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On smoothing and order reduction effects for implicit Runge–Kutta formulae

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Abstract

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It is well known that many important classes of Runge–Kutta methods suffer an order reduction phenomenon when applied to certain classes of stiff problems. In particular, the s-stage Gauss methods with stage order s and order of consistency $2s$ behave like methods of order s when applied to the class of singularly perturbed problems. In this paper we will show that the process of smoothing can ameliorate this effect, when dealing with initial-value problems, by first studying the effect of smoothing on the standard Prothero–Robinson problem and then by extending the analysis to the general class of singularly perturbed problems.

Keywords: Order reduction; Gauss methods; singular perturbation; symmetrizer.

1. Introduction

A symmetric Runge–Kutta method has the property of admitting (classical) asymptotic error expansions in even powers of the stepsize. When applied to stiff problems, however, the observed order of accuracy is usually less than the classical order. Such an order reduction phenomenon was first observed by Prothero and Robinson [14] and led to the concept of B-convergence introduced by Frank et al. [9]. Stiffness may also destroy the structure of asymptotic error expansions since the coefficients may depend on stiffness and can become

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unbounded [1–3]. These difficulties of symmetric Runge–Kutta methods with stiff problems have important implications for the application of acceleration techniques such as extrapolation.

Symmetric methods that have been implemented in extrapolation codes for stiff problems have included the implicit midpoint and trapezoidal rules [8], and the linearly implicit midpoint rule of Rosenbrock type [4]. An important strategy for improving the accuracy of the numerical solutions is the idea of smoothing with a formula such as

$$\hat{y}_n = \tfrac{1}{4}[y_{n-1} + 2y_n + y_{n+1}], \tag{1.1}$$

suggested in [12] but first used in [10] in connection with the explicit midpoint rule. When applied in the context of extrapolation or other acceleration techniques, it is important that the smoothing formula preserves the h^2-asymptotic error expansion. In a previous study, Chan [7] has generalized the idea of smoothing to arbitrary symmetric Runge–Kutta methods and in [6] the order of smoothers for Gauss methods is studied. In this paper we study the effects of smoothing on the order reduction phenomenon for the Prothero–Robinson problem. The analysis provides valuable insight into the behaviour of smoothing of symmetric methods for stiff initial-value problems, singular perturbation problems and differential algebraic equations. In order to introduce the ideas involved in our study we begin with an analysis of the scalar Prothero–Robinson problem.

Let $\mathscr{R}$ denote a symmetric Runge–Kutta method generated by the triple (A, b, c). For an s-stage method, A is the $s \times s$ Runge–Kutta matrix, b and c are $s \times 1$ vectors of weights and abscissae satisfying the following symmetry relations [16]:

$$A + PAP^{\mathrm{T}} = eb^{\mathrm{T}}, \quad Pb = b, \ Pc = e - c, \tag{1.2}$$

where e is a vector of units, and P is a permutation matrix whose (i, j)-th element is given by the Kronecker $\delta_{i,s+1-j}$. If the method is applied to a Prothero–Robinson problem

$$y'(x) = \lambda(y(x) - g(x)) + g'(x), \quad y(0) = g(0), \ \lambda < 0, \tag{1.3}$$

with $g(x)$ sufficiently smooth and the exact solution given by $y(x) = g(x)$, then it can be shown (see, for example, [5,7]) that the global error after n steps with constant stepsize h, $\Delta y_n = y_n - y(x_n)$, satisfies a recursion formula

$$\Delta y_n = R(z)\, \Delta y_{n-1} + S_n(z), \quad z = h\lambda, \tag{1.4}$$

where

$$R(z) = 1 + zb^{\mathrm{T}}(I - zA)^{-1}e, \tag{1.5a}$$

$$S_n(z) = -\sum_j \frac{h^j}{j!}\psi_j(z)g^{(j)}(x_{n-1}), \tag{1.5b}$$

$$\psi_j(z) = 1 - jb^{\mathrm{T}}c^{j-1} + zb^{\mathrm{T}}(I - zA)^{-1}(c^j - jAc^{j-1}). \tag{1.5c}$$

The simplifying assumptions $B(q)$ and $C(q)$ that will be used subsequently are defined by

$$B(q): \quad jb^{\mathrm{T}}c^{j-1} = 1, \ j = 1, \ldots, q,$$

$$C(q): \quad jAc^{j-1} = c^j, \ j = 1, \ldots, q.$$

If the method has stage order q, then $B(q)$ and $C(q)$ hold, and $\psi_j(z)=0$ for all z for $j=1,\dots,q$. Iteration of (1.4), with $\Delta y_0=0$, then gives

$$\Delta y_n = \sum_{i=1}^{n} R^{n-i}(z) S_i(z)$$
$$= -\sum_{j=q+1}^{\infty} \frac{h^j}{j!}\psi_j(z) \sum_{i=1}^{n} R^{n-i}(z) g^{(j)}(x_{i-1}).$$

For the s-stage Gauss method, $q=s$ and $R(\infty)=(-1)^s$, and it is easy to show that as $z\to\infty$ and $h\to 0$,

$$\Delta y_n = \begin{cases} O(h^{s+1}), & \text{if } s \text{ is odd,} \\ O(h^s), & \text{if } s \text{ is even.} \end{cases} \tag{1.6}$$

Except for the implicit midpoint rule, given by $s=1$, the order is less than the classical order of $2s$. If, on the other hand, $z=O(h)$, then $\Delta y_n = O(h^{2s})$ as $h\to 0$. Thus order reduction is expected for Gauss methods with $s\geqslant 2$ when applied to stiff problems.

In what follows it will always be assumed that the stepsize is constant. Thus consider replacing the method $\mathscr{R}$ in the last step by a method $\tilde{\mathscr{R}}=(\tilde{A}, \tilde{b}, \tilde{c})$, and denote the numerical solution by $\hat{y}_n$. Thus, while y_n is the numerical solution of the composite method $\mathscr{R}_n=\mathscr{R}^n/n$, $\hat{y}_n$ is the numerical solution of the modified composite method $\hat{\mathscr{R}}_n=(\mathscr{R}^{n-1}\circ\tilde{\mathscr{R}})/n$. The recursion formula for the last step is now given by

$$\Delta \hat{y}_n = \tilde{R}(z)\,\Delta y_{n-1} + \tilde{S}_n(z), \tag{1.7}$$

where

$$\tilde{S}_n(z) = -\sum_j \frac{h^j}{j!}\tilde{\psi}_j(z) g^{(j)}(x_{n-1}), \tag{1.8a}$$

$$\tilde{\psi}_j(z) = 1 - j\tilde{b}^{\mathrm{T}}\tilde{c}^{j-1} + z\tilde{b}^{\mathrm{T}}(I-z\tilde{A})^{-1}\left(\tilde{c}^j - j\tilde{A}\tilde{c}^{j-1}\right). \tag{1.8b}$$

The idea is to choose a method $\tilde{\mathscr{R}}$ so that the order behaviour of $\Delta\tilde{y}_n$ is significantly better than that of Δy_n. That is, the method $\tilde{\mathscr{R}}$ is introduced in the last (nth) step so as to minimize the order reduction effect for the symmetric method. We observe that if the global error Δy_{n-1} can be sufficiently damped by the stability function $\tilde{R}(z)=1+z\tilde{b}^{\mathrm{T}}(I-z\tilde{A})^{-1}\tilde{e}$ for large $|z|$, then the global error $\Delta\tilde{y}_n$ is essentially determined by the local error $\tilde{S}_n(z)$ for the last step. Besides the damping property, the parameters carried by the method $\tilde{\mathscr{R}}$ are chosen to reduce this local error. Thus, if q is the stage order of the symmetric method, then we would require that

$$\tilde{\psi}_j(z)=0, \quad \text{for all } z,\ j=1,\dots,q, \tag{1.9}$$

and, in addition, that $\tilde{\psi}_j(z)\to 0$ as $z\to\infty$ for as many values of $j=q+1,\dots,q+t$ as possible to achieve.

An important feature of symmetric methods is the existence of asymptotic error expansions in even powers of the stepsize h. Thus another requirement in the choice of $\tilde{\mathscr{R}}$ is the preservation of this desirable property. Such a method is called a *symmetrizer*. Chan [7] has shown how symmetrizers can be constructed for a given symmetric method. In Section 2 we present a summary of the construction of one-step symmetrizers and study the effects of smoothing on Gauss methods for the Prothero-Robinson problem, while in Section 3 we investigate the effect of smoothing in a more general setting by analysing the order behaviour of smoothing on symmetric methods when applied to singularly perturbed problems.

2. One-step symmetrizers

A symmetrizer $\tilde{\mathscr{R}}$ for a symmetric method $\mathscr{R}$ satisfying

$$\tilde{\mathscr{R}} \circ \left(-\tilde{\mathscr{R}}^{-1}\right) = \mathscr{R}^2$$

leads to the symmetry property $\hat{\mathscr{R}}_n = \hat{\mathscr{R}}_{-n}$ for all nonzero integers n, where $\hat{\mathscr{R}}_n = (\mathscr{R}^{n-1} \circ \tilde{\mathscr{R}})/n$. For an s-stage symmetric method $\mathscr{R}$ generated by (A, b, c), $\tilde{\mathscr{R}}$ is generated by

$$\begin{array}{c|cc} c & A & 0 \\ e+c & eb^{\mathrm{T}} & A \\ \hline & b^{\mathrm{T}} - w^{\mathrm{T}}P & w^{\mathrm{T}} \end{array} \tag{2.1}$$

where P is the permutation matrix corresponding to the symmetry of $\mathscr{R}$. The weight vector w carries s parameters which are chosen to satisfy certain order and stability conditions so as to minimise the phenomenon of order reduction. By construction, the method $\tilde{\mathscr{R}}$ is almost the composition of two steps of the method $\mathscr{R}$ but with different weights. Since the condition $C(q)$ for $\tilde{\mathscr{R}}$ does not depend on the weight vector w, $\tilde{\mathscr{R}}$ satisfies $C(q)$ if $\mathscr{R}$ has stage order q. This can be seen from the resulting decomposition

$$\tilde{c}^j - j\tilde{A}\tilde{c}^{j-1} = \begin{bmatrix} c^j - jAc^{j-1} \\ \sum_{i=1}^{j} \binom{j}{i}\left(c^i - iAc^{i-1}\right) + e\left(1 - jb^{\mathrm{T}}c^{j-1}\right) \end{bmatrix}.$$

In addition, it can be observed that

$$\tilde{b}^{\mathrm{T}}\tilde{c}^{j-1} - 1 = b^{\mathrm{T}}c^{j-1} - 1 + w^{\mathrm{T}}\left((e+c)^{j-1} - (e-c)^{j-1}\right),$$

so that if (A, b, c) satisfies $B(r)$, then $\tilde{\mathscr{R}}$ will satisfy $B(r)$ if

$$w^{\mathrm{T}}c^{2k-1} = 0, \quad k = 1, \ldots, \left[\tfrac{1}{2}r\right]. \tag{2.2}$$

In [6] the classical order of symmetrizers for Gauss methods was studied. It was shown that unique and L-stable symmetrizers of order $2s-1$ exist for Gauss methods with $s = 1, 2, 3$ stages, while $2s-3$ is the maximum attainable order for symmetrizers of Gauss methods with $s = 4, 5, 6$ stages. The order behaviour studied took no special account of the degree of stiffness. In the present paper we study the order behaviour of the symmetrized solution under conditions that are considered to be strongly stiff, that is, $z \to \infty$ and $h \to 0$, but subject to various degrees of stiffness, for example, $|\lambda|^{-1} \leqslant Ch^2$ (see, for example, [1,2]). This restriction is not a serious one for highly stiff problems, but our results can be compromised if the stiffness is only moderate. In addition, further difficulties can arise when systems of stiff equations are studied due to the types of coupling between the components that can arise (see [1,2] again).

The stability function of the method $\tilde{\mathscr{R}}$ is given by

$$\begin{aligned}\tilde{\mathscr{R}}(z) &= 1 + z\tilde{b}^{\mathrm{T}}(I - z\tilde{A})^{-1}\tilde{e}\\ &= R(z)\big(1 + zw^{\mathrm{T}}(I - zA)^{-1}e - zw^{\mathrm{T}}(I + zA)^{-1}e\big)\\ &\to \left(R(\infty) + \mathrm{O}\left(\frac{1}{z}\right)\right)\left(1 - 2w^{\mathrm{T}}A^{-1}e - \frac{2}{z^2}w^{\mathrm{T}}A^{-3}e + \mathrm{O}\left(\frac{2}{z^4}\right)\right), \quad \text{as } z \to \infty, \end{aligned} \tag{2.3}$$

where A is assumed to be nonsingular. As the stability function for a symmetric method is given by $R(z) = \det(I + zA)/\det(I - zA) \to \pm 1$ as $z \to \infty$, it then follows that $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$ if and only if $\tilde{R}(z) = \mathrm{O}(z^{-2})$ as $z \to \infty$. Furthermore, (1.8b) yields, as $z \to \infty$,

$$\tilde{\psi}_j(z) \to \tilde{\psi}_j^{(0)} + \tilde{\psi}_j^{(1)}\frac{1}{z} + \tilde{\psi}_j^{(2)}\frac{1}{z^2} + \cdots, \tag{2.4a}$$

$$\tilde{\psi}_j^{(0)} = 1 - \tilde{b}^{\mathrm{T}}\tilde{A}^{-1}\tilde{c}^j, \tag{2.4b}$$

$$\tilde{\psi}_j^{(1)} = j\tilde{b}^{\mathrm{T}}\tilde{A}^{-1}\tilde{c}^{j-1} - \tilde{b}^{\mathrm{T}}\tilde{A}^{-2}\tilde{c}^j, \tag{2.4c}$$

$$\tilde{\psi}_j^{(2)} = j\tilde{b}^{\mathrm{T}}\tilde{A}^{-2}\tilde{c}^{j-1} - \tilde{b}^{\mathrm{T}}\tilde{A}^{-3}\tilde{c}^j. \tag{2.4d}$$

In terms of the coefficients of the method,

$$\tilde{b}^{\mathrm{T}}\tilde{A}^{-1}\tilde{c}^j = 1 + 2\binom{j}{2}w^{\mathrm{T}}A^{-1}c^2 + 2\binom{j}{4}w^{\mathrm{T}}A^{-1}c^4 + \cdots, \tag{2.5a}$$

$$\tilde{b}^{\mathrm{T}}\tilde{A}^{-2}\tilde{c}^j = j + 2\binom{j}{3}w^{\mathrm{T}}A^{-2}c^3 + 2\binom{j}{5}w^{\mathrm{T}}A^{-2}c^5 + \cdots, \tag{2.5b}$$

$$\tilde{b}^{\mathrm{T}}\tilde{A}^{-3}\tilde{c}^j = 2w^{\mathrm{T}}A^{-3}e(1 - b^{\mathrm{T}}A^{-1}c^j) + 2\binom{j}{2}w^{\mathrm{T}}A^{-3}c^2 + 2\binom{j}{4}w^{\mathrm{T}}A^{-3}c^4 + \cdots, \tag{2.5c}$$

where $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$ and $c = Ae$ have been assumed. The order behaviour of the global error $\Delta\tilde{y}_n$ as $z \to \infty$ and $h \to 0$ now follows from (1.6)–(1.8), (2.3)–(2.5). The results for Gauss methods with s stages satisfying $C(s)$ for $s \leqslant 6$ are given below.

$s = 1$: If the condition $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$ is satisfied, then $\Delta\tilde{y}_n = \mathrm{O}(h^2)$ in the nonstiff case, that is when $z = \mathrm{O}(h)$ as $h \to 0$. In the stiff case, as $z \to \infty$ and $h \to 0$,

$$\Delta\tilde{y}_n = \mathrm{O}\left(\frac{1}{\lambda^2}\right) + \mathrm{O}(h^2).$$

The unique symmetrizer is determined by $w = \frac{1}{4}$ and gives the smoothing formula (1.1). If $|\lambda|^{-1} \leqslant Ch$, then $\Delta\tilde{y}_n = \mathrm{O}(h^2)$.

$s = 2$: If $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$ and $w^{\mathrm{T}}c = 0$, then $\Delta\tilde{y}_n = \mathrm{O}(h^4)$ in the nonstiff case. In the stiff case we have

$$\Delta\tilde{y}_n = \mathrm{O}\left(\frac{1}{\lambda^2}\right) + \mathrm{O}\left(\frac{h^2}{\lambda}\right) + \mathrm{O}(h^4).$$

Since $C(2)$ holds, the conditions are equivalent to $w^{\mathrm{T}}A^{-1}[e, c^2] = [\frac{1}{2}, 0]$ which yields $w^{\mathrm{T}} = [\frac{1}{2}, 0][e, c^2]^{-1}A = [\frac{1}{24}(\sqrt{3}+1), -\frac{1}{24}(\sqrt{3}-1)]$. If $|\lambda|^{-1} \leqslant Ch^2$, then $\Delta\tilde{y}_n = \mathrm{O}(h^4)$ and there is no order reduction in the strongly stiff case. Thus, the order reduction is eliminated by the symmetrizer since $\Delta y_n = \mathrm{O}(h^2)$ in the stiff case.

$s = 3$: If $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$, $w^{\mathrm{T}}c = 0$ and $w^{\mathrm{T}}c^3 = 0$, then $\Delta\tilde{y}_n = \mathrm{O}(h^6)$ in the nonstiff case, while the stiff order behaviour is given by

$$\Delta\tilde{y}_n = \mathrm{O}\left(\frac{h^2}{\lambda^2}\right) + \mathrm{O}(h^4).$$

If $|\lambda|^{-1} \leqslant Ch^2$, then $\Delta\tilde{y}_n = \mathrm{O}(h^4)$, which gives no improvement over the stiff order behaviour without symmetrization.

On the other hand, if instead of $w^{\mathrm{T}}c^3 = 0$ the condition was replaced by $w^{\mathrm{T}}A^{-1}c^4 = 0$, then $\Delta\tilde{y}_n = \mathrm{O}(h^4)$ in the nonstiff case, but in the stiff case

$$\Delta\tilde{y}_n = \mathrm{O}\left(\frac{h^2}{\lambda^2}\right) + \mathrm{O}\left(\frac{h^4}{\lambda}\right) + \mathrm{O}(h^6).$$

If $|\lambda|^{-1} \leqslant Ch^2$, then $\Delta\tilde{y}_n = \mathrm{O}(h^6)$ and there is no order reduction in the strongly stiff case. This is an interesting example in which the order in the strongly stiff case is higher than in the nonstiff case.

$s = 4$: In this case the nonstiff order is 6 with the conditions $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$, $w^{\mathrm{T}}c = 0$ and $w^{\mathrm{T}}c^3 = 0$. For the stiff case there are two choices. If $w^{\mathrm{T}}A^{-2}c^5 = 0$, then

$$\Delta\tilde{y}_n = \mathrm{O}\left(\frac{h^2}{\lambda^2}\right) + \mathrm{O}(h^6),$$

and if $|\lambda|^{-1} \leqslant Ch^2$, then $\Delta\tilde{y}_n = \mathrm{O}(h^6)$. Thus, in this case, symmetrization increases the order by 2 in the strongly stiff situations since $\Delta y_n = \mathrm{O}(h^4)$. On the other hand, if $w^{\mathrm{T}}A^{-1}c^6 = 0$, then

$$\Delta\tilde{y}_n = \mathrm{O}\left(\frac{h^2}{\lambda^2}\right) + \mathrm{O}\left(\frac{h^4}{\lambda}\right) + \mathrm{O}(h^8).$$

Thus the full order with $\Delta\tilde{y}_n = \mathrm{O}(h^8)$ can be achieved only if $|\lambda|^{-1} \leqslant Ch^4$.

$s = 5$: The classical order of 8 is attained with the choice of the conditions $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$, $w^{\mathrm{T}}c = 0$, $w^{\mathrm{T}}c^3 = 0$ and $w^{\mathrm{T}}c^5 = 0$. If $w^{\mathrm{T}}A^{-1}c^6 = 0$, then the stiff order behaviour is given by

$$\Delta\hat{y}_n = \mathrm{O}\left(\frac{h^4}{\lambda^2}\right) + \mathrm{O}\left(\frac{h^6}{\lambda}\right) + \mathrm{O}(h^8),$$

and if $|\lambda|^{-1} \leqslant Ch^2$, then $\Delta\hat{y}_n = \mathrm{O}(h^8)$, which is an improvement over $\Delta y_n = \mathrm{O}(h^6)$, a stiff order of 6 without symmetrization.

$s = 6$: The order conditions for order 10 are given by $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$, $w^{\mathrm{T}}c = 0$, $w^{\mathrm{T}}c^3 = 0$, $w^{\mathrm{T}}c^5 = 0$, $w^{\mathrm{T}}c^7 = 0$ and $w^{\mathrm{T}}Ac^6 = 0$. The stiff order behaviour is given by

$$\Delta\hat{y}_n = \mathrm{O}\left(\frac{h^4}{\lambda^2}\right) + \mathrm{O}\left(\frac{h^6}{\lambda}\right) + \mathrm{O}(h^8),$$

and if $|\lambda|^{-1} \leqslant Ch^2$, then $\Delta\hat{y}_n = \mathrm{O}(h^8)$, which is two orders higher than without symmetrization, since $\Delta y_n = \mathrm{O}(h^6)$.

If the order conditions for order 8 only are imposed, that is the first four listed above, then two conditions remain. If these are chosen to be $w^{\mathrm{T}}A^{-2}c^7 = 0$ and $w^{\mathrm{T}}A^{-3}e = 0$, then

$$\Delta \hat{y}_n = \mathrm{O}\left(\frac{h^2}{\lambda^4}\right) + \mathrm{O}\left(\frac{h^4}{\lambda^3}\right) + \mathrm{O}(h^8),$$

and if $|\lambda|^{-1} \leqslant Ch^{1.5}$, then $\Delta \hat{y}_n = \mathrm{O}(h^8)$. On the other hand, if $w^{\mathrm{T}}A^{-2}c^7 = 0$ and $w^{\mathrm{T}}A^{-1}c^8 = 0$, then

$$\Delta \hat{y}_n = \mathrm{O}\left(\frac{h^4}{\lambda^2}\right) + \mathrm{O}\left(\frac{h^8}{\lambda}\right) + \mathrm{O}(h^{10}),$$

and if $|\lambda|^{-1} \leqslant Ch^3$, then $\Delta \hat{y}_n = \mathrm{O}(h^{10})$.

Thus, in summary, appropriate symmetrizers for Gauss methods can be chosen so that the corresponding global error for the Prothero–Robinson problem behaves like $\mathrm{O}(h^{s+2})$ for $s = 2$, 4, 6 and $\mathrm{O}(h^{s+3})$ for $s = 5$. In these cases the improvement in order over the global error behaviour without symmetrization is two.

3. Singularly perturbed problems and DAEs

Singularly perturbed problems represent an important class of problems arising, for example, in control theory and take the form

$$y' = f(y, z), \qquad \epsilon z' = g(y, z), \quad 0 < \epsilon \ll 1. \tag{3.1}$$

It is well known (see [13], for example) that, on an interval outside of the initial transient phase, the solution has an ϵ-expansion of the form

$$y(x) = y_0(x) + \epsilon y_1(x) + \cdots + \epsilon^N y_N(x) + \mathrm{O}(\epsilon^{N+1}),$$
$$z(x) = z_0(x) + \epsilon z_1(x) + \cdots + \epsilon^N z_N(x) + \mathrm{O}(\epsilon^{N+1}),$$

where the y_k and z_k are smooth and independent of ϵ.

In fact, these coefficients can be found as solutions of a sequence of differential algebraic equations (DAEs) of increasingly higher index.

In [11] is shown that the numerical solution of a Runge–Kutta method applied to (3.1) also possesses an ϵ-expansion whose coefficients are the global errors of the Runge–Kutta method applied to a sequence of DAEs of increasing index. In particular they have shown that, for an A-stable method with $|R(\infty)| < 1$ and the Runge–Kutta matrix A having eigenvalues with positive real part, the numerical solution (y_n, z_n) satisfies

$$\begin{aligned} y_n - y(x_n) &= [\Delta y_0]_n + \epsilon[\Delta y_1]_n + \mathrm{O}(\epsilon^2 h^q), \\ z_n - z(x_n) &= [\Delta z_0]_n + \epsilon[\Delta z_1]_n + \mathrm{O}(\epsilon^2 h^{q-1}), \end{aligned} \tag{3.2}$$

for $\epsilon \leqslant h \leqslant h_0$. Here it is assumed that the stage order is q and the classical order $p \geqslant q + 1$. $[\Delta y_0]_n$, $[\Delta z_0]_n$ and $[\Delta y_1]_n$, $[\Delta z_1]_n$ represent the global errors of the Runge–Kutta method applied to semi-explicit DAEs of index 1 and 2, respectively, with constant stepsize.

In the case of an index-1 DAE,

$$[\Delta y_0]_n = \mathrm{O}(h^p), \tag{3.3}$$

while the convergence of the z-component is heavily influenced by the stage order q. In particular, it can be shown that if $p \geqslant q+1$, then
(a) $[\Delta z_0]_n = O(h^q)$ if $R(\infty) = 1$;
(b) $[\Delta z_0]_n = O(h^{q+1})$ if $-1 \leqslant R(\infty) < 1$;
(c) $[\Delta z_0]_n = O(h^p)$ if $b^T = e_s^T A$, the stiffly accurate case.
Note that $b^T = e_s^T A$ implies $b^T A^{-1} e = 1$ (which is equivalent to $R(\infty) = 0$). However, this latter condition is not a sufficient condition for $O(h^p)$.

In the case that a method is not stiffly accurate, the order estimates in (a) and (b) can still be improved upon by the analysis of the order conditions in the Taylor series expansion of the local error in the z-component (see [15]).

Before doing this, we will introduce two additional sets of simplifying assumptions which relate to index-1 and index-2 problems and which are denoted, respectively, by

$$\begin{aligned} S_1(r)&: \quad b^T A^{-1} c^k = 1, \ k = 1, \ldots, r, \\ S_2(r)&: \quad b^T A^{-2} c^k = k, \ k = 1, \ldots, r, \end{aligned} \tag{3.4}$$

where it is assumed that A is nonsingular. We note that if $B(q)$ and $C(q)$ hold, then $S_1(q)$ and $S_2(q)$ hold.

In what follows we will always assume that the Runge–Kutta matrix A is nonsingular, that $|R(\infty)| < 1$ and that a method is of order $p \geqslant q$ satisfying $B(p)$ and $C(q)$. Thus, using Roche's analysis (see [15]), it is possible to show that for semi-explicit DAEs of index 1,

$$[\Delta z_0]_n = O(h^{q+d}), \tag{3.5}$$

with

$$\begin{aligned} d = 1 \ &\Leftrightarrow \ B(q+1) \quad \text{(which implies} \, p = q+1), \\ d = 2 \ &\Leftrightarrow \ B(q+2), \ b^T v_{q+1} = 0, \ v_{q+1} = c^{q+1} - (q+1) A c^q \quad \text{(so that } p = q+2) \\ &\qquad \text{and } S_1(q+1). \end{aligned} \tag{3.6}$$

This latter result arises because a necessary condition for $[\Delta z_0]_n = O(h^p)$ is that all the standard order conditions for a Runge–Kutta method to be of order p must be satisfied (see [15]). In [11] the order theory of Roche is extended to semi-explicit DAEs of index 2 of the form

$$y' = f(y, z), \qquad 0 = g(y),$$

where f and g are sufficiently differentiable and where

$$\left\| g_y(y) f_z(y, z)^{-1} \right\| \leqslant M,$$

in a neighbourhood of the exact solution. Under the given assumptions and assuming consistent initial values, it can be shown with the use of this tree theory that

$$[\Delta y_1]_n = O(h^{q+d_1}), \qquad [\Delta z_1]_n = O(h^{q+d_2}), \tag{3.7}$$

with

$$
\begin{aligned}
d_1 = 1 \quad &\Leftrightarrow \quad B(q+1), \\
d_2 = 1 \quad &\Leftrightarrow \quad S_2(q+1), \\
d_1 = 2 \quad &\Leftrightarrow \quad B(q+2),\ b^{\mathrm{T}}v_{q+1} = 0 \quad (\text{so that } p = q+2) \\
&\qquad \text{and } S_1(q+1),\ b^{\mathrm{T}}CA^{-1}v_{q+1} = b^{\mathrm{T}}DA^{-1}v_{q+1} = 0, \\
&\qquad \text{where } D = \operatorname{diag}(A^{-1}C^2),\ C = \operatorname{diag}(c_1, \dots, c_s).
\end{aligned}
\tag{3.8}
$$

We must take some care in applying the above convergence order results to the methods being considered in this paper because these results are derived under the assumption that the same method is applied at each step. In the case of the symmetrizing process we apply a symmetric method with constant stepsize h over $N-1$ steps and then the symmetrizer. Thus the basic method can be considered to be $\hat{\mathscr{R}} = (\mathscr{R}^{N-1} \circ \tilde{\mathscr{R}})/N$. Consequently, in the case of a method in which $\mathscr{R}$ is of order p_1 and the symmetrizer over one step is of order $p_2 < p_1$, then p in (3.3) is to be interpreted as $p = p_2 + 1$. Furthermore, the stepsize associated with $\hat{\mathscr{R}}$ is denoted by H. It should be noted that the implementational approach intended here is the standard one used in extrapolation methods — as typified, for example, by the Bulirsch and Stoer algorithm. That is, extrapolation takes place on a specified subinterval. When this is completed, a new large stepsize H is chosen from the behaviour in the previous H. The smoothing takes place at the end of each major step.

In addition, the stability function $\hat{R}$ for this method is given by

$$\hat{R}(z) = R^{N-1}\left(\frac{z}{N}\right)\tilde{R}\left(\frac{z}{N}\right), \quad z = \lambda H. \tag{3.9}$$

Now it is known from [11] that, in the case of Gauss methods, two orders of convergence are lost on the z-component for index-2 problems if $R(\infty) = 1$, while one order is lost if $R(\infty) = -1$. Consequently, in (3.9) we will require

$$\hat{R}(\infty) \neq \pm 1,$$

and from (2.3) this can only happen if

$$w^{\mathrm{T}}A^{-1}e = \tfrac{1}{2}. \tag{3.10}$$

We are now in a position to write down the general order formulas for the $s = 2$ and $s = 3$ symmetrizing cases when applied to (3.1). It should be noted that in the following formulae the subscript n refers to the number of applications of the composite method $\hat{\mathscr{R}}$.

$s = 2$: If $w^{\mathrm{T}}A^{-1}e = \frac{1}{2}$, then $|\hat{R}(\infty)| < 1$ and if, in addition, $w^{\mathrm{T}}c = 0$, then the order of the symmetrizer is 3. Consequently, since the stage order is 2, we have

$$
\begin{aligned}
y_n - y(x_n) &= \mathrm{O}(H^4) + \epsilon \mathrm{O}(H^3), \\
z_n - z(x_n) &= \mathrm{O}(H^3) + \epsilon \mathrm{O}(H^p),
\end{aligned}
\tag{3.11}
$$

where p is 2 or 3.

Now from (3.8) and (2.5b), $p = 3$ if and only if

$$\tilde{b}^{\mathrm{T}}\tilde{A}^{-2}\tilde{c}^3 = 3 \quad \Leftrightarrow \quad w^{\mathrm{T}}A^{-2}c^3 = 0,$$

and this can be shown to be impossible, so that $p = 2$ in (3.11).

$s=3$: It can be shown that the one-step symmetrizer has order 5 and that $|\hat{R}(\infty)|<1$ if

$$w^{\mathrm{T}}c=0, \qquad w^{\mathrm{T}}c^3=0, \qquad w^{\mathrm{T}}A^{-1}e=\tfrac{1}{2}.$$

In this case

$$\begin{aligned} y_n-y(x_n)&=\mathrm{O}(H^6)+\epsilon\mathrm{O}(H^4),\\ z_n-z(x_n)&=\mathrm{O}(H^4)+\epsilon\mathrm{O}(H^p), \end{aligned} \tag{3.12}$$

where p is 3 or 4. From (3.8) and (2.5b), $p=4$ if and only if

$$\tilde{b}^{\mathrm{T}}\tilde{A}^{-2}\tilde{c}^4=4 \Leftrightarrow w^{\mathrm{T}}A^{-2}c^3=0,$$

which holds by $C(3)$, so that $p=4$ in (3.12).

4. Conclusions

We have shown that smoothing can have a significant effect on the behaviour of, for example, a Gauss method. However, in the case where the number of stages exceeds 1 and the smoothing process is a one-step process, there are not enough free parameters (as in (3.11)) to obtain the best possible effect. Thus in the $s=3$ case if a two-step smoothing was applied, there would be enough free parameters to allow both

$$w^{\mathrm{T}}(c^4-4Ac^3)=0, \qquad w^{\mathrm{T}}A^{-1}c^4=0,$$

and this would guarantee

$$\begin{aligned} y_n-y(x_n)&=\mathrm{O}(H^6)+\epsilon\mathrm{O}(H^4),\\ z_n-z(x_n)&=\mathrm{O}(H^5)+\epsilon\mathrm{O}(H^4). \end{aligned}$$

We hope to study the smoothing effects of two- (and higher-) step smoothing in a later paper.

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