3}$$

Here, h_n denotes the integration step $x_{n+1} - x_n$ and $\sigma(J_1)$ the spectral radius of the Jacobian matrix J_1 of the function $\vec{f}$.

It may be interesting to compare the above stability conditions with the conditions which are obtained when equation (1.1) is first written in first order form, i.e.

$$\begin{aligned} \frac{d\vec{y}}{dx} &= \vec{z} \\ \frac{d\vec{z}}{dx} &= \vec{f}(\vec{y}), \end{aligned} \tag{1.1'}$$

and then solved by a stabilized Runge-Kutta method for *first order equations*. Since the Jacobian matrix of the right-hand side of (1.1') is given by

$$J = \begin{pmatrix} 0 & I \\ J_1 & 0 \end{pmatrix}, \tag{1.4}$$

we have eigenvalues of the form $\pm\sqrt{\delta}$, where δ are the eigenvalues of J_1. Hence, when J_1 has *negative* eigenvalues, we have *purely imaginary* eigenvalues in the first order representation (1.1'). It is known (cf. VAN DER HOUWEN [1972]) that the stability condition for second order Runge-Kutta methods with optimal imaginary stability interval reads

$$h_n \leq \frac{m-1}{\sigma(J)}, \qquad m = 1,2,2i+1, \qquad i = 1,2,\ldots, \tag{1.5}$$

where $\sigma(J)$ denotes the spectral radius of J. Seeing that

$$\sigma(J) = \sqrt{\sigma(J_1)}, \tag{1.6}$$

we may conclude from (1.2) and (1.5) that a reduction to first order form makes the maximal allowable integration step a factor $(m-1)/2m$ smaller than direct integration of the second order equation. For third order accuracy, the classical Heun formula is available with an imaginary stability limit of $\sqrt{3}$. Since Heun's formula requires 3 right-hand-side evaluations we have effectively a stability limit of $\sqrt{3}/3 \cong .5$, whereas (1.3) yields an effective stability limit of $2.66/2 \cong 1.3$, i.e. more than twice as large.

Apart from a relaxed stability condition, the new formulas have the

advantage that at the cost of a slightly smaller maximal integration step, perturbations due to rounding errors can be damped out by an appropriate choice of some control parameter.

Finally, the new formulas are chosen in such a way that storage requirements are low, so that they are suitable for the integration of partially discretized hyperbolic equations, e.g. the wave equation.

In the near future numerical results will be reported obtained by the new formulas.

2. CONSISTENCY CONDITIONS

The general m-point Runge-Kutta method for the autonomous, second order system

$$\frac{d^2\vec{y}}{dx^2} = \vec{f}(\vec{y}, \frac{d\vec{y}}{dx}) \tag{2.1}$$

reads as follows:

$$\begin{aligned}
&\vec{y}^{(0)}_{n+1} = \vec{y}_n, \quad \vec{w}^{(0)}_{n+1} = \vec{y}'_n, \\
&\vec{y}^{(j)}_{n+1} = \vec{y}^{(0)}_{n+1} + \mu_j h_n \vec{w}^{(0)}_{n+1} + \sum_{\ell=0}^{j-1} \lambda_{j\ell} h_n^2 \vec{f}^{(\ell)}_{n+1}, \\
&\vec{w}^{(j)}_{n+1} = \vec{w}^{(0)}_{n+1} + \sum_{\ell=0}^{j-1} \beta_{j\ell} h_n \vec{f}^{(\ell)}_{n+1}, \\
&\vec{y}_{n+1} = \vec{y}^{(m)}_{n+1}, \quad \vec{y}'_{n+1} = \vec{w}^{(m)}_{n+1}, \quad \mu_m = 1.
\end{aligned} \tag{2.2}$$

Here, $\vec{y}_{n+1}$ and $\vec{y}'_{n+1}$ denote the numerical approximations to the solution $\vec{y}$ and its derivative $d\vec{y}/dx$ at the point $x = x_n + h_n$; furthermore, we have

$$\vec{f}(\vec{y}^{(\ell)}_{n+1}, \vec{w}^{(\ell)}_{n+1}) = \vec{f}^{(\ell)}_{n+1}.$$

The order equations for scheme (2.2) are well known and can be found in, e.g., ZONNEVELD [1964] and FEHLBERG [1972]. Therefore, we only present the

final conditions for orders p up to 3 (see table 2.1). These conditions hold for the general second order equation (2.1). When the first derivative does not occur in the right-hand side, the last condition in table 2.1 may be omitted. It should be remarked that table 2.1 presents for p = 3 the "additional" conditions, i.e. the conditions for p = 3 consist of the conditions listed for p = 2 and p = 3.

Table 2.1. Consistency conditions for scheme (2.2)

p = 2	$\sum_{\ell=0}^{m-1} \lambda_{m\ell} = \frac{1}{2}, \quad \sum_{\ell=0}^{m-1} \beta_{m\ell} = 1, \quad \sum_{\ell=1}^{m-1} \beta_{m\ell}\mu_\ell = \frac{1}{2}$
p = 3	$\sum_{\ell=1}^{m-1} \lambda_{m\ell}\mu_\ell = \frac{1}{6}, \quad \sum_{\ell=1}^{m-1} \beta_{m\ell}\mu_\ell^2 = \frac{1}{3},$ $\sum_{\ell=2}^{m-1} \beta_{m\ell} \sum_{j=1}^{\ell-1} \beta_{\ell j}\mu_\ell = \frac{1}{6}$

3. STABILITY ANALYSIS

Let us introduce the vectors

$$\vec{\eta}^{(j)} = \begin{pmatrix} \vec{y}^{(j)}_{n+1} \\ h_n \vec{w}^{(j)}_{n+1} \end{pmatrix}, \qquad \vec{F}^{(j)} = \begin{pmatrix} \vec{f}^{(j)}_{n+1} \\ \vec{f}^{(j)}_{n+1} \end{pmatrix}; \tag{3.1}$$

then we can represent scheme (2.2) in a more compact form by

$$\vec{\eta}^{(j)} = M_j \vec{\eta}^{(0)} + h_n^2 \sum_{\ell=0}^{j-1} N_{j\ell} \vec{F}^{(\ell)}, \qquad j = 1(1)m, \tag{3.2}$$

where M_j and $N_{j\ell}$ are matrices defined by

$$M_j = \begin{pmatrix} I & \mu_j I \\ 0 & I \end{pmatrix}, \qquad N_{j\ell} = \begin{pmatrix} \lambda_{j\ell} I & 0 \\ 0 & \beta_{j\ell} I \end{pmatrix}. \tag{3.3}$$

If J_1 and J_2 denote the Jacobian matrices of the right-hand side $\vec{f}$ with respect to $\vec{y}$ and $\vec{y}'$, respectively, and if we write

$$J = \begin{pmatrix} J_1 & h_n^{-1} J_2 \\ J_1 & h_n^{-1} J_2 \end{pmatrix}, \tag{3.4}$$

then it is easily verified that a perturbation $\Delta\vec{\eta}^{(0)}$ of $\vec{\eta}^{(0)}$ gives rise to a perturbation $\Delta\vec{\eta}^{(m)}$ in $\vec{\eta}^{(m)}$ which is approximately given by

$$\Delta\vec{\eta}^{(j)} = M_j \Delta\vec{\eta}^{(0)} + h_n^2 \sum_{\ell=0}^{j-1} N_{j\ell} J \Delta\vec{\eta}^{(\ell)}, \tag{3.5}$$

or alternatively,

$$\Delta\vec{\eta}^{(j)} = R^{(j)} \Delta\vec{\eta}^{(0)}$$

$$R^{(j)} = \begin{pmatrix} R_{11}^{(j)} & R_{12}^{(j)} \\ R_{21}^{(j)} & R_{22}^{(j)} \end{pmatrix}, \tag{3,5'}$$

where the submatrices $R_{\ell k}^{(j)}$ are defined by the recurrence relation

$$\begin{pmatrix} R_{11}^{(j)} & R_{12}^{(j)} \\ R_{21}^{(j)} & R_{22}^{(j)} \end{pmatrix} = \begin{pmatrix} I & \mu_j I \\ 0 & I \end{pmatrix} + \sum_{\ell=0}^{j-1} \begin{pmatrix} \lambda_{j\ell} h_n^2 J_1 & \lambda_{j\ell} h_n J_2 \\ \beta_{j\ell} h_n^2 J_1 & \beta_{j\ell} h_n J_2 \end{pmatrix} \begin{pmatrix} R_{11}^{(\ell)} & R_{12}^{(\ell)} \\ R_{21}^{(\ell)} & R_{22}^{(\ell)} \end{pmatrix} \tag{3.6}$$

and the initial condition

$$R_{11}^{(0)} = R_{22}^{(0)} = I, \quad R_{21}^{(0)} = R_{12}^{(0)} = 0.$$

We will call method (2.2) *stable* when $R^{(m)}$ has all its eigenvalues within the unit circle; when one or more eigenvalues are on the unit circle we will call the method *weakly stable*.

In the general case the analysis of the eigenvalues of the matrix $R^{(m)}$ is very difficult. Therefore, in this report we have confined ourselves to the special case where $J_2 = 0$, that is we consider equations *without first derivatives*. A possible approach for equations *with first derivatives* might be a separate treatment of perturbations of $\vec{y}_n$ and $\vec{y}'_n$, respectively. In the near future we intend to publish results of such a stability analysis.

EXAMPLE 3.1. Consider the second order method generated by (cf. ZONNEVELD [1964])

$$\text{m = 2:} \quad \mu_1 = \mu_2 = 1, \quad \lambda_{10} = \lambda_{21} = 0, \quad \lambda_{20} = \tfrac{1}{2}, \qquad \beta_{10} = 1, \quad \beta_{20} = \beta_{21} = \tfrac{1}{2}. \tag{3.7}$$

According to (3.6) we have

$$R^{(1)} = \begin{pmatrix} 1 & 1 \\ h_n^2 J_1 & 1 + h_n J_2 \end{pmatrix},$$

$$R^{(2)} = \begin{pmatrix} I + \frac{1}{2} h_n^2 J_1 & I + \frac{1}{2} h_n J_2 \\ h_n^2 (I + \frac{1}{2} h_n J_2) J_1 & I + \frac{1}{2} h_n^2 J_1 + h_n J_2 (I + \frac{1}{2} h_n J_2) \end{pmatrix}.$$

It is not clear how to derive manageable conditions from $R^{(2)}$ by requiring that its eigenvalues are within or on the unit circle. Only when some relation between the eigenvectors of J_1 and J_2 is known can we say

more about the stability region. For instance, when J_1 and J_2 have the same eigenvectors $\vec{e}^{(j)}$ with eigenvalues $\delta_1^{(j)}$ and $\delta_2^{(j)}$, respectively, then $R^{(2)}$ has eigenvectors of the form $(a_j\vec{e}^{(j)}, b_j\vec{e}^{(j)})^T$ with eigenvalues that are the same as those of the matrix

$$\tilde{R}^{(2)} = \begin{pmatrix} 1 + \frac{1}{2} h_n^2\delta_1^{(j)} & 1 + \frac{1}{2} h_n\delta_2^{(j)} \\ h_n^2\delta_1^{(j)}(1+\frac{1}{2}h_n\delta_2^{(j)}) & 1 + \frac{1}{2} h_n^2\delta_1^{(j)} + h_n\delta_2^{(j)}(1+\frac{1}{2} h_n\delta_2^{(j)}) \end{pmatrix}.$$

Denoting these eigenvalues by α and putting

$$z = h_n^2\delta_1^{(j)}, \quad w = h_n\delta_2^{(j)},$$

we have for the eigenvalues of $R^{(2)}$ the equation

$$\alpha^2 - [2+z+w+\tfrac{1}{2}w^2]\alpha + [1+w+\tfrac{1}{2}w^2-\tfrac{1}{2}wz+\tfrac{1}{4}z^2]. \tag{3.8}$$

We shall derive the *real* stability region of method (3.7), that is we derive the region of real z- and w-values where $|\alpha| \le 1$. The most simple way to do this is the application of the Hurwitz criterion: *the roots of the equation*

$$\alpha^2 - S\alpha + P = 0$$

are within or on the unit circle when the coefficients S *and* P *are real and satisfy the inequalities*

$$|S| \le P + 1, \quad P \le 1. \tag{3.9}$$

Application to (3.8) yields the inequalities

$$w + \frac{1}{2} w^2 - \frac{1}{2} wz + \frac{1}{4} z^2 \le 0,$$

$$z(1+\tfrac{1}{2}w-\tfrac{1}{4}z) \le 0,$$

$$4 + z + 2w + w^2 - \frac{1}{2} wz + \frac{1}{4} z^2 \ge 0.$$

The last inequality is trivially satisfied; the first two inequalities result in the shaded region of figure 3.1. This implies that method (3.7) is only stable when the Jacobian matrices J_1 and J_2 both have negative eigenvalues. Consequently, differential equations without first derivatives cannot be integrated in a stable way by (3.7).

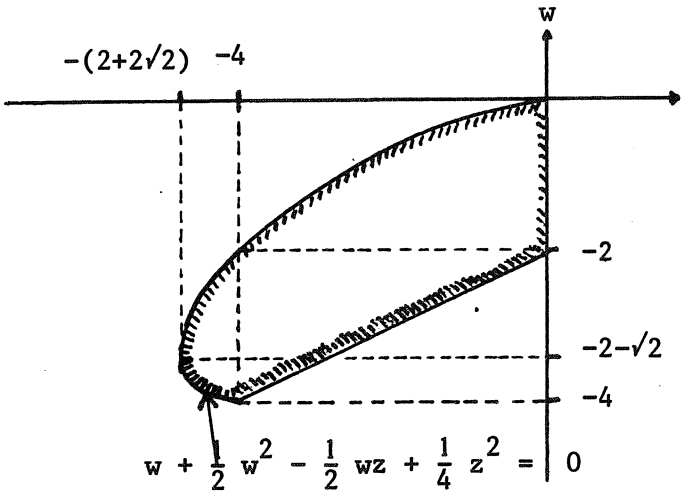

Fig. 3.1. Real stability region of formula (3.7) when J_1 and J_2 have the same set of eigenvectors

4. STABILIZED FORMULAS FOR EQUATIONS WITHOUT FIRST DERIVATIVES

When $\vec{f}$ does not depend on $d\vec{y}/dx$ we have $J_2 = 0$ and we may put, without loss of generality,

$$\beta_{j\ell} = 0, \quad j = 1,2,\ldots,m-1, \quad \ell = 0,1,\ldots,j-1. \tag{4.1}$$

The matrices $R^{(j)}$ are now defined by (cf. (3.6))

$$R^{(0)} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix},$$

$$R^{(j)} = \begin{pmatrix} I & \mu_j I \\ 0 & I \end{pmatrix} + h_n^2 \sum_{\ell=0}^{j-1} \begin{pmatrix} \lambda_{j\ell} J_1 & 0 \\ 0 & 0 \end{pmatrix} R^{(\ell)}, \quad j = 1(1)m-1,$$

$$R^{(m)} = \begin{pmatrix} I & I \\ 0 & I \end{pmatrix} + h_n^2 \sum_{\ell=0}^{m-1} \begin{pmatrix} \lambda_{m\ell} J_1 & 0 \\ \beta_{m\ell} J_1 & 0 \end{pmatrix} R^{(\ell)}.$$

From this it follows that $R^{(m)}$ is a matrix-valued function of $h_n^2 J_1$ given by

$$(4.2) \qquad R^{(m)}(z) = \begin{pmatrix} 1 + \sum_{\ell=0}^{m-1} \lambda_{m\ell} z R_{11}^{(\ell)}(z) & 1 + \sum_{\ell=0}^{m-1} \lambda_{m\ell} z R_{12}^{(\ell)}(z) \\ \sum_{\ell=0}^{m-1} \beta_{m\ell} z R_{11}^{(\ell)}(z) & 1 + \sum_{\ell=0}^{m-1} \beta_{m\ell} z R_{12}^{(\ell)}(z) \end{pmatrix},$$

where $R_{11}^{(\ell)}$ and $R_{12}^{(\ell)}$ satisfy the recurrence relations

$$R_{11}^{(j)} = 1 + \sum_{\ell=0}^{j-1} \lambda_{j\ell} z R_{11}^{(\ell)},$$

$$j = 1,2,\ldots,m-1.$$

$$R_{12}^{(j)} = \mu_j + \sum_{\ell=0}^{j-1} \lambda_{j\ell} z R_{12}^{(\ell)},$$

Let Δ denote the eigenvalue spectrum of the matrix J_1. Then the eigenvalues of $R^{(m)}(h_n^2 J_1)$ are given by the eigenvalues of $R^{(m)}(h_n^2 \delta)$ where $\delta \in \Delta$. Thus, we have stability when the eigenvalues of $R^{(m)}(h_n^2 \delta)$ are within the unit circle for all $\delta \in \Delta$. When one or more eigenvalues are on the unit circle, we have weak stability. Furthermore, we define the region where $|R^{(m)}(z)| < 1$ as the *strong stability region* and the region where $|R^{(m)}(z)| \leq 1$ as the *weak stability region*.

It may be interesting to see how analytically perturbations are approximately propagated when x increases from x_n to $x_n + h_n$. To that end we consider the variational equation

$$(\Delta\vec{y})'' = J_1 \Delta\vec{y},$$

where $\Delta\vec{y}$ denotes a perturbation of $\vec{y}$. Formally, we may write

$$\Delta\vec{y} = \exp(Dx)\vec{a} + \exp(-Dx)\vec{b},$$

where

$$D^2 = J_1,$$
$$\vec{a} = \frac{1}{2}\,[\Delta\vec{y}(0) + D^{-1}\Delta\vec{y}'(0)],$$
$$\vec{b} = \frac{1}{2}\,[\Delta\vec{y}(0) - D^{-1}\Delta\vec{y}'(0)].$$

From this explicit solution we can derive that

$$\Delta\vec{\eta} = \begin{pmatrix} \Delta\vec{y} \\ h_n \Delta\vec{y}' \end{pmatrix} = \begin{pmatrix} \exp(Dx) & \exp(-Dx) \\ Dh_n\exp(Dx) & -Dh_n\exp(-Dx) \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \end{pmatrix},$$

so that errors are amplified according to

$$\Delta\vec{\eta}(x_{n+1}) = A\,\Delta\vec{\eta}(x_n), \quad A = \begin{pmatrix} \cosh(Dh_n) & (Dh_n)^{-1}\sinh(Dh_n) \\ Dh_n\sinh(Dh_n) & \cosh(Dh_n) \end{pmatrix}. \tag{4.3}$$

Note that the matrix A is the analytical analogue of the matrix $R^{(m)}$. The eigenvalues α of the amplification matrix A are defined by

$$\alpha^2 - 2\cosh\sqrt{z}\,\alpha + 1 = 0,$$

where $z = h_n^2\delta$, $\delta \in \Delta$. A simple calculation yields

$$\alpha_{\pm} = \exp(\pm\sqrt{z}).$$

Hence the formula which gives us the analytical solution is weakly stable at points on the negative z-axis and unstable at other points. Consequently, it is realistic to require that the Runge-Kutta method (2.2) is also stable at points on the negative z-axis. In subsections 4.1 and 4.2 we shall try to maximize the negative stability interval under the by-condition that storage requirements are low. The resulting formulas are suitable for the integration of many propagation problems arising in mathematical physics. Below we give two examples of this class of problems. These examples are taken from the partial differential equations governing important physical processes. By applying the *method of lines* the partial differential equations are converted into a large set of ordinary differential equations of type (1.1). As a consequence, we should take into account the large number of equations (thousand or more equations) when we actually construct a stabilized Runge-Kutta method (see the following subsection).

Sound waves

The propagation of sound waves in fluids can be described by the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} ,$$

where t is the time, x the space coordinate and c the velocity of the waves. By replacing $\partial^2/\partial x^2$ by a second order difference quotient and restricting the function u to a discrete set of lines $x = x_j$ in the (x,t)-plane, we may write

$$\frac{d^2\vec{y}}{dt^2} = c^2 D\vec{y},$$

where the components y_j of the vector $\vec{y}$ represent the function u restricted to the line $x = x_j$ (method of lines). D is a tridiagonal matrix with definite subdiagonal elements. Such matrices have real eigenvalues; hence the Jacobian matrix

$$J_1 = c^2 D$$

also has real eigenvalues. A further investigation reveals that all eigenvalues are negative, so that the wave equation belongs to the class mentioned above.

Bar under tension

The vibration of a bar under tension is described by (cf. RICHTMYER & MORTON [1967])

$$\frac{\partial^2 u}{\partial t^2} = - a^2 \frac{\partial^4 u}{\partial x^4} + b^2 \frac{\partial^2 u}{\partial x^2} ,$$

where a is a measure for the stiffness and b for the tension. Applying the method of lines yields the system

$$\frac{d^2 \vec{y}}{dt^2} = - a^2 E\vec{y} + b^2 D\vec{y},$$

where E is a quindiagonal matrix and D is the same matrix as in the preceding example. It is easily verified that E has positive eigenvalues and the same eigenvectors as D, provided that the boundary conditions are periodic (cf. RICHTMYER & MORTON). Hence the Jacobian matrix

$$J_1 = - a^2 E + b^2 D$$

has negative eigenvalues.

4.1. Second order formulas with reduced storage requirements

It is readily seen from scheme (2.2) that storage needed in a computer to implement this method is minimal when

$$\lambda_{j\ell} = \beta_{j,\ell} = 0 \quad \text{for } \ell < j-1. \tag{4.4}$$

Substitution of these conditions into table 2.1 shows that we have at most second order accuracy; this is achieved by putting ($m \geq 2$)

$$\lambda_{m\ m-1} = \frac{1}{2}, \quad \beta_{m\ m-1} = 1, \quad \mu_{m-1} = \frac{1}{2}. \tag{4.5}$$

With these simplifications formula (4.2) reduces to

$$R^{(m)}(z) = \begin{pmatrix} 1 + \frac{1}{2} zR_{11}^{(m-1)}(z) & 1 + \frac{1}{2} zR_{12}^{(m-1)}(z) \\ zR_{11}^{(m-1)}(z) & 1 + zR_{12}^{(m-1)}(z) \end{pmatrix},$$

where

$$R_{11}^{(m-1)}(z) = 1 + \lambda_{m-1\ m-2}\, z + \lambda_{m-1\ m-2}\, \lambda_{m-2\ m-3}\, z^2 + \ldots + \lambda_{m-1\ m-2} \cdots \lambda_{10}\, z^{m-1},$$

$$R_{12}^{(m-1)}(z) = \frac{1}{2} + \lambda_{m-1\ m-2}\, \mu_{m-2}\, z + \lambda_{m-1\ m-2}\, \lambda_{m-2\ m-3}\, \mu_{m-3}\, z^2 + \ldots + \lambda_{m-1\ m-2} \cdots \lambda_{21}\, \mu_1\, z^{m-2}.$$

The eigenvalues α of $R^{(m)}(z)$ (the *amplification factors* of the method) satisfy the equation

$$\alpha^2 - S(z)\alpha + P(z) = 0, \tag{4.6}$$

where

$$S(z) = 2 + z + \sigma_2 z^2 + \ldots + \sigma_m z^m$$

and

$$P(z) = 1 + \pi_2 z^2 + \ldots + \pi_{m-1} z^{m-1} - \sigma_m z^m.$$

The coefficients σ_j and π_j can be expressed in terms of the Runge-Kutta parameters $\lambda_{j\ j-1}$ and μ_j in the following way

$$\sigma_j = \prod_{m-j+1}^{m-1} \lambda_{i\ i-1}(\tfrac{1}{2}+\mu_{m-j}), \quad \sigma_m = \tfrac{1}{2}\prod_{1}^{m-1} \lambda_{i\ i-1},$$

(4.7)

$$\pi_j = \prod_{m-j+1}^{m-1} \lambda_{i\ i-1}(\mu_{m-j}-\tfrac{1}{2}), \qquad j = 2,\ldots,m-1.$$

Conversely, we can express the Runge-Kutta parameters in terms of the coefficients σ_j and π_j, implying that $\sigma_2,\ldots,\sigma_m$ and $\pi_2,\ldots,\pi_{m-1}$ can be freely chosen; for $m > 2$ we find

$$\lambda_{10} = \frac{2\sigma_m}{\sigma_{m-1}-\pi_{m-1}},$$

$$\lambda_{j\ j-1} = \frac{\sigma_{m-j+1}-\pi_{m-j+1}}{\sigma_{m-j}-\pi_{m-j}}, \qquad j = 2(1)m-2,$$

(4.7')

$$\lambda_{m-1\ m-2} = \sigma_2 - \pi_2,$$

$$\mu_j = \frac{1}{2}\frac{\sigma_{m-j}+\pi_{m-j}}{\sigma_{m-j}-\pi_{m-j}}, \qquad j = 1(1)m-2.$$

For $m = 2$ we have

(4.7'') $\qquad \lambda_{10} = 2\sigma_2.$

Thus, we have arrived at the problem of choosing S and P in such a way that the roots of (4.6) are within or on the unit circle for as large a range of z as possible. We recall that we would only consider negative eigenvalues δ; this means that z only assumes negative values, so that the Hurwitz criterion can be applied to equation (4.6) (cf. condition (3.9)). Substitution of the polynomials S and P into (3.9) yields the inequalities

$$|1 + \tfrac{1}{2}\sigma_2 z^2 + \ldots + \tfrac{1}{2}\sigma_m z^m| \le 1 + \tfrac{1}{2}\pi_2 z^2 + \ldots + \tfrac{1}{2}\pi_{m-1} z^{m-1} - \tfrac{1}{2}\sigma_m z^m,$$

(4.8)

$$\tfrac{1}{2}\pi_2 z^2 + \ldots + \tfrac{1}{2}\pi_{m-1} z^{m-1} - \tfrac{1}{2}\sigma_m z^m \le 0.$$

We first consider the simplified case

(4.9) $$\sigma_m = 0; \quad \pi_j = 0, \quad j = 2,\ldots,m-1.$$

We then have the following minimax problem: determine the coefficients σ_j, $j = 2,\ldots,m-1$, in such a way that the polynomial

(4.10) $$\tfrac{1}{2}S(z) = 1 + \tfrac{1}{2}z + \tfrac{1}{2}\sigma_2 z^2 + \ldots + \tfrac{1}{2}\sigma_{m-1} z^{m-1}$$

remains between -1 and +1 over the longest possible interval $[-\beta,0]$. This type of minimax problem is well known and is solved by

(4.11) $$\tfrac{1}{2}S(z) = T_{m-1}\left(1 + \frac{z}{2(m-1)^2}\right),$$

where T_{m-1} is the Chebyshev polynomial of degree m-1 (cf. VAN DER HOUWEN [1968]). For β we have

(4.12) $$\beta = 4(m-1)^2.$$

The stability condition now becomes $|h_n^2\delta| \le \beta$, where δ runs through the (negative) eigenvalues of J_1. Thus

(4.13) $$h_n \le \frac{2(m-1)}{\sqrt{\sigma(J_1)}},$$

where $\sigma(J_1)$ denotes the spectral radius of J_1. It is convenient to define the *effective integration step* h_{eff} of a method:

(4.14) $$h_{eff} = \frac{\text{maximal integration step}}{\text{number of right-hand-side evaluations}};$$

this step h_{eff} indicates the maximal progress the method can make at the cost of one function evaluation. In case (4.9) we have a maximal integration step determined by (4.13) at the cost of m - 1 right-hand-side evaluations ($\sigma_m = 0$ implies, by virtue of (3.7'), that $\lambda_{10} = 0$ so that $\vec{f}(\vec{y}_n)$ does not need to be evaluated!). Consequently,

$$h_{eff} = \frac{2}{\sqrt{\sigma(J_1)}} . \tag{4.15}$$

Note that h_{eff} does not depend on m; hence, with regard to stability, there is no reason to choose m larger than 2 in the case determined by (4.9) and (4.11).

One may wonder whether it is possible to increase h_{eff} by choosing other values for π_j and σ_m than those defined by (4.9). The answer is no. Whatever π_j and σ_m are, we always have to satisfy the condition

$$\tfrac{1}{2}S(z) \le 1.$$

By a similar argument to that used above, this condition implies that $\beta \le 4m^2$, so that $h_n \le 2m/\sqrt{\sigma(J_1)}$ and $h_{eff} \le 2/\sqrt{\sigma(J_1)}$ because now *m* right-hand-side evaluations are to be made ($\sigma_m \neq 0$ implies $\lambda_{10} \neq 0$!).

When we substitute (4.9) and (4.11) into (4.6) we obtain for the amplification factors α

$$\alpha_{1,2} = T_{m-1}\left(1+\frac{h_n^2\delta}{2(m-1)^2}\right) \pm \sqrt{T_{m-1}^2\left(1+\frac{h_n^2\delta}{2(m-1)^2}\right) - 1}, \tag{4.16}$$

revealing that the interval $[-4(m-1)^2,0]$ is the interval of *weak* stability; there are no points of *strong* stability. This is in accordance with the analytical propagation of errors which are also multiplied by amplification factors α of magnitude 1 (cf. relation (4.3)). In practice, however, it is often desirable to have a *strongly stable* formula; therefore, instead of (3.9), we require

$$|S| \le P + \rho, \quad P \le \rho, \; 0 \le p \le 1, \tag{4.17}$$

by which it is guaranteed that the amplification factors $\alpha_1(z)$ and $\alpha_2(z)$ are bounded by $\sqrt{\rho(z)}$. In particular, we are interested in damping functions $\sqrt{\rho}$ which are decreasing when $|z| = h_n^2|\delta|$ increases. In other words, we are looking for functions which damp out the higher frequencies (eigenvectors with large negative eigenvalues). By again choosing $\sigma_m = 0$, conditions (4.17) may be written as

$$(4.17') \qquad \tfrac{1}{2}|S(z)| \le \rho(z),$$

where $\rho(z)$ is of the form

$$(4.18) \qquad \rho(z) \equiv P(z) = 1 + \pi_2 z^2 + \ldots + \pi_{m-1} z^{m-1}.$$

We first consider the special case m = 3 and then we will investigate higher-point formulas for damping functions $\sqrt{\rho}$ close to unity. (Notice that m = 2 always results in a weakly stable formula.)

Two-point formulas

For m = 3 we obtain a two-point formula (remember that we have set $\sigma_m = 0$ which implies $\lambda_{10} = 0$ so that $\vec{f}(\vec{y}_n)$ is not to be evaluated). The functions S and ρ are of second degree and should be chosen as illustrated in figure 4.1.

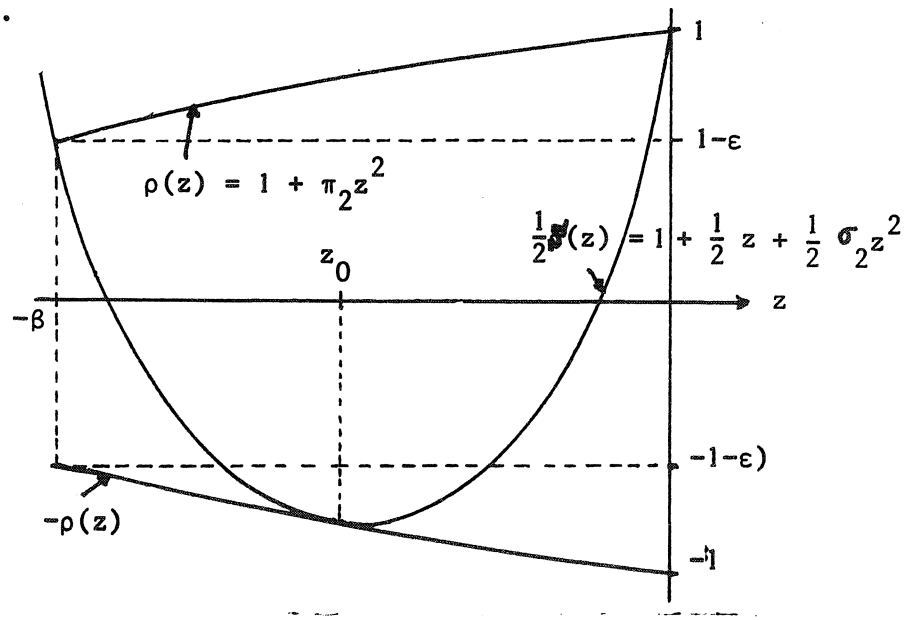

Fig. 4.1. Functions S and ρ for m = 3

It is easily seen that this optimal choice for S and ρ is determined by the relations

$$
\begin{aligned}
&\rho(-\beta) = 1 - \varepsilon, \\
&\tfrac{1}{2} S(-\beta) = 1 - \varepsilon, \\
&\tfrac{1}{2} S(z_0) = -\rho(z_0), \\
&\tfrac{1}{2} S'(z_0) = -\rho'(z_0),
\end{aligned}
\tag{4.19}
$$

where ε denotes the maximal deviation of the function ρ from unity. These relations are easily solved to obtain

$$
\begin{aligned}
&\sigma_2 = \frac{\beta-2\varepsilon}{\beta^2}, \quad \pi_2 = -\frac{\varepsilon}{\beta^2}, \\
&\beta = 8\left(1+\sqrt{1-\varepsilon}\right) \cong 16 - 4\varepsilon \qquad \text{as } \varepsilon \to 0.
\end{aligned}
\tag{4.20}
$$

The integration formula assumes the form

$$
\begin{aligned}
\vec{y}_{n+1} = \vec{y}_n + h_n \vec{y}_n' + \tfrac{1}{2} h_n^2 \vec{f}\Big(\vec{y}_n + \tfrac{1}{2} h_n \vec{y}_n' + \\
+ \frac{\beta-\varepsilon}{\beta^2} h_n^2 \vec{f}\Big(\vec{y}_n + \tfrac{1}{2} \frac{\beta-3\varepsilon}{\beta-\varepsilon} h_n \vec{y}_n'\Big)\Big),
\end{aligned}
\tag{4.21}
$$

$$
\vec{y}_{n+1}' = 2 \frac{\vec{y}_{n+1} - \vec{y}_n}{h_n} - \vec{y}_n',
$$

with the stability condition

$$
h_n \le 2\sqrt{\frac{2(1+\sqrt{1-\varepsilon})}{\sigma(J_1)}} \cong 2\sqrt{\frac{4-\varepsilon}{\sigma(J_1)}} = 2h_{\text{eff}},
\tag{4.22}
$$

and a damping function

$$\sqrt{\rho(h_n^2\delta)} \doteq \sqrt{1 - \frac{\varepsilon}{\beta^2} h_n^4 \delta^2}. \tag{4.23}$$

Three-point formulas

The case m = 4 will be treated for $\varepsilon << 1$. Analogous to the two-point case we determine the function S by imposing the "equal ripple" conditions (see figure 4.2):

$$\begin{aligned}
&\rho(-\beta) = 1 - \varepsilon, \\
&\tfrac{1}{2} S(-\beta) = -(1-\varepsilon), \\
&\tfrac{1}{2} S(z_0) = -\rho(z_0), \\
&\tfrac{1}{2} S(z_1) = \rho(z_1), \\
&\tfrac{1}{2} S'(z_0) = -\rho'(z_0), \\
&\tfrac{1}{2} S'(z_1) = \rho'(z_1).
\end{aligned} \tag{4.24}$$

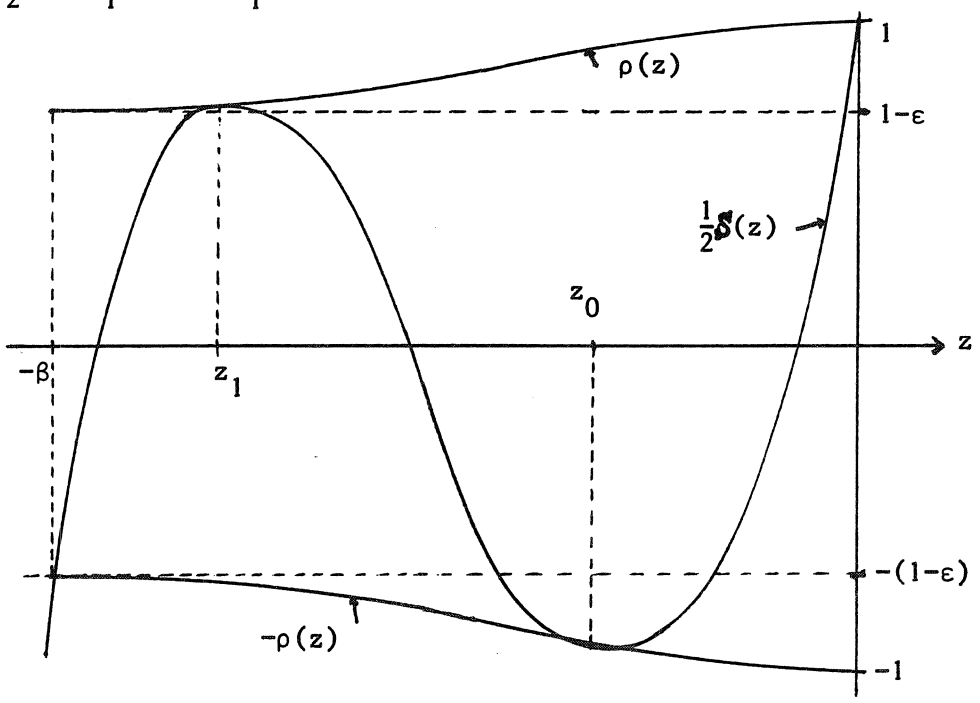

Fig. 4.2. Functions S and ρ for m = 4

By choosing for ρ a function with vanishing first derivative at $z = -\beta$, i.e.

$$(4.25) \qquad \rho(z) = 1 + \pi_2 z^2 + \pi_3 z^3 = 1 - 3\frac{\varepsilon}{\beta^2} z^2 - 2\frac{\varepsilon}{\beta^3} z^3,$$

the first condition of (4.24) is satisfied. Thus, we have 5 equations for σ_2, σ_3, z_0, z_1 and β, leaving ε as a free parameter. We solve these equations for $\varepsilon \to 0$. Firstly, the coefficients σ_2 and σ_3 are expressed in terms of z_0. From the third and fifth equations of (4.24) it follows that

$$(4.26) \qquad \sigma_2 = -2\frac{6+z_0+\pi_2 z_0^2}{z_0^2}, \qquad \sigma_3 = \frac{8+z_0-2\pi_3 z_0^3}{z_0^3}.$$

Furthermore, from the fourth and sixth equations it follows that

$$z_1 = \frac{2}{2\pi_2-\sigma_2} = \frac{z_0^2}{6+z_0+2\pi_2 z_0^2}.$$

Substitution of σ_2, σ_3 and z_1 into the sixth equation yields for z_0 the equation

$$(4.27) \qquad (\pi_3+\pi_2^2) z_0^4 + \pi_2 z_0^3 + 6\pi_2 z_0^2 + z_0 + 9 = 0.$$

For small values of ε we see from (4.25) that π_2 and π_3 are close to zero, and hence

$$(4.27') \qquad z_0 \cong -9 + c\varepsilon \qquad \text{as } \varepsilon \to 0$$

where

$$c = 243\frac{\pi_2-27\pi_3-27\pi_2^2}{\varepsilon} \cong -\frac{729}{\beta^2}\left[1 - \frac{18}{\beta}\right].$$

Substitution of σ_2 and σ_3 into the second equation yields for β the equation

$$(4.28) \qquad (8+z_0)\beta^3 + 2z_0(6+z_0)\beta^2 + z_0^3\beta - 4z_0^3 = 0.$$

For $\varepsilon = 0$, i.e. $z_0 = -9$, this equation is solved by $\beta = 36$ in accordance with formula (4.12). Therefore we may write for z_0 (cf.(4.27'))

$$(4.27'') \qquad z_0 \cong -9 - \frac{9}{32}\varepsilon \qquad \text{as } \varepsilon \to 0.$$

We now substitute for β in (4.28) the expression $\beta = 36 - b\varepsilon$ and for z_0 expression (4.27''). Neglecting terms of order ε^2 we find for b the value 9, so that

$$(4.28') \qquad \beta \cong 36 - 9\varepsilon \qquad \text{as } \varepsilon \to 0.$$

Summarizing, the relations (4.26), (4.27) and (4.28) determine a second order, three-point formula with (4.25) as its damping function and the stability condition

$$h_n \leq 6\sqrt{\frac{1-\frac{1}{4}\varepsilon}{\sigma(J_1)}} \qquad \text{as } \varepsilon \to 0.$$

The effective integration step behaves as

$$h_{eff} \cong \sqrt{\frac{4-\varepsilon}{\sigma(J_1)}} \qquad \text{as } \varepsilon \to 0,$$

which is identical to the effective integration step of the two-point formula.

One may ask whether the three-point formula has advantages when compared with the two-point formula. Since the efficiencies of both formulas are equal, the only advantage could be the damping effect of ρ. In order to compare the damping effect we consider the damping function of the two-point formula and the three-point formula after three and two maximal integration steps, respectively (notice that the same integration interval is then covered). For m = 3 we deduce from (4.23) the damping function

$$\left[1 - \varepsilon\left[\frac{\delta}{\sigma(J_1)}\right]^2\right]^{3/2},$$

and for m = 4 we deduce from (4.25) the damping function

$$1 - 3\varepsilon\left[\frac{\delta}{\sigma(J_1)}\right]^2 - 2\varepsilon\left[\frac{\delta}{\sigma(J_1)}\right]^3.$$

In figure 4.3 the behaviour of these functions is illustrated for small ε.

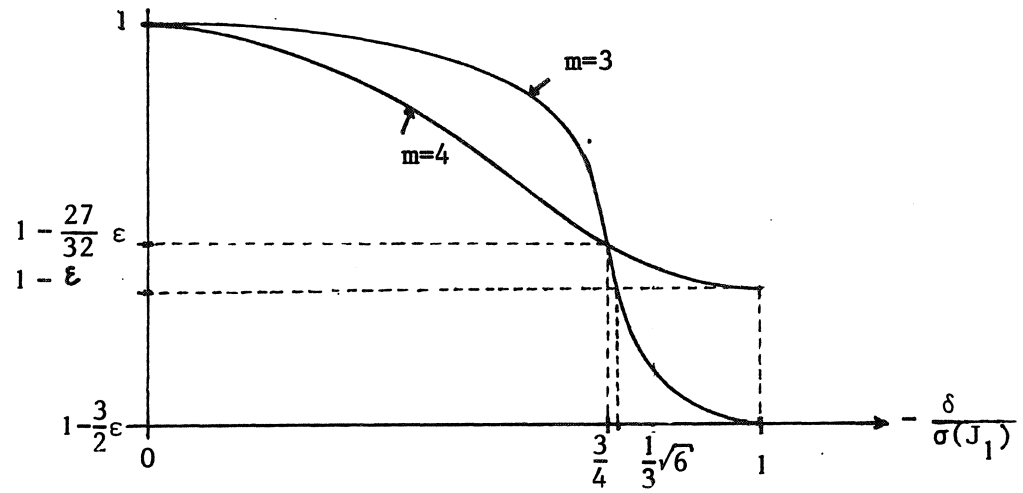

Fig. 4.3. Behaviour of the damping functions of the two- and three-point formulas after equal integration intervals and for $\varepsilon \to 0$

From this figure it may be concluded that the three-point formula has a better overall damping, whereas the two-point formula has a better damping of the higher frequencies. This conclusion does not justify investigating higher point formulas at this moment, since the efficiency will not become better for larger m-values and the damping effect will only be smeared out over the eigenvalue interval instead of being concentrated in the large eigenvalue region.

4.2. Third order formulas

By adding new Runge-Kutta parameters to the formulas considered in the preceding section, we can achieve third order consistency. Let us take λ_{m1} and β_{m1} as additional parameters and let us set ($m \geq 3$)

$$\lambda_{10} = 0 \tag{4.29}$$

(compare the preceding subsection).

From table 2.1 we find the order equations

$$\begin{aligned}
&\lambda_{m1} + \lambda_{m\,m-1} = \frac{1}{2},\\
&\lambda_{m1}\mu_1 + \lambda_{m\,m-1}\mu_{m-1} = \frac{1}{6},\\
&\beta_{m1} + \beta_{m\,m-1} = 1,\\
&\beta_{m1}\mu_1 + \beta_{m\,m-1}\mu_{m-1} = \frac{1}{2},\\
&\beta_{m1}\mu_1^2 + \beta_{m\,m-1}\mu_{m-1}^2 = \frac{1}{3},
\end{aligned} \tag{4.30}$$

and from (4.2) we derive

$$R^{(m)}(z) = \begin{pmatrix} 1 + (\lambda_{m1}+\lambda_{m\,m-1} R_{11}^{(m-1)}(z) & 1 + (\lambda_{m1}\mu_1+\lambda_{m\,m-1} R_{12}^{(m-1)}(z) \\ (\beta_{m1}+\beta_{m\,m-1} R_{11}^{(m-1)}(z) & 1 + (\beta_{m1}\mu_1+\beta_{m\,m-1} R_{12}^{(m-1)}(z) \end{pmatrix},$$

where $R_{11}^{(m-1)}$ and $R_{12}^{(m-1)}$ are defined as in the preceding section.

The eigenvalues of $R^{(m)}(z)$ are given by

$$\alpha^2 - S(z)\alpha + P(z) = 0 \tag{4.31}$$

where

$$S(z) = 2 + (\lambda_{m1}+\beta_{m1}\mu_1)z + [\lambda_{m\,m-1} R_{11}^{(m-1)}(z) + \beta_{m\,m-1} R_{12}^{(m-1)}(z)]z,$$

$$P(z) = S(z) - 1 - [\beta_{m1} + \beta_{m\,m-1}\, R_{11}^{(m-1)}(z)]z +$$

$$+ [\lambda_{m1}\beta_{m\,m-1} - \lambda_{m\,m-1}\beta_{m1}][R_{12}^{(m-1)}(z) - \mu_1\, R_{11}^{(m-1)}(z)]z^2.$$

Substitution of $R_{11}^{(m-1)}$ and $R_{12}^{(m-1)}$ and of the consistency conditions (4.30) yields

$$S(z) = 2 + z + \sigma_2 z^2 + \ldots + \sigma_{m-1} z^{m-1},$$

$$P(z) = 1 + \pi_2 z^2 + \ldots + \pi_{m-1} z^{m-1},$$

(4.32)

where

$$\sigma_2 = (\lambda_{m\,m-1} + \beta_{m\,m-1}\mu_{m-2})\, \lambda_{m-1\,m-2},$$

$$\sigma_3 = (\lambda_{m\,m-1} + \beta_{m\,m-1}\mu_{m-3}) \prod_{m-2}^{m-1} \lambda_{j\,j-1},$$

$$\vdots$$

$$\sigma_{m-1} = (\lambda_{m\,m-1} + \beta_{m\,m-1}\mu_1) \prod_{2}^{m-1} \lambda_{j\,j-1},$$

$$\pi_2 = \sigma_2 - [\beta_{m\,m-1}\lambda_{m-1\,m-2} - C(\mu_{m-1} - \mu_1)],$$

$$\pi_3 = \sigma_3 - \left[\beta_{m\,m-1} - C\,\frac{\mu_{m-2} - \mu_1}{\lambda_{m-2\,m-3}}\right] \prod_{m-2}^{m-1} \lambda_{j\,j-1},$$

$$\vdots$$

$$\pi_{m-1} = \sigma_{m-1} - \left[\beta_{m\,m-1} - C\,\frac{\mu_2 - \mu_1}{\lambda_{21}}\right] \prod_{2}^{m-1} \lambda_{j\,j-1},$$

(4.33)

$$C = \lambda_{m1}\beta_{m\,m-1} - \lambda_{m\,m-1}\beta_{m1}.$$

Notice that by virtue of our choice (4.29) both S(z) and P(z) are of degree m-1 in z. Since (4.29) also implies that only m-1 right-hand-side evaluations are involved, we have a similar situation as in the second order

case provided that we are able to convert the relations (4.30) and (4.33), i.e. when we succeed in expressing the Runge-Kutta parameters in terms of the coefficients σ_j and π_j. Hitherto we have not succeeded in solving this conversion problem for $m > 3$. We have therefore confined our considerations to the special case $m = 3$.

Two-point formulas

For $m = 3$ we have 7 equations to solve

$$
\begin{aligned}
&\lambda_{31} + \lambda_{32} = \tfrac{1}{2},\\
&\lambda_{31}\mu_1 + \lambda_{32}\mu_2 = \tfrac{1}{6},\\
&\beta_{31}\mu_1 + \beta_{32}\mu_2 = \tfrac{1}{2},\\
&\beta_{31} + \beta_{32} = 1,\\
&\beta_{31}\mu_1^2 + \beta_{32}\mu_2^2 = \tfrac{1}{3},\\
&(\lambda_{32}+\mu_1\beta_{32})\lambda_{21} = \sigma_2,\\
&\beta_{32}\lambda_{21} - C(\mu_2-\mu_1) = \sigma_2 - \pi_2,
\end{aligned}
\tag{4.34}
$$

where

$$C = \lambda_{31}\beta_{32} - \lambda_{32}\beta_{31}.$$

From the first five equations we find

$$
\begin{aligned}
&\lambda_{31} = \tfrac{1}{2} - \lambda_{32}, \quad \beta_{31} = 1 - 3\,\frac{1-2\mu_1}{1-3\mu_1}\,\lambda_{32},\\
&\beta_{32} = 3\,\frac{1-2\mu_1}{1-3\mu_1}\,\lambda_{32}, \quad \mu_2 = \mu_1 + \frac{1-3\mu_1}{6\lambda_{32}},\\
&\lambda_{32} = \frac{(1-2\mu_1)(1-3\mu_1)}{12(\mu_1^2-\mu_1+\frac{1}{3})},
\end{aligned}
\tag{4.35}
$$

leaving μ_1 as a free parameter.

By observing that

$$C = \frac{(1-2\mu_1)}{24(\mu_1^2-\mu_1+\frac{1}{3})} \tag{4.36}$$

the last two equations yield for λ_{21} the expression

$$\lambda_{21} = \frac{12(\mu_1^2-\mu_1+\frac{1}{3})}{(1-2\mu_1)(1-6\mu_1^2)}\sigma_2 \tag{4.37}$$

and for μ_1 the equation

$$(6\sigma_2-6\pi_2+\tfrac{1}{2})\mu_1^2 - 6\sigma_2\mu_1 + 2\sigma_2 + \pi_2 - \frac{1}{12} = 0. \tag{4.38}$$

Of course, we are only interested in real values for μ_1, and thus we require

$$9\sigma_2^2 \geq [6(\sigma_2-\pi_2) + \tfrac{1}{2}][2\sigma_2 + \pi_2 - \tfrac{1}{12}]. \tag{4.39}$$

This condition should be taken into account when we optimize the real stability boundary. An elementary analysis reveals that the above condition implies that the optimal situation is as illustrated in figure 4.4.

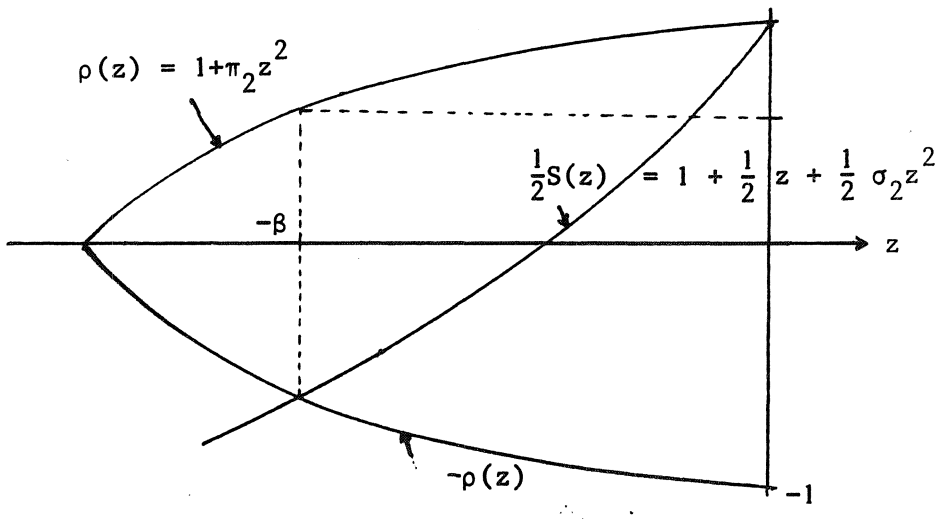

Fig. 4.4. Functions S and ρ for m = 3

Thus, β is determined by the relation

$$\frac{1}{2} S(-\beta) = - \rho(-\beta),$$

i.e.

$$\beta = \frac{1-\sqrt{1-16(\sigma_2+2\pi_2)}}{2(\sigma_2+2\pi_2)} . \tag{4.40}$$

It is easily verified that β is maximized by

$$\sigma_2 + 2\pi_2 = \frac{1}{16} .$$

Henceforth, we shall try to choose $\sigma_2 + 2\pi_2$ as close as possible to 1/16 as is allowed by (4.39). From (4.39) it can be derived that

$$3\sigma_2^2 + (\tfrac{1}{2}-6\pi_2)\sigma_2 - \frac{1}{24} + \pi_2 - 6\pi_2^2 \leq 0,$$

or

$$3\pi_2 - \frac{1}{12} - \frac{1}{12}\sqrt{3-72\pi_2+432\pi_2^2} \leq \sigma_2 + 2\pi_2 \leq 3\pi_2 - \frac{1}{12} + \frac{1}{12}\sqrt{3-72\pi_2+432\pi_2^2}.$$

Since the upper bound for $\sigma_2 + 2\pi_2$ is always less than 1/16 for $\pi_2 < 0$ and is an increasing function of π_2 we may conclude that

$$\sigma_2 + 2\pi_2 = 3\pi_2 - \frac{1}{12} + \frac{1}{12}\sqrt{3-72\pi_2+432\pi_2^2} \cong \tag{4.41}$$

$$\cong \frac{1}{12}(\sqrt{3}-1) + (3-\sqrt{3})\pi_2 \qquad \text{as } \pi_2 \to 0$$

is the best choice to be made for $\sigma_2 + 2\pi_2$. For β we then have

$$\beta \cong \frac{6 - 6\sqrt{\frac{7-4\sqrt{3}}{3} - 16(3-\sqrt{3})\pi_2}}{\sqrt{3} - 1 + 12(3-\sqrt{3})\pi_2} \cong \tag{4.40'}$$

$$\cong 7 \qquad \text{as } \pi_2 \to 0.$$

Finally, we express π_2 in terms of the maximal deviation of $\rho(z)$ from unity, i.e. in terms of ε:

$$\pi_2 = -\frac{\varepsilon}{\beta^2} . \tag{4.42}$$

Formulas (4.35), (4.37), (4.38), (4.41), (4.40') and (4.42) determine a one-parameter family (ε is a free parameter) of third order, two-point formulas with effective integration step

$$h_{eff} = \frac{1}{2}\sqrt{\frac{\beta}{\sigma(J_1)}} \simeq \frac{1.32}{\sqrt{\sigma(J_1)}} \quad \text{as } \varepsilon \to 0. \tag{4.43}$$

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