Construction and implementation of highly stable two-step continuous methods for stiff differential systems

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Abstract

We describe a class of two-step continuous methods for the numerical integration of initial-value problems based on stiff ordinary differential equations (ODEs). These methods generalize the class of two-step Runge–Kutta methods. We restrict our attention to methods of order $p = m$, where m is the number of internal stages, and stage order $q = p$ to avoid order reduction phenomenon for stiff equations, and determine some of the parameters to reduce the contribution of high order terms in the local discretization error. Moreover, we enforce the methods to be A-stable and L-stable. The results of some fixed and variable stepsize numerical experiments which indicate the effectiveness of two-step continuous methods and reliability of local error estimation will also be presented.

Keywords: Two-step almost collocation methods, two-step continuous methods, order conditions, error propagation, local error estimation, A-stability, L-stability, variable stepsize implementation.

1. Introduction

Assume that the function $f : \mathbb{R}^d \to \mathbb{R}^d$ is sufficiently smooth and consider the initial-value problem for systems of ordinary differential equations (ODEs)

$$\begin{cases} y'(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0. \end{cases} \tag{1.1}$$

Let be given a constant stepsize $h > 0$ and define the grid $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, where $Nh = T - t_0$. For the numerical solution of (1.1) consider the class of two-step m-stage continuous methods defined by

$$\begin{cases} P(t_n + sh) = \varphi_0(s)y_{n-1} + \varphi_1(s)y_n + h\displaystyle\sum_{j=1}^{m}\Big(\chi_j(s)f(P(t_{n-1} + c_jh)) + \psi_j(s)f(P(t_n + c_jh))\Big), \\ y_{n+1} = P(t_{n+1}), \end{cases} \tag{1.2}$$

$s \in (0, 1]$, $n = 1, 2, \ldots, N-1$. Here, $c = [c_1, \ldots, c_m]^T$ is the abscissa vector, $P(t_n + sh)$ is an approximation to $y(t_n + sh)$ on the interval $[t_n, t_{n+1}]$, and $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$, and $\psi_j(s)$, $j = 1, 2, \ldots, m$, are polynomials which define the method. Setting

$$Y_j^{[n-1]} = P(t_{n-1} + c_jh), \qquad Y_j^{[n]} = P(t_n + c_jh),$$

$j = 1, 2, \ldots, m$, two-step continuous methods (1.2) can be regarded as a special class of two-step Runge–Kutta methods [20], having the form

$$\begin{cases} y_{n+1} = \varphi_0(1)y_{n-1} + \varphi_1(1)y_n + h\displaystyle\sum_{i=1}^{m}\Big(\chi_i(1)f(Y_i^{[n-1]}) + \psi_i(1)f(Y_i^{[n]})\Big), \\ Y_i^{[n]} = \varphi_0(c_i)y_{n-1} + \varphi_1(c_i)y_n + h\displaystyle\sum_{j=1}^{m}\Big(\chi_j(c_i)f(Y_j^{[n-1]}) + \psi_j(c_i)f(Y_j^{[n]})\Big), \end{cases} \tag{1.3}$$

$i = 1, 2, \dots, m$, or equivalently, in tensor form,

$$\begin{cases} y_{n+1} = \theta y_{n-1} + \widetilde{\theta} y_n + h\Big((v^T \otimes I)F^{[n-1]} + (w^T \otimes I)F^{[n]}\Big), \\ Y^{[n]} = (u \otimes I)y_{n-1} + (\widetilde{u} \otimes I)y_n + h\Big((A \otimes I)F^{[n-1]} + (B \otimes I)F^{[n]}\Big), \end{cases} \tag{1.4}$$

where

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} & Y_2^{[n]} & \dots & Y_m^{[n]} \end{bmatrix}^T \in \mathbb{R}^{md}, \qquad F^{[n]} = \begin{bmatrix} f(Y_1^{[n]}) & f(Y_2^{[n]}) & \dots & f(Y_m^{[n]}) \end{bmatrix}^T \in \mathbb{R}^{md},$$

and

$$\begin{array}{llll} \theta = \varphi_0(1), & \widetilde{\theta} = \varphi_1(1), & v_j = \chi_j(1), & w_j = \psi_j(1), \\ u_i = \varphi_0(c_i), & \widetilde{u}_i = \varphi_1(c_i), & a_{ij} = \chi_j(c_i), & b_{ij} = \psi_j(c_i). \end{array}$$

Two-step continuous methods (1.2) were introduced in [12, 13] and further investigated in [9, 14, 15], also in the context of Volterra Integral Equations [10, 11]. In this paper we follow a similar approach to that in [13], but restrict our attention to methods of order $p = m$ and stage order $q = p$ to avoid order reduction phenomenon [3] for stiff equations. Moreover, we are mainly interested in methods which are A-stable and L-stable. In the follow up paper [9] we investigate algebraic stability properties of these methods. In the next section we review continuous order conditions obtained before in [13] and investigate error propagation of these methods up to the terms of order $p + 2$, in order to derive methods of type (1.2) with narrowed contribution of such high order terms. In Sections 3–6 we describe the construction of methods with $p = q = m$ for $m = 1$, 2, 3, and 4. In Section 7 we describe the variable stepsize implementation of these methods for stiff differential systems. In Section 8 we present the results of some fixed and variable stepsize numerical experiments which indicate the effectiveness of two-step continuous methods and reliability of local error estimation. Finally, in Section 9 some concluding remarks are given and plans for future research are briefly outlined.

2. Error propagation

Let us consider the local discretization error $\xi(t_n + sh)$ associated to the method (1.2), which is defined as the residuum obtained by replacing in (1.2) $P(t_n + sh)$ by $y(t_n + sh)$, y_{n-1} by $y(t_{n-1})$ and y_n by $y(t_n)$, where $y(t)$ is the solution to the problem (1.1). That is,

$$\xi(t_n + sh) = y(t_n + sh) - \varphi_0(s)y(t_{n-1}) - \varphi_1(s)y(t_n) - h\sum_{j=1}^{m}\Big(\chi_j(s)f(P(t_{n-1} + c_jh)) + \psi_j(s)f(P(t_n + c_jh))\Big). \tag{2.1}$$

We now analyze the local discretization error considering the terms up to order $p + 2$. The following result arises.

Theorem 2.1. *If $P(t_n + sh)$ is an approximation of uniform order p to $y(t_n + sh)$, $s \in [0, 1]$, then the local truncation error (2.1) of the method (1.2) takes the form*

$$\xi(t_n + sh) = h^{p+1}C_p(s)y^{(p+1)}(t_n) + h^{p+2}C_{p+1}(s)y^{(p+2)}(t_n) + h^{p+2}G_{p+1}(s)\frac{\partial f}{\partial y}\Big(y(t_n)\Big)y^{(p+1)}(t_n) + O(h^{p+3}), \tag{2.2}$$

where

$$C_\nu(s) = \frac{s^{\nu+1}}{(\nu+1)!} - \frac{(-1)^{\nu+1}}{(\nu+1)!}\varphi_0(s) - \sum_{j=1}^{m}\Big(\chi_j(s)\frac{(c_j-1)^\nu}{\nu!} + \psi_j(s)\frac{c_j^\nu}{\nu!}\Big), \tag{2.3}$$

with $\nu = p,\ p + 1$, and

$$G_{p+1}(s) = \sum_{j=1}^{m}\eta_j\Big(\chi_j(s) + \psi_j(s)\Big). \tag{2.4}$$

Proof: It is known that (see for example [13]), if $P(t_n + sh)$ is an approximation of uniform order p to $y(t_n + sh)$, $s \in [0, 1]$, the stage order is also equal to p and the local discretization error (2.1) takes the form

$$\xi(t_n + sh) = h^{p+1}C_p(s)y^{(p+1)}(t_n) + O(h^{p+2}), \tag{2.5}$$

where $C_p(s)$ is the error function of the method (1.2). Hence, the stage values $P(t_{n-1} + c_j h)$ and $P(t_n + c_j h)$ in (1.2) satisfy the relations

$$P(t_{n-1} + c_j h) = y(t_{n-1} + c_j h) - \eta_j h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}), \tag{2.6}$$

$$P(t_n + c_j h) = y(t_n + c_j h) - \eta_j h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}), \tag{2.7}$$

where

$$\eta_j = C_p(c_j), \quad j = 1, 2, \ldots, m,$$

are the stage error constants, which we put together in the vector

$$\eta = \begin{bmatrix} \eta_1 & \eta_2 & \ldots & \eta_m \end{bmatrix}^T.$$

We now analyze the local discretization error considering the terms up to order $p + 2$. Substituting the relations (2.6) and (2.7) into (2.1), we obtain

$$\begin{aligned} \xi(t_n + sh) &= y(t_n + sh) - \varphi_0(s)y(t_n - h) - \varphi_1(s)y(t_n) - h\sum_{j=1}^{m}\Big(\chi_j(s)f\Big(y(t_{n-1} + c_j h) - \eta_j h^{p+1}y^{(p+1)}(t_n)\Big) \\ &+ \psi_j(s)f\Big(y(t_n + c_j h) - \eta_j h^{p+1}y^{(p+1)}(t_n)\Big)\Big) + O(h^{p+3}), \end{aligned}$$

and since f is sufficiently smooth, this formula can be rewritten as

$$\begin{aligned} \xi(t_n + sh) &= y(t_n + sh) - \varphi_0(s)y(t_n - h) - \varphi_1(s)y(t_n) - h\sum_{j=1}^{m}\Big(\chi_j(s)y'(t_{n-1} + c_j h) + \psi_j(s)y'(t_n + c_j h)\Big) \\ &+ h^{p+2}\sum_{j=1}^{m}\Big(\eta_j\big(\chi_j(s) + \psi_j(s)\big)\frac{\partial f}{\partial y}\big(y(t_n)\big)y^{(p+1)}(t_n)\Big) + O(h^{p+3}). \end{aligned}$$

Expanding $y(t_n + sh)$, $y(t_n - h)$, $y'(t_{n-1} + c_j h)$ and $y'(t_n + c_j h)$ into Taylor series around t_n and collecting the terms with the same powers of h, we obtain

$$\begin{aligned} \xi(t_n + sh) &= (1 - \varphi_0(s) - \varphi_1(s))y(t_n) \\ &+ \sum_{k=1}^{p+2}\Big(\frac{s^k}{k!} - \frac{(-1)^k}{k!}\varphi_0(s)\Big)h^k y^{(k)}(t_n) \\ &- \sum_{k=1}^{p+2}\sum_{j=1}^{m}\Big(\chi_j(s)\frac{(c_j - 1)^{k-1}}{(k-1)!} + \psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\Big)h^k y^{(k)}(t_n) \\ &+ \sum_{j=1}^{m}\Big(\eta_j\big(\chi_j(s) + \psi_j(s)\big)h^{p+2}\frac{\partial f}{\partial y}\big(y(t_n)\big)y^{(p+1)}(t_n)\Big) + O(h^{p+3}). \end{aligned}$$

Equating to zero terms of order $O(h^k)$, $k = 0, 1, \ldots, p$, we obtain the continuous order conditions (see [12, 13])

$$\begin{cases} \varphi_0(s) + \varphi_1(s) = 1, \\ \dfrac{(-1)^k}{k!}\varphi_0(s) + \displaystyle\sum_{j=1}^{m}\Big(\chi_j(s)\frac{(c_j - 1)^{k-1}}{(k-1)!} + \psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\Big) = \dfrac{s^k}{k!}, \end{cases} \tag{2.8}$$

$s \in [0, 1]$, $k = 1, 2, \ldots, p$ and, considering the remaining terms, we can conclude that the local discretization error of two-step continuous methods takes the form (2.2), with $C_\nu(s)$, $\nu = p,\ p + 1$, and $G_{p+1}(s)$ are given by (2.3) and (2.4) respectively.

□

We have previously provided in [13] an estimation to the leading term of the local truncation error (2.5), having the form

$$h^{p+1}y^{(p+1)}(t_n) = \alpha_0 y_{n-1} + \alpha_1 y_n + h\sum_{j=1}^{m}\Big(\beta_j f(P(t_{n-1}+c_j h)) + \gamma_j f(P(t_n + c_j h))\Big). \tag{2.9}$$

The following result holds (see [12, 13]).

Theorem 2.2. *Assume that the solution* $\widetilde{y}(t)$ *to the problem (1.1) is sufficiently smooth. Then the constants* α_0, α_1, β_j, *and* γ_j, $j = 1, 2, \ldots, m$ *appearing in (2.9) satisfy the system of equations*

$$\begin{cases} \alpha_0 + \alpha_1 = 0, \\ \dfrac{(-1)^k}{k!}\alpha_0 + \displaystyle\sum_{j=1}^{m}\Big(\beta_j \frac{(c_j-1)^{k-1}}{(k-1)!} + \gamma_j \frac{c_j^{k-1}}{(k-1)!}\Big) = 0, \quad k = 1, 2, \ldots, p, \\ \Big(\dfrac{(-1)^{p+1}}{(p+1)!} - C_p(-1)\Big)\alpha_0 + \displaystyle\sum_{j=1}^{m}\Big(\beta_j \frac{(c_j-1)^{p}}{p!} + \gamma_j \frac{c_j^{p}}{p!}\Big) = 1. \end{cases}$$

Concerning the high order terms, in order to narrow their contribution in the local discretization error (2.5), we derive in the following sections methods such that the stage error constant $G_{p+1}(1)$ is equal to zero. This condition implies that terms of order $p+2$ only depend on the derivatives of the solution and not on the form of the equation. Moreover, this feature is of practical utility in the implementation of such methods in a variable stepsize-variable order environment (which will be treated in forthcoming papers), since it simplifies the order changing strategy.

3. Construction of methods with $m = 1$

We now analyze two-step continuous methods (1.2) with $p = q = m = 1$, assuming that the continuous approximant $P(t_n + sh)$ satisfies the interpolation condition

$$P(t_n) = y_n, \tag{3.1}$$

which implies that

$$\varphi_0(0) = 0, \quad \varphi_1(0) = 1, \quad \chi(0) = 0, \quad \psi(0) = 0.$$

Let us assume the following expression for the basis functions

$$\varphi_0(s) = p_0 + p_1 s, \quad \chi(s) = r_0 + r_1 s, \quad \varphi_1(s) = q_0 + q_1 s, \quad \psi(s) = s_0 + s_1 s.$$

Therefore, we have $p_0 = r_0 = s_0 = 0$ and $q_0 = 1$. We next impose the set of order conditions (2.8), obtaining

$$p_1 = -q_1, \qquad r_1 = 1 - q_1 - s_1.$$

Hence, the resulting family of one stage methods (1.2) depends on q_1, s_1, and c, which must be determined in order to achieve the desired stability properties (e.g. A-stability and L-stability). We next consider the associated local truncation error (2.2)

$$\xi(t_n + sh) = h^2 E(s) y^{(2)}(t_n) + h^3\Big(F(s)y^{(3)}(t_n) + G(s)\frac{\partial f}{\partial y}(y(t_n))y^{(2)}(t_n)\Big) + O(h^4), \tag{3.2}$$

where $E(s) = C_1(s)$, $F(s) = C_2(s)$ and $G(s) = G_2(s)$ can be derived from formulae (2.3) and (2.4). In particular, the constant $G(s)$ takes the following form

$$G(s) = \frac{c^2}{2}(1-q_1)(2 - c - q_1 + 2cq_1 - 2s_1)s.$$

Solving the equation $G(1) = 0$ with respect to s_1 we obtain

$$s_1 = \frac{2 - c - q_1 + 2cq_1}{2}.$$

As a consequence, the basis functions in (1.2) for $m = 1$, which now depend only on the parameter q_1 and the value of the abscissa c, take the following form

$$\begin{aligned} \varphi_0(s) &= -q_1 s, \qquad \chi(s) = -\frac{s}{2}(q_1 + 2cq_1 - c), \\ \varphi_1(s) &= 1 + q_1 s, \quad \psi(s) = -\frac{s}{2}(q_1 - 2cq_1 + c - 2). \end{aligned} \tag{3.3}$$

We next consider the linear stability analysis of this class of methods, first deriving the expression of the stability polynomial, i.e. the characteristic polynomial of the stability matrix (see [12, 13])

$$M(z) = \begin{bmatrix} M_{11}(z) & M_{12}(z) & M_{13}(z) \\ 1 & 0 & 0 \\ Q(z)\varphi_1(c) & Q(z)\varphi_0(c) & zQ(z)A \end{bmatrix} \in \mathbb{C}^{(m+2)\times(m+2)}, \tag{3.4}$$

where

$$\begin{aligned} M_{11}(z) &= \varphi_1(1) + zw^T Q(z)\varphi_1(c), \\ M_{12}(z) &= \varphi_0(1) + zw^T Q(z)\varphi_0(c), \\ M_{13}(z) &= z(v^T + zw^T Q(z)A), \end{aligned}$$

and $A = (\chi_j(c_i))_{i,j=1}^m$, $B = (\psi_j(c_i))_{i,j=1}^m$, $v = (\chi_j(1))_{j=1}^m$, $w = (\psi_j(1))_{j=1}^m$, $Q(z) = (I - zB)^{-1} \in \mathbb{C}^{m\times m}$ and I is the identity matrix of order m.

In the case $m = 1$, the stability function takes the form

$$p(\omega, z) = \omega(p_2(z)\omega^2 + p_1(z)\omega + p_0(z)), \tag{3.5}$$

where $p_0(z)$, $p_1(z)$ and $p_2(z)$ are polynomials of degree less than or equal 2 with respect to z. Applying the Schur criterion (see [22, 25]) to the polynomial (3.5), we obtain the following result, which characterizes A-stable methods with $p = m = 1$.

Theorem 3.1. *Each one stage continuous method of type (1.2) which satisfies the restrictions discussed above is A-stable if and only if*

$$c > 1, \qquad \frac{c-1}{2c} \le q_1 \le 1. \tag{3.6}$$

Figure 3.1 shows the corresponding region of A-stability in the parameter space (c, q_1).

Let us provide an example of A-stable method. Setting $c = \frac{5}{4}$ and $q_1 = \frac{1}{2}$, the basis functions (3.3) take the form

$$\varphi_0(s) = -\frac{s}{2}, \quad \varphi_1(s) = \frac{2+s}{2}, \quad \chi(s) = -\frac{s}{4}, \quad \psi(s) = \frac{3s}{4}. \tag{3.7}$$

We can estimate the local truncation error associated to this method with the one-parameter family of estimators (2.9), where

$$\alpha_1 = -\alpha_0, \quad \beta = \frac{5}{8}\alpha_0, \quad \gamma = \frac{3}{8}\alpha_0. \tag{3.8}$$

The derived A-stable methods are also L-stable if

$$\lim_{z\to-\infty} \frac{p_0(z)}{p_2(z)} = 0 \quad \text{and} \quad \lim_{z\to-\infty} \frac{p_1(z)}{p_2(z)} = 0.$$

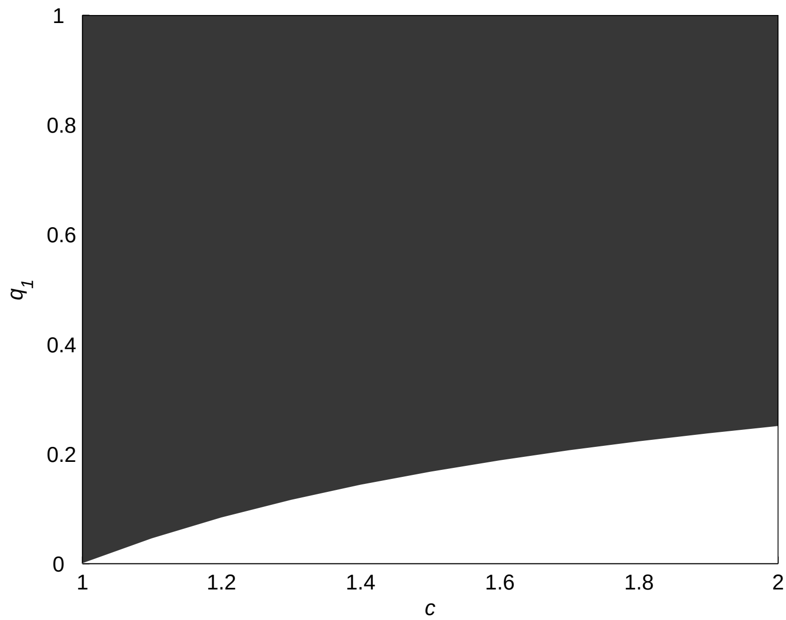

Figure 3.1: Region of A-stability in the (c, q_1)-plane for two-step methods (2.1) with $p = q = m = 1$ and satisfying the restrictions discussed above.

These conditions are equivalent to the system of equations

$$\begin{cases} (-1+c)(-c+q_1+2cq_1) = 0, \\ 2-3c+2c^2-(1-2c+4c^2)q_1 = 0, \end{cases}$$

which has a unique solutions $(c, q_1) = (1, \frac{1}{3})$. Correspondingly, we obtain the L-stable method with

$$\varphi_0(s) = -\frac{s}{3}, \quad \varphi_1(s) = \frac{3+s}{3}, \quad \chi(s) = 0, \quad \psi(s) = \frac{2s}{3},$$

and a one-parameter family of local error estimators of the type (2.9), with

$$\alpha_1 = -\alpha_0, \quad \beta = \frac{1}{2}\alpha_0, \quad \gamma = \frac{1}{2}\alpha_0.$$

We also observe that the derived L-stable method is also superconvergent since $E(1) = 0$ and, therefore, its uniform order is equal to 2.

4. Construction of methods with $m = 2$

We now consider two-stage continuous methods (2.1) with $p = q = m = 2$. We always assume that $[c_1, c_2] = [\frac{1}{2}, 1]$. We next impose the interpolation condition (3.1), which leads to

$$\varphi_0(0) = 0, \quad \chi_1(0) = 0, \quad \chi_2(0) = 0,$$
$$\varphi_1(0) = 1, \quad \psi_1(0) = 0, \quad \psi_2(0) = 0.$$

Correspondingly, we set

$$\varphi_0(s) = s(p_1 + p_2 s), \quad \chi_1(s) = s(q_1 + q_2 s), \quad \chi_2(s) = s(r_1 + r_2 s),$$

and derive $\varphi_1(s)$, $\psi_1(s)$ and $\psi_2(s)$ by imposing the system of order conditions (2.8) up to $p = 2$, obtaining

$$\begin{array}{rcl} \varphi_1(s) & = & 1 - p_1 s - p_2 s^2, \\ \psi_1(s) & = & s(2 + 3p_1 - 3q_1 - 2r_1 - s + 3p_2 s - 3q_2 s - 2r_2 s), \\ \psi_2(s) & = & -s(1 + 2p_1 - 2q_1 - r_1 - s + 2p_2 s - 2q_2 s - r_2 s). \end{array}$$

This leads to a six-parameter family of methods depending on p_1, p_2, q_1, q_2, r_1 and r_2. These parameters will be chosen in order to obtain methods which are A-stable and L-stable. We next consider the linear stability analysis, deriving the stability polynomial (compare [12, 13])

$$p(\omega, z) = \omega(p_3(z)\omega^3 + p_2(z)\omega^2 + p_1(z)\omega + p_0(z)), \tag{4.1}$$

where

$$p_0(z) = (p_2 q_1 - p_1 q_2)z, \tag{4.2}$$

and $p_1(z)$, $p_2(z)$, $p_3(z)$ are polynomials of degree 2 with respect to z. However, by imposing

$$q_1 = \frac{p_1 q_2}{p_2},$$

the polynomial (4.2) annihilates and, correspondingly, the stability function (4.1) takes the form

$$p(\omega, z) = \omega^2(\widetilde{p}_2(z)\omega^2 + \widetilde{p}_1(z)\omega + \widetilde{p}_0(z)),$$

where $\widetilde{p}_0(z)$, $\widetilde{p}_1(z)$, $\widetilde{p}_2(z)$ are polynomials of degree 2 with respect to z. Therefore, the stability properties of the resulting methods depend on the quadratic function (see [8])

$$\widetilde{p}(\omega, z) = \widetilde{p}_2(z)\omega^2 + \widetilde{p}_1(z)\omega + \widetilde{p}_0(z).$$

We next impose the system of equations leading to L-stability, i.e.

$$\lim_{z\to-\infty} \frac{\widetilde{p}_0(z)}{\widetilde{p}_2(z)} = 0, \qquad \lim_{z\to-\infty} \frac{\widetilde{p}_1(z)}{\widetilde{p}_2(z)} = 0.$$

This system takes the form

$$\begin{cases} p_2 r_1 - p_1 r_2 = 0, \\ p_2(-q_2 - r_1 + 3p_2 r_1 - 2q_2 r_1 - 2r_2) - p_1(q_2 + 3p_2 r_2 - 2q_2 r_2) = 0 \end{cases}$$

and has a unique solution given by

$$p_1 = -\frac{p_2(q_2 + 2r_2)}{q_2 + r_2}, \quad r_1 = -\frac{r_2(q_2 + 2r_2)}{q_2 + r_2}.$$

This leads to a three-parameter family of methods depending on p_2, q_2, r_2. We next apply the Schur criterion to determine the set of conditions involving these parameters, in order to be the corresponding methods A- and L-stable. Let us fix, for example, q_2=2: we carry out a computer search of L-stable methods in the parameter space (p_2, r_2), using this criterion. The result is shown in Fig. 4.2.

We now consider the expression of the corresponding local truncation error (2.2)

$$\xi(t_n + sh) = h^3 E(s) y^{(3)}(t_n) + h^4\Big(F(s) y^{(4)}(t_n) + G(s)\frac{\partial f}{\partial y}(y(t_n)) y^{(3)}(t_n)\Big) + O(h^5),$$

where $E(s) = C_2(s)$, $F(s) = C_3(s)$ and $G(s) = G_3(s)$ can be derived from formulas (2.3) and (2.4). For $r_2 = 1$, we obtain

$$G(1) = 945 - 714p_2 + 133p_2^2,$$

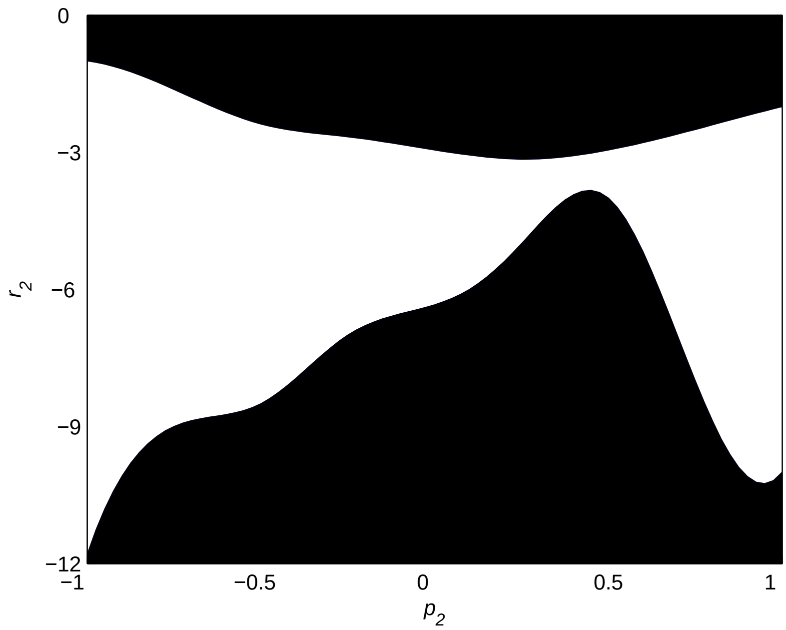

Figure 4.2: Region of L-stability in the (p_2, r_2)-plane for two-step methods (1.2) with $p = q = m = 2$, $q_2 = 2$ and satisfying the restriction discussed above.

and its roots are p_2=3, $p_2 = \frac{45}{19}$. Anyway, only in correspondence to the values $p_2 = \frac{45}{19}$ and $r_2 = 1$ the Schur criterion together with the L-stability requirements are satisfied. The basis functions of the corresponding L-stable method take the form

$$\begin{aligned} \varphi_0(s) &= -\frac{15s}{19}(4-3s), \qquad \varphi_1(s) = 1 + \frac{60}{19}s - \frac{45}{19}s^2, \\ \chi_1(s) &= -2s\left(\frac{4}{3} - s\right), \qquad \chi_2(s) = -s\left(\frac{4}{3} - s\right), \\ \psi_1(s) &= \frac{2s}{19}\left(\frac{91}{3} - 18s\right), \quad \psi_2(s) = -\frac{s}{19}\left(\frac{77}{3} - 24s\right). \end{aligned} \tag{4.3}$$

We next estimate the local truncation error associated to this method, using a two-parameter family of estimators of the type (2.9), with

$$\alpha_1 = -\alpha_0, \quad \beta_1 = \frac{8}{3} + \frac{4}{9}\alpha_0 + \frac{1}{3}\gamma_1, \quad \beta_2 = -4 + \frac{4}{3}\alpha_0 - \gamma_1, \quad \gamma_2 = \frac{4}{3} - \frac{7}{9}\alpha_0 - \frac{1}{3}\gamma_1.$$

We observe that the error constant $E(1)$ is equal to 0 and, therefore, the above method has uniform order of convergence equal to 3.

5. Construction of methods with $m = 3$

We now focus our attention on two-step continuous methods of order $p = q = m = 3$, assuming that $\varphi_0(s) = 0$ and imposing not only the interpolation condition (3.1), but also the collocation condition

$$P'(t_n + c_i h) = f(t_n + c_i h, P(t_n + c_i h)), \tag{5.1}$$

for $i = 1, 2, 3$. We next assume $[c_1, c_2, c_3] = [\frac{1}{2}, \frac{3}{4}, 1]$ and

$$\begin{aligned}
\chi_1(s) &= p_0 + p_1 s + p_2 s^2 + p_3 s^3 + p_4 s^4, \\
\chi_2(s) &= r_0 + r_1 s + r_2 s^2 + r_3 s^3 + r_4 s^4, \\
\chi_3(s) &= s_0 + s_1 s + s_2 s^2 + s_3 s^3 + s_4 s^4.
\end{aligned}$$

Therefore, imposing the set of conditions (3.1) and (5.1), we obtain

$$\begin{aligned}
\chi_1(s) &= \frac{s}{4}(-6p_4 + 13p_4 s - 12p_4 s^2 + 4p_4 s^3), \\
\chi_2(s) &= \frac{s}{4}(-6r_4 + 13r_4 s - 12r_4 s^2 + 4r_4 s^3), \\
\chi_3(s) &= \frac{s}{4}(-6s_4 + 13s_4 s - 12s_4 s^2 + 4s_4 s^3).
\end{aligned}$$

We next compute the remaining basis functions via order conditions (2.8) for $p = m = 3$, whose expressions are here omitted for brevity. We have now 3 free parameters (p_4, r_4 and s_4) to play with in order to achieve the desired stability properties. We next analyze the stability polynomial associated to this family of methods, i.e.

$$p(\omega, z) = \omega^3 (p_2(z)\omega^2 + p_1(z)\omega + p_0(z)),$$

where $p_0(z)$, $p_1(z)$ and $p_2(z)$ are polynomials of degree 3 with respect to z. The stability property of resulting methods now depend on the quadratic function (compare [8])

$$\widetilde{p}(\omega, z) = p_2(z)\omega^2 + p_1(z)\omega + p_0(z).$$

We next solve the system of equations leading to L-stability

$$\lim_{z\to-\infty} \frac{p_0(z)}{p_2(z)} = 0, \qquad \lim_{z\to-\infty} \frac{p_1(z)}{p_2(z)} = 0,$$

with respect to s_4, obtaining

$$s_4 = -\frac{1}{8}(4p_4 - 3r_4).$$

At this point, everything depends on the parameters $p_4,\ r_4$. We have next applied the Schur criterion to determine the set of conditions involving $p_4,\ r_4$, in order to be the corresponding methods L-stable and carried out a computer search of L-stable methods in the parameter space (p_4, r_4), according to these conditions. The results are given in Fig. 5.3.

We now consider the expression of the local truncation error which is, in our case,

$$\xi(t_n + sh) = h^4 E(s) y^{(4)}(t_n) + h^5 \Big(F(s) y^{(5)}(t_n) + G(s) \frac{\partial f}{\partial y}(y(t_n)) y^{(4)}(t_n) \Big) + O(h^6),$$

where $E(s) = C_3(s)$, $F(s) = C_4(s)$ and $G(s) = G_4(s)$ are computed using formulas (2.6) and (2.7). In particular, the expression of $G_4(1)$ is

$$G(1) = -(784 + 60p_4 + 57r_4)(16 + 108p_4 + 69r4),$$

and it annihilates for

$$r_4 = -\frac{-4(196 + 15p_4)}{57}, \quad r_4 = -\frac{4(4 + 27p_4)}{69},$$

but only the first one is acceptable for us, because the line $r_4 = -\frac{4(4+27p_4)}{69}$ does not lie inside the L-stability region in Fig. 5.3. Correspondingly, in order to achieve L-stability, we obtain from the Schur criterion that

$$\mu < p_4 < \frac{554}{21},$$

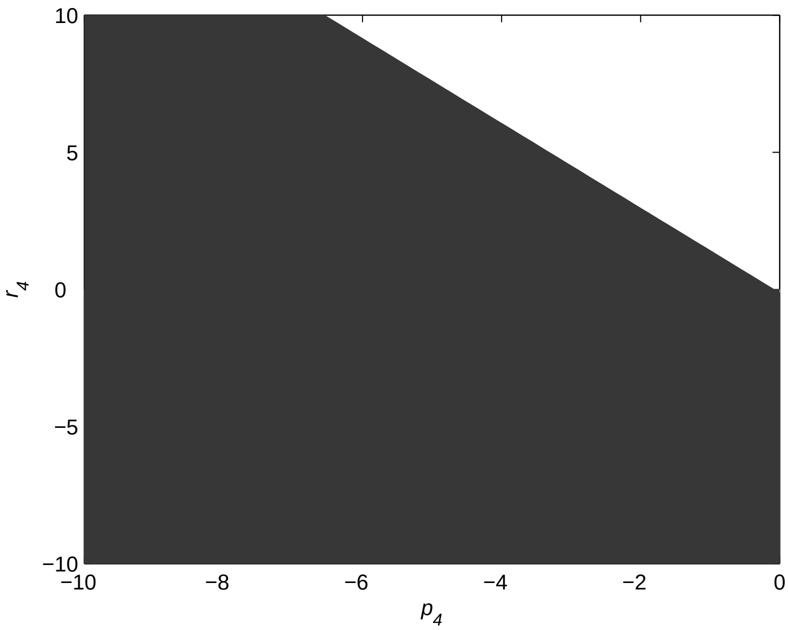

Figure 5.3: Region of L-stability in the (p_4, r_4)-plane for two-step methods (2.1) with $p = q = m = 3$ satisfying the restrictions discussed above.

where μ is the negative root of the polynomial

$$\begin{aligned} q(x) &= -5045494028660092 - 341657542579860x - 5937877049931x^2 \\ &+ 80771782176x^3 + 136188864x^4. \end{aligned}$$

Moreover, we have

$$E(1) = \frac{554 - 21p_4}{912}, \quad F(1) = \frac{16841 - 315p_4}{54720}.$$

We observe that the error constant $E(1)$ annihilates in $p_4 = \frac{554}{21}$: in correspondence of this value, we gain one order more of convergence, but the L-stability constraint are not satisfied. Therefore, we decide to choose a value of p_4 which allows us to achieve L-stability and, at the same time, provides a small error constant. For example, taking $p_4 = 20$, we obtain the L-stable method with $E(1) = \frac{67}{456}$, $F(1) = \frac{10541}{54720}$, $G(1) = 0$, and basis functions

$$\begin{aligned} &\varphi_0(s) = 0, \quad \varphi_1(s) = 1, \\ &\chi_1(s) = 5s(-6 + 13s - 12s^2 + 4s^3), \quad \chi_2(s) = -\frac{496s}{57}(-3 + 2s)(2 - 3s + 2s^2), \\ &\chi_3(s) = -\frac{219s}{38}(-3 + 2s)(2 - 3s + 2s^2), \quad \psi_1(s) = -\frac{s}{37}(15594 - 34129s + 31720s^2 - 10624s^3), \\ &\psi_2(s) = \frac{16\,s}{57}(1182 - 2580s + 2402s^2 - 807s^3), \quad \psi_3(s) = -\frac{s}{6}(684 - 1491s + 1388s^2 - 468s^3). \end{aligned}$$

We can estimate the local truncation error of this method, using a three-parameter family of estimators of type (2.9), with

$$\begin{aligned} \alpha_1 &= -\alpha_0, \\ \beta_1 &= -\frac{96}{5} + \frac{5723}{57}\alpha_0 + \frac{3}{10}\beta_3 + \frac{1}{2}\gamma_3, \quad \beta_2 = 32 - \frac{9437}{57}\alpha_0 - \beta_3 - \gamma_3, \\ \gamma_1 &= -32 + \frac{9418}{57}\alpha_0 - \frac{1}{2}\beta_3 + \frac{5}{2}\gamma_3, \qquad \gamma_2 = \frac{96}{5} - \frac{5647}{57}\alpha_0 + \frac{1}{5}\beta_3 - 3\gamma_3. \end{aligned}$$

6. Construction of methods with $m = 4$

We now derive four-stage continuous methods (1.2) of order $p = q = m = 4$, with $\varphi_0(s) = 0$ and satisfying the interpolation condition (3.1) and the collocation condition (5.1) for $i = 1, 2, 3, 4$. We assume in advance the collocation abscissa $[c_1,\ c_2,\ c_3,\ c_4] = [0, \frac{1}{2},\ \frac{3}{4},\ 1]$ and the following form for the basis functions

$$\begin{aligned} \chi_1(s) &= s(p_1 + p_2 s + p_3 s^2 + p_4 s^3 + p_5 s^4), \\ \chi_2(s) &= s(q_1 + q_2 s + q_3 s^2 + q_4 s^3 + q_5 s^4), \\ \chi_3(s) &= s(r_1 + r_2 s + r_3 s^2 + r_4 s^3 + r_5 s^4), \\ \chi_4(s) &= s(s_1 + s_2 s + s_3 s^2 + s_4 s^3 + s_5 s^4), \end{aligned}$$

where p_i, q_i, r_i, s_i, for $i = 1, 2, 3, 4$, are derived in order to satisfy the collocation conditions. We next derive $\psi_i(s)$, for $i = 1, 2, 3, 4$ imposing the set of order conditions (2.8), for $p = m = 4$. We omit their expressions for brevity. We have now 4 free parameters (p_4, q_4, r_4 and s_4) to compute in order to achieve the desired stability properties.

We next develop the linear stability analysis, studying the stability polynomial

$$p(\omega, z) = \omega^4(p_2(z)\omega^2 + p_1(z)\omega + p_0(z)),$$

where $p_0(z),\ p_1(z),\ p_2(z),\ p_3(z)$ are polynomials of degree 4 with respect to z. Hence, the stability properties of the stability polynomial depend on the quadratic function

$$\widetilde{p}(\omega, z) = p_2(z)\omega^2 + p_1(z)\omega + p_0(z).$$

We next solve the conditions for L-stability

$$\lim_{z\to-\infty} \frac{p_0(z)}{p_2(z)} = 0, \quad \lim_{z\to-\infty} \frac{p_1(z)}{p_2(z)} = 0,$$

with respect to p_5 and r_5, obtaining

$$p_5 = \frac{3072 + 17792q_5 - 21s_5}{99840}, \quad r_5 = -\frac{3072 + 9472q_5 - 21s_5}{3120}.$$

At this point, everything depends on the parameters $q_5,\ s_5$. We now consider the expression of the local truncation error (2.2)

$$\xi(t_n + sh) = h^5 E(s) y^{(5)}(t_n) + h^6\Big(F(s)y^{(6)}(t_n) + G(s)\frac{\partial f}{\partial y}(y(t_n))y^{(5)}(t_n)\Big) + O(h^7),$$

where $E(s) = C_4(s)$, $F(s) = C_5(s)$ and $G(s) = G_5(s)$ have been computed using (2.3) and (2.4). In particular, $G(1)$ takes the form

$$G(1) = -s_5(5768192 - 258048q_5 - 265631s_5),$$

and annihilates for

$$q_5 = \frac{5768192 - 265631s_5}{258048}.$$

With this position, it is possible to prove using the Schur criterion that, for any $s_5 < 0$, the corresponding method is A-stable and L-stable. If we choose $s_5 = -1$, we obtain

$$
\begin{aligned}
\varphi_0(s) &= 0, \quad \varphi_1(s) = 1,\\
\chi_1(s) &= -\frac{12999029s^2}{148635648}(45-130s+135s^2-48s^3),\\
\chi_2(s) &= -\frac{6033823s^2}{12386304}(45-130s+135s^2-48s^3),\\
\chi_3(s) &= \frac{3482603s^2}{2322432}(45-130s+135s^2-48s^3),\\
\chi_4(s) &= \frac{s^2}{48}(45-130s+135s^2-48s^3),\\
\psi_1(s) &= s\left(1-\frac{58553863}{8257536}s+\frac{602930779}{37158912}s^2-\frac{42497543}{2752512}s^3+\frac{8132507}{1548288}s^4\right),\\
\psi_2(s) &= -\frac{s^2}{1769472}(364272993-1066499978s+1117591587s^2-399882480s^3),\\
\psi_3(s) &= \frac{s^2}{2322432}(603731871-1755124342s+1835968221s^2-657192720s^3),\\
\psi_4(s) &= -\frac{s^2}{1835008}(164345193-476610010s+497623099s^2-178237552s^3),
\end{aligned}
\tag{6.1}
$$

and $E(1) = \frac{1}{36864}$, $F(1) = \frac{69411889}{1486356480}$, $G(1) = 0$. We finally estimate the local truncation error of this method using a four-parameter family of estimators (2.9) with

$$
\begin{aligned}
\alpha_1 &= -\alpha_0, & \beta_1 &= \frac{128}{3}+\frac{517}{1440}\alpha_0-\frac{5}{12}\gamma_3-\frac{5}{3}\gamma_4,\\
\beta_2 &= -384-\frac{511}{480}\alpha_0+\frac{21}{4}\gamma_3+20\gamma_4, & \beta_3 &= \frac{2048}{3}+\frac{277}{90}\alpha_0-\frac{35}{3}\gamma_3-\frac{128}{3}\gamma_4,\\
\gamma_1 &= -384-\frac{751}{480}\alpha_0-\beta_4+\frac{35}{4}\gamma_3+30\gamma_4, & \gamma_2 &= \frac{128}{3}+\frac{277}{1440}\alpha_0-\frac{35}{12}\gamma_3-\frac{20}{3}\gamma_4.
\end{aligned}
$$

7. Implementation of two-step continuous methods

This section is devoted to the description of the issues we have considered for the variable stepsize implementation of two-step continuous methods (1.2) for the numerical solution of stiff problems (1.1). In particular, we discuss the following aspects:

- the construction of a starting procedure;
- a reliable estimation of the local truncation error and its assessment for large values of the stepsize;
- a stepsize control strategy;
- the solution of the nonlinear system of equations in the internal stages.

Starting procedure.
Concerning the starting procedure, we proceed as follows. We choose an initial stepsize h_0 and compute the missing starting values $y_1 \approx y(t_0 + h_0)$ and $Y^{[0]} \approx (y(t_0 + c_j h_0))_{j=1}^m$, using the m-stage Runge–Kutta method

$$
\begin{cases}
y_1 = y_0 + h_0(b^T \otimes I)F^{[0]},\\
Y^{[0]} = (e \otimes I)y_0 + h_0(A \otimes I)F^{[0]},
\end{cases}
\tag{7.1}
$$

based on the Gaussian nodes (see [3]), of order $p = 2m$ and stage order $q = m$. In the integration of stiff systems, such methods suffer from order reduction (for instance, see [4]) and, therefore, their effective order is equal to m. These are implicit methods and, therefore, the stage vector $Y^{[0]}$ has to be determined by solving the nonlinear system in (7.1): its solution is computed by using Newton iterations, in the following way. We set

$$\Phi(Y^{[0]}) = Y^{[0]} - (e \otimes I)y_0 - h_0(A \otimes I)F^{[0]}$$

and aim to solve the system $\Phi(Y^{[0]}) = 0$, of dimension $md \times md$. We take as initial guess the vector

$$Y^{[0],0} = [y_0, \ldots, y_0]^T \in \mathbb{R}^{md},$$

and start the following Newton-type iterative procedure

$$Y^{[0],i+1} = Y^{[0],i} - (\partial\Phi(Y^{[0],i}))^{-1}\Phi(Y^{[0],i}), \tag{7.2}$$

for $i = 0, 1, \ldots, \nu - 1$, where

$$\partial\Phi(Y^{[0]}) = I_{md} - h(A \otimes I_d)J \in \mathbb{R}^{md \times md},$$

and J is the Jacobian matrix of $F^{[0]}$, i.e. the block diagonal matrix

$$J = \begin{bmatrix} \partial f(Y_1^{[0]}) & & \\ & \ddots & \\ & & \partial f(Y_m^{[0]}) \end{bmatrix},$$

where $\partial f(Y_j^{[0]})$ is the Jacobian matrix of f evaluated in $Y_j^{[0]}$, for $j = 1, 2, \ldots, m$. The expression (7.2) is equivalent to the linear system

$$-\partial\Phi(Y^{[0],i})\delta Y^{[0]} = \Phi(Y^{[0],i}), \tag{7.3}$$

where $\delta Y^{[0]} = Y^{[0],i+1} - Y^{[0],i}$. We next solve the system (7.3) with respect to $\delta Y^{[0]}$, for example by Gaussian elimination, and derive

$$Y^{[0],i+1} = Y^{[0],i} + \delta Y^{[0]}.$$

We stop the iterative scheme at the ν-th step, when $\|\delta Y^{[0]}\|_\infty < tol$ and $\|\Phi Y^{[0],\nu}\|_\infty < tol$, and take $Y^{[0]} = Y^{[0],\nu}$. We next compute the value $\widehat{y}_1$, applying the Runge–Kutta methods twice, i.e. with two steps of stepsize $h_0/2$, in order to estimate the local error by means of Richardson extrapolation (see [17])

$$est(t_1) = \frac{2^{2m}(y_1 - \widehat{y}_1)}{1 - 2^{2m}}.$$

It is well known that Richardson extrapolation is accurate, but also expensive. However, its usage in our implementation is only restrict to the very first step of the integration, so its contribution to the overall cost of the algorithm is not significant. Finally, the stepsize h_0 is adjusted until $\|est(t_1)\| < tol$.

Assessment of the local error estimation for large step sizes

We have provided in Section 2 the estimation (2.9) to the local truncation error, following the ideas reported in [12, 13]. Such an estimate is asymptotically correct for h_n tending to 0: this property can be tested by means of Taylor series expansion arguments, or may be obvious from its construction. However, in order to approach stiff systems, this property of correctness is not sufficient, since their solution also requires the usage of large stepsizes with respect to certain features of the problem. Shampine and Baca in [24] focused their attention on the assessment of the quality of the error estimate for large values of the stepsize, by using similar arguments as in the classical theory of absolute stability. We now specialize the results proposed in [24] to our class of methods (1.2).

Following the lines drawn in [24], we consider a restricted class of problems of the form $y' = Jy$, where J is a constant matrix that can be diagonalized by a similarity transformation $M^{-1}JM = \mathrm{diag}(\xi_i)$. Then, it is sufficient to consider the scalar problem

$$\begin{cases} y'(t) = \xi y, & t \geq 0, \\ y(0) = 1, \end{cases} \tag{7.4}$$

where $\xi \in \mathbb{C}$ is one the eigenvalues of J, which is supposed to have negative real part. The solution of the problem (7.4) is $y(t) = e^{\xi t}$ and, therefore,

$$Y^{[n]} = e^{\xi(t_n + \mathbf{c}h_n)} + O(h_n^{p+1})$$

and

$$Y^{[n-1]} = e^{\xi(t_n + (\mathbf{c}-\mathbf{e})h_{n-1})} + O(h_n^{p+1}).$$

As a consequence, we obtain

$$\mathrm{le}(t_n) = e^{\xi t_n}\Big(e^{z\delta_n} - \varphi_0(1)e^{-z} - \varphi_1(1) - z\delta_n(v^T \otimes I)e^{z(\mathbf{c}-\mathbf{e})} - z\delta_n(w^T \otimes I)e^{z\mathbf{c}\delta_n}\Big) + O(z^{p+2}),$$

where $z = \xi h_{n-1}$ and $\delta_n = \frac{h_n}{h_{n-1}}$. We next achieve an analogous expression also for the error estimate $\mathrm{est}(t_n)$, obtaining

$$\mathrm{est}(t_n) = C_p(1)e^{\xi t_n}\Big(\alpha_0 e^{-z} + \alpha_1 + z\delta_n(\beta^T \otimes I)e^{z(\mathbf{c}-\mathbf{e})} + z\delta_n(\gamma^T \otimes I)e^{z\mathbf{c}\delta_n}\Big) + O(z^{p+2}).$$

To investigate the behaviour of error estimates for large values of z, we define the functions $R_{\mathrm{le}}(z,\delta)$ and $R_{\mathrm{est}}(z,\delta)$, respectively defined by

$$R_{\mathrm{le}}(z,\delta) = e^{z\delta} - \varphi_0(1)e^{-z} - \varphi_1(1) - z\delta(v^T \otimes I)e^{z\mathbf{c}\delta} - z\delta(w^T \otimes I)e^{z(\mathbf{c}-\mathbf{e})\delta},$$

$$R_{\mathrm{est}}(z,\delta) = \alpha_0 e^{-z} + \alpha_1 + z\delta(\beta^T \otimes I)e^{z(\mathbf{c}-\mathbf{e})\delta} + z\delta(\gamma^T \otimes I)e^{z\mathbf{c}\delta},$$

corresponding to $\mathrm{le}(t_n)$ and $\mathrm{est}(t_n)$. To assess the quality of $\mathrm{est}(t_n)$ for large step sizes, we examine the ratio

$$r(z,\delta) = \frac{R_{\mathrm{est}}(z,\delta)}{R_{\mathrm{le}}(z,\delta)}. \tag{7.5}$$

If $r(z,\delta) \sim \text{constant} \cdot z^{\mu}$, for $\mathrm{Re}(z) < 0$ as $|z| \to \infty$ with a positive integer μ, the error is grossly overestimated for large z. To compensate for this, Shampine and Baca proposed in [24], in the context of RK methods, premultiplying $\mathrm{est}(t_n)$ by the so-called *filter matrix*,

$$(I - h_n\mathbf{J}(t_n))^{-\mu}$$

where $\mathbf{J}(t_n)$ is an approximation to th Jacobian matrix of the problem (1.1) at the point t_n. This choice is suitable to damp the large, stiff error components.

Concerning two-step continuous methods (1.2), we observe that the ratio (7.5) behaves in the following way:

$$r(z,\delta) \sim -\frac{\alpha_1}{\varphi_0(1)}, \quad |z| \to \infty, \quad \mathrm{Re}(z) < 0,$$

and this behaviour would suggest that the original estimate $\mathrm{est}(t_n)$ can be used for all the values of the stepsize. However, it is important to observe that the denominator appearing in the above expression is equal to $\varphi_0(1)$ which, for zero-stability requirements, is always between -1 and 1: this means that, for small values of $\varphi_0(1)$ close to zero, the ratio $r(z,\delta)$ results to be very large and, therefore, the error estimate $\mathrm{est}(t_n)$ would not be reliable at all. On the contrary, the filtered estimation

$$\mathrm{est}'(t_n) = (I - h_n J)^{-1}\mathrm{est}(t_n), \tag{7.6}$$

corresponding to the filter matrix $(I - h_n J)^{-1}$ proposed in [24], results to be much more reliable than the original estimation $\mathrm{est}(t_n)$, as it has also been verified experimentally. As observed in [24], the improved error estimator does not alter the behaviour for small h_n but it corrects the behaviour of the estimate for large values of h_n.

Stepsize control strategy

Once we have derived an estimation to the local error, we can decide whether to increase or decrease the stepsize in the advancing from the point t_n to the point t_{n+1} according to the following control (see [1])

$$||est(n)|| \le Rtol \cdot \max\{||y_{n-1}||, ||y_n||\} + Atol, \tag{7.7}$$

where *Atol* and *Rtol* are given absolute and relative tolerances. In our numerical experiments we have used $Atol = Rtol = tol$. If the control (7.7) is not satisfied, the stepsize h_n is halved. Otherwise, the stepsize is accepted and a new stepsize for the following step is computed, according to a suitable control strategy. The standard step control strategy (see [17])

$$h_{n+1} = h_n \cdot \min\left(2, \left(\frac{fac \cdot tol}{\|est(t_n)\|}\right)^{\frac{1}{p+1}}\right), \tag{7.8}$$

which only depends on the estimate computed in the previous step, can often determine useless stepsize rejections, “with disruptive and wasteful increases and decreases” of the stepsize (see [4]). Gustafsson, Lundh and Söderlind [16, 26, 27] introduced a different stepsize control, the so-called PI stepsize control, based on control theory arguments. The PI control involve the estimation of the local errors related to the two most recent step points, as follows

$$h_{n+1} = h_n \cdot \min\left(2, \left(\frac{tol}{\|est(t_n)\|}\right)^{\sigma_1}\left(\frac{tol}{\|est(t_{n-1})\|}\right)^{\sigma_2}\right), \tag{7.9}$$

where σ_1 and σ_2 must be suitably chosen. In [18, 26, 27] the derivation of σ_1 and σ_2 is discussed, according to some control theory arguments. In our case, we have experimentally found some values for σ_1 and σ_2 in order to obtain a PI stepsize control which is competitive with the standard one in the implementation of our methods: they are $\sigma_1 \approx 0.3$ and $\sigma_2 \approx 0.04$.

When we advance from t_n to t_{n+1} with stepsize h_n, another problem occurs, i.e. the computation of the missing approximations $\widetilde{y}_{n-1}$ to $y(\widetilde{t}_{n-1})$, with $\widetilde{t}_{n-1} = t_n - h_n$, and $\widetilde{Y}_i^{[n-1]}$ to $y(\widetilde{t}_{n-1} + c_i h_n)$, with $i = 1, 2, \ldots, m$. The computation of such approximations can be efficiently derived taking into account the special structure of the methods we are implementing: continuous methods are particularly suitable for the design of a numerical solver in a variable stepsize environment, since every time the stepsize changes, the missing approximations to the solution in previous points can be suitably computed by evaluating the continuous approximant in these points. In fact, let us suppose that k is the minimum integer such that $\widetilde{t}_{n-1}$ belongs to the interval $[t_k, t_{k+1}]$ of length h_k. The point $\widetilde{t}_{n-1}$ is then uniquely determined by the time scaled variable

$$\widetilde{s} = \frac{\widetilde{t}_{n-1} - t_k}{h_k}.$$

The value of $\widetilde{y}_{n-1}$ can next be computed by evaluating the continuous approximant $P(t_k + sh_k)$ (1.2) in correspondence to $s = \widetilde{s}$, obtaining

$$\widetilde{y}_{n-1} = \varphi_0(\widetilde{s})y_{k-1} + \varphi_1(\widetilde{s})y_k + h_k \sum_{i=1}^{m} \left(\chi_i(\widetilde{s}) f(Y_i^{[k-1]}) + \psi_i(s) f(Y_i^{[k]})\right).$$

In an analogous way, we can derive the values of $\widetilde{Y}_i^{[n-1]}$, $i = 1, 2, \ldots, m$. Let us assume that r is the minimum integer such that $\widetilde{t}_{n-1} + c_i h$, for a fixed value of the index i, belongs to the interval $[t_r, t_{r+1}]$ of length h_r. The point $\widetilde{t}_{n-1} + c_i h$ corresponds to the value of the time scaled variable

$$\widetilde{s}_i = \frac{\widetilde{t}_{n-1} + c_i h_r - t_r}{h_r}.$$

The missing value of $\widetilde{Y}_i^{[n-1]}$ can then be computed by evaluating the continuous approximant $P(t_r + sh_r)$ (1.2) in correspondence to $s = \widetilde{s}_i$, obtaining

$$\widetilde{Y}_i^{[n-1]} = \varphi_0(\widetilde{s}_i)y_{r-1} + \varphi_1(\widetilde{s}_i)y_r + h_r \sum_{j=1}^{m} \left(\chi_j(\widetilde{s}_i) f(Y_j^{[r-1]}) + \psi_j(s_i) f(Y_j^{[r]})\right).$$

Computation of the stage values

Two-step continuous methods are implicit formulae and, therefore, they require the solution of a system of nonlinear equations of dimension $md \times md$ at each time step. We solve this system by means of Newton-type iterations, in the following way. We define

$$\Phi(Y^{[n]}) = Y^{[n]} - (u \otimes I)y_{n-1} - (\widetilde{u} \otimes I)y_n - h\left((A \otimes I)F^{[n-1]} - (B \otimes I)F^{[n]}\right),$$

and aim to solve the system $\Phi(Y^{[n]}) = 0$. We take as initial guess the vector

$$Y^{[n],0} = [y_n, \ldots, y_n]^T \in \mathbb{R}^{md},$$

and start the following Newton-type iterative procedure

$$Y^{[n],i+1} = Y^{[n],i} - (\partial\Phi(Y^{[n],i}))^{-1}\Phi(Y^{[n],i}), \tag{7.10}$$

for $i = 0, 1, \ldots, \mu - 1$, where

$$\partial\Phi(Y^{[0]}) = I_{md} - h(B \otimes I_d)J \in \mathbb{R}^{md\times md},$$

and J is the Jacobian matrix of $F^{[n]}$, i.e. the block diagonal matrix

$$J = \begin{bmatrix} \partial f(Y_1^{[n]}) & & \\ & \ddots & \\ & & \partial f(Y_m^{[n]}) \end{bmatrix},$$

where $\partial f(Y_j^{[n]})$ is the Jacobian matrix of f evaluated in $Y_j^{[n]}$, for $j = 1, 2, \ldots, m$. The expression (7.10) is equivalent to the linear system

$$-\partial\Phi(Y^{[n],i})\delta Y^{[n]} = \Phi(Y^{[n],i}), \tag{7.11}$$

where $\delta Y^{[n]} = Y^{[n],i+1} - Y^{[n],i}$. We next solve the system (7.11) with respect to $\delta Y^{[n]}$, for instance by Gaussian elimination, and derive

$$Y^{[n],i+1} = Y^{[n],i} + \delta Y^{[n]}.$$

We stop the iterative scheme at the μ-th step, when $\|\delta Y^{[n]}\|_\infty < tol$ and $\|\Phi Y^{[n],\mu}\|_\infty < tol$, and take $Y^{[n]} = Y^{[n],\mu}$.

The numerical solution of the nonlinear system $\Phi(Y^{[n]}) = 0$ can be efficiently approached if the matrix B has a structured shape, e.g. lower triangular or diagonal: in these cases, instead of solving a nonlinear system of dimension md, we solve m successive or independent nonlinear systems of dimension d and, in particular, when these systems are independent, their solution can be fastly computed in a parallel environment. The construction of such numerical methods is treated in [15].

8. Numerical examples

In this section we present some fixed and variable stepsize numerical experiments which aim to indicate the effectiveness of two-step continuous methods, especially in the implementation of stiff problems, and the reliability of the local error estimation. The implementation issues we have used in order to carry out the following experiments are the ones described in Section 7. We aim to solve the following problems:

1. The Prothero-Robinson problem

$$\begin{cases} y'(t) = \lambda(y(t) - G(t)) + G'(t), \quad t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{8.1}$$

   where $\mathrm{Re}(\lambda) < 0$ and $G(t)$ is a slowly varying function on the interval $[t_0, T]$. As observed by Hairer and Wanner [18] in the context of Runge-Kutta methods this equation provides much new insight into the behaviour of numerical methods for stiff problems. This equation with $t_0 = 0$, $G(t) = \exp(\mu t)$, and $y_0 = 1$, was also used by Butcher [3] to investigate the order reduction for Runge-Kutta-Gauss methods of order $p = 2m$;
2. The van der Pol oscillator (see VDPOL problem in [18])

$$\begin{cases} y_1'(t) = y_2(t), & t \in [0, T], \\ y_2'(t) = \dfrac{(1 - y_1^2(t))y_2(t) - y_1(t)}{\varepsilon}, & \\ y_1(0) = 2, & \\ y_2(0) = 0, & \end{cases} \tag{8.2}$$

k	$\lambda = -10$			k	$\lambda = -10^5$		
	$e_h^{RK}(T)$	fe	p		$e_h^{RK}(T)$	fe	p
6	$3.70 \cdot 10^{-6}$	384		6	$7.90 \cdot 10^{-9}$	384	
7	$4.74 \cdot 10^{-7}$	768	2.96	7	$1.98 \cdot 10^{-9}$	768	1.99
8	$6.00 \cdot 10^{-8}$	1536	2.98	8	$4.96 \cdot 10^{-10}$	1536	2.00
9	$7.55 \cdot 10^{-9}$	3072	2.99	9	$1.23 \cdot 10^{-10}$	3072	2.01
10	$9.46 \cdot 10^{-10}$	6144	3.00	10	$3.03 \cdot 10^{-11}$	6144	2.02
11	$1.18 \cdot 10^{-10}$	12288	3.00	11	$7.36 \cdot 10^{-12}$	12288	2.04

Table 8.1: Numerical results for Radau IIA method of order $p = 3$ and stage order $q = 2$ for the Prothero-Robinson problem.

with $T > 0$ and $\varepsilon = 10^{-6}$. This equation constitutes a challenging problem for numerical methods: small oscillations are amplified, while large oscillations are damped (compare [17]).

8.1. Fixed stepsize experiments

We first present some fixed stepsize numerical results which confirm that two-step continuous methods do not suffer from order reduction in the integration of stiff differential systems, which is the case for classical Runge-Kutta formulae. This phenomenon does not occur for two-step continuous methods (1.2), because they possess high stage order equal to their order of convergence. Indeed the order convergence of (1.2) is the same over the entire integration interval. On the other hand, Runge-Kutta methods do not possess the same feature, because their stage order is only equal to m, where m is the number of stages. To illustrate this we have applied the two-stage Radau IIA method (compare [3, 22]) of order $p = 3$ and stage order $q = 2$ and the L-stable two-step continuous method (4.3) of uniform order order $p = 3$ to the Prothero-Robinson problem (8.1), with $G(t) = G'(t) = \exp(t)$, $y_0 = 1$, $t_0 = 0$ and $T = 2$. We have implemented both methods with fixed stepsize $h = (T - t_0)/2^k$, in correspondence to different integer values of k, and listed norms of errors $\|e_h(T)\|$ at the endpoint of integration T, the number fe of function evaluations and the observed order of convergence p computed from the formula

$$p = \frac{\log\left(\|e_h(T)\|/\|e_{h/2}(T)\|\right)}{\log(2)},$$

where $e_h(T)$ and $e_{h/2}(T)$ are errors corresponding to stepsizes h and $h/2$.

The results are presented in Tables 8.1 and 8.2, for the Radau IIA method and the two-step continuous one respectively, in correspondence to two values of the stiffness parameter λ.

We can observe that in the case $\lambda = -10$, for which the Prothero-Robinson problem is nonstiff, both methods are convergent with expected order $p = 3$. However, for $\lambda = -10^5$, the problem is stiff and the Radau IIA method exhibits the order reduction phenomenon: in fact, its order of convergence drops to about $p = 2$ which corresponds to the stage order $q = 2$. This is not the case for the method (4.3), which preserves order of convergence $p = q = 3$ and provides higher accuracy. Therefore, the two-step continuous method (4.3) is able to achieve better accuracy for the stiff Prothero-Robinson problem (8.1) at a lower computational cost.

Additional results confirming that two-step continuous methods preserve the order of convergence for stiff problems can be found in [12, 14, 15].

8.2. Variable stepsize experiments

We now present the results originated by implementing the A-stable two-step continuous method (1.2) of uniform order 2, corresponding to the basis functions

	$\lambda = -10$				$\lambda = -10^5$		
k	$e_h^{TSC}(T)$	fe	p	k	$e_h^{TSC}(T)$	fe	p
6	$2.31 \cdot 10^{-6}$	378		3	$6.60 \cdot 10^{-8}$	42	
7	$4.01 \cdot 10^{-7}$	762	2.53	4	$9.11 \cdot 10^{-9}$	90	2.86
8	$6.01 \cdot 10^{-8}$	1530	2.74	5	$1.20 \cdot 10^{-9}$	186	2.92
9	$8.28 \cdot 10^{-9}$	3066	2.86	6	$1.55 \cdot 10^{-10}$	378	2.95
10	$1.09 \cdot 10^{-9}$	6138	2.92	7	$1.87 \cdot 10^{-11}$	762	3.05
11	$1.40 \cdot 10^{-10}$	12282	2.95	8	$2.48 \cdot 10^{-12}$	1530	2.92

Table 8.2: Numerical results for two-step continuous method (4.3) of uniform order $p = 3$ for the Prothero-Robinson problem.

$$\begin{array}{ll} \varphi_0 = 0, & \varphi_1 = 1, \\ \chi_1 = \dfrac{s}{6}(7-3s), & \chi_2 = -2s\left(\frac{7}{3}-s\right), \\ \psi_1 = \dfrac{s}{6}(47-21s), & \psi_2 = -\dfrac{2}{3}s(5-3s). \end{array} \tag{8.3}$$

The used implementation issues are the ones described in Section 7. Concerning the Prothero-Robinson problem (8.1), we choose $G(t) = \sin(t)$, $y_0 = 1$, $t_0 = 0$ and $T = 2\pi$. It is known that the problem (8.1) is much more stiff when the stiffness parameter λ is negative and large in modulus. The experimental results reported in Figures 8.4 and 8.5 are referred to the case $\lambda = -1e6$, while Figure 8.6 contains the results regarding the case $\lambda = -1e10$. We observe that, in correspondence to both these values, the problem (8.1) is very stiff. In particular, Figures 8.5 and 8.6 (bottom) show the reliability of the error estimate, also when the problem is very stiff. Moreover, as suggested by Figures 8.4 and 8.6 (top), the stepsize pattern is very smooth, especially because of the high stability properties of the implemented method and in force of the used stepsize control strategy: this control also avoid useless stepsize refusions. In particular, we observe that the stepsize refusions at the beginning of the integration are only due to the presence of an initial transient in the point t_0: the exact solution, i.e. $y(t) = \sin(t)$, is equal to 0 in $t_0 = 0$, while we have chosen $y_0 = 1$. This causes an initial transient in the solution, which requires a certain effort to be overcome.

Figures 8.7 and 8.8 report the results concerning the numerical solution of the Van der Pol problem for $\varepsilon = 1e-6$ and $tol = 1e-4$. In correspondence to this value of the stiffness parameter ε, the problem is stiff. We observe that also in this case the error estimate is absolutely reliable and the stepsize pattern is very smooth. Also the number of refused stepsize is very low: its percentage with respect to the total number of steps is lower then 1%: most of the refusions occur at the very first step point, because of the presence of an initial transient. We also observe that no hump phenomena (see [18]) occur: this is due to the L-stability of the method we have implemented.

9. Concluding remarks

We have introduced a class of highly stable continuous methods of the type (1.2) based on a modification of the two-step collocation technique [12, 13]. We have analyzed the local truncation error, with special attention to the terms of order $p + 2$, in order to narrow their contribution in the error propagation. We have constructed A-stable and L-stable methods with m stages, $m = 1, 2, 3, 4$ having uniform order of convergence $p = m$. We have presented the issues for their variable stepsize implementation: some of them take special advantage from the special structure of the considered methods. For instance, by suitably evaluating the continuous approximant associated to the method,

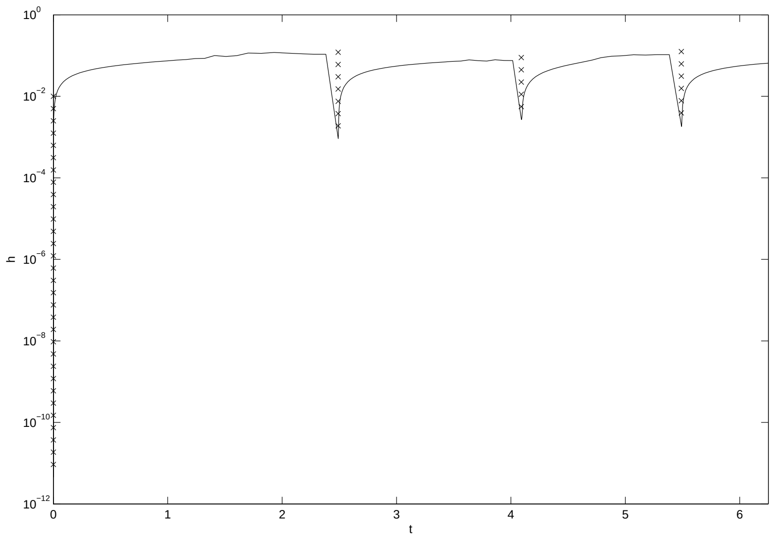

Figure 8.4: Stepsize pattern related to the solution of the Prothero-Robinson problem (8.1) with $tol = 1e-6$ and $\lambda = -1e6$, using the method (8.3). The crosses represent the refused stepsizes.

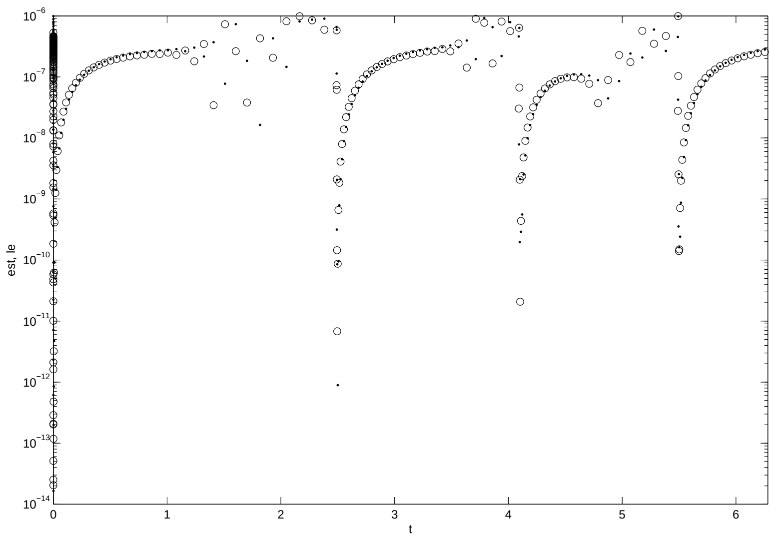

Figure 8.5: Comparison between the local error and its estimate for the solution of the Prothero-Robinson problem (8.1) with $tol = 1e-6$ and $\lambda = -1e6$, using the method (8.3). The circles represent the true local error in each step point, while the dots represent the corresponding estimation.

we are able to recover the starting values needed whenever the stepsize is changed. Moreover, the integration of stiff systems takes benefit from the usage of two-step continuous methods since they have high stage order and, therefore,

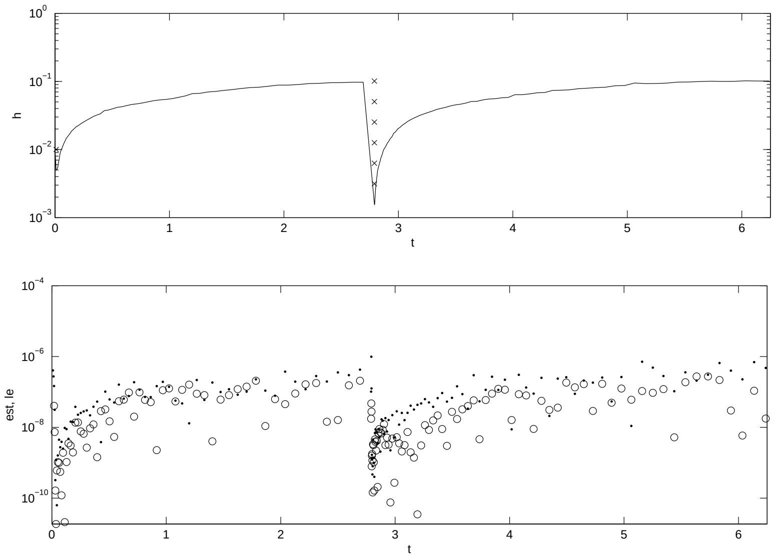

Figure 8.6: Numerical results for Prothero-Robinson problem (8.1) with $tol = 1e-6$ and $\lambda = -1e10$, using the method (8.3). Top: stepsize pattern related to the solution. Bottom: comparison between the local error and its estimate.

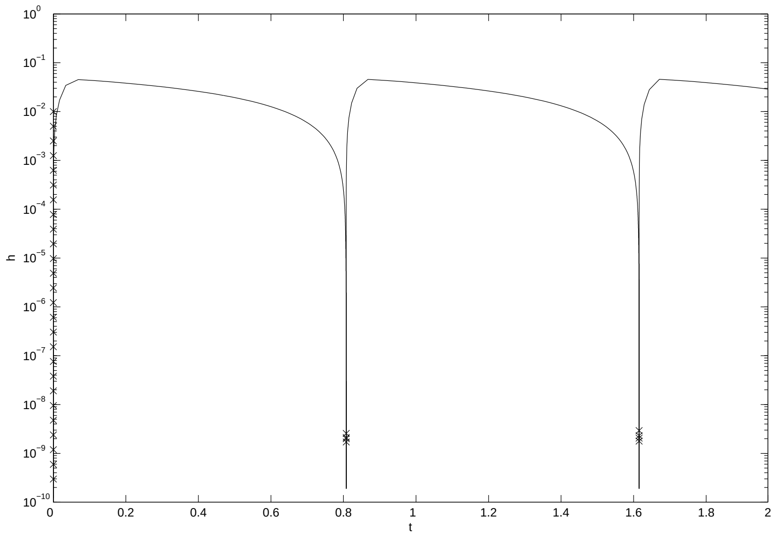

Figure 8.7: Stepsize pattern related to the solution of the Van der Pol oscillator (8.2) with $tol = 1e-4$ and $\varepsilon = 1e-6$, using the method (8.3).

no order reduction phenomena occur when these methods are applied, in contrast with Runge–Kutta methods, which exhibit order reduction. Some experiments on stiff problems have also been reported.

Future investigation will address the construction of highly stable methods (e.g. *A*-stable, *L*-stable, algebraically stable) of high order (e.g. up to 8) and their variable step-variable order implementation, also addressing large stiff problems.

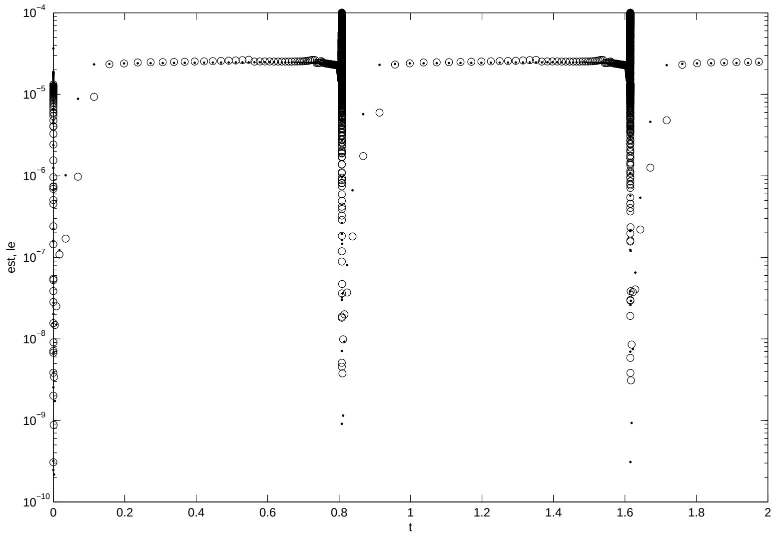

Figure 8.8: Comparison between the local error and its estimate for the solution of the Van der Pol oscillator (8.2) with $tol = 1e - 4$ and $\varepsilon = 1e - 6$, using the method (8.3).

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