STABILITY OF COLLOCATION AT GAUSSIAN POINTS

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ABSTRACT

Symmetric Runge-Kutta schemes are particularly useful for solving stiff two-point boundary value problems. Such A-stable schemes perform well in many cases, but it is demonstrated that in some instances the stronger property of algebraic stability is required.

A characterization of symmetric, algebraically stable Runge-Kutta schemes is given. The class of schemes thus defined turns out not to be very rich: The only collocation schemes in it are those based on Gauss points, and other schemes in the class do not seem to offer any advantage over collocation at Gaussian points.

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1. INTRODUCTION

The use of symmetric difference schemes for the numerical solution of ordinary differential equations (ODEs) is particularly attractive for stiff boundary value problems (BVPs). Here, unlike initial value ODEs, the Jacobian of a well-posed problem may have both eigenvalues with a large negative real part and eigenvalues with a large positive real part. Hence, invariance with respect to the direction of integration is a very desirable property, which symmetric schemes possess.

There are many collocation schemes, and more generally Runge-Kutta schemes, which are symmetric and A-stable. That is, for the test equation

$$y' = \lambda y \qquad t \geq 0,\ \lambda\, constant \tag{1}$$

the approximate solution does not grow in magnitude when $re(\lambda) \leq 0$. However, this is not always a sufficient stability requirement. To see this, let us compare the midpoint (box) scheme and the trapezoidal scheme for the problem

$$y' = \lambda(t) y \qquad t \geq 0,\ re(\lambda(t)) < 0. \tag{2}$$

Thus consider a mesh

$$0 = t_1 < t_2 < \cdots < t_{N+1}; \quad h_i := t_{i+1} - t_i,\ 1 \leq i \leq N \tag{3}$$

and denote the approximation of $y(t_i)$ by y_i. With $h = h_i$, the midpoint scheme gives

$$y_{i+1} = \frac{1 + \frac{1}{2} h\, \lambda(t_{i+1/2})}{1 - \frac{1}{2} h\, \lambda(t_{i+1/2})}\, y_i \qquad t_{i+1/2} = t_i + \frac{1}{2} h$$

and clearly

$$|y_{i+1}| \leq |y_i| \qquad 1 \leq i \leq N. \tag{4}$$

The trapezoidal scheme, on the other hand, gives

$$y_{i+1} = \frac{1 + \frac{1}{2} h \lambda(t_i)}{1 - \frac{1}{2} h \lambda(t_{i+1})} y_i$$

and when $|\lambda|$ is very large, so that $|\lambda h| >> 1$,

$$y_{i+1} \approx -\frac{\lambda(t_i)}{\lambda(t_{i+1})} y_i \approx \frac{\lambda(t_{i-1})}{\lambda(t_{i+1})} y_{i-1} \approx \ldots \approx (-1)^i \frac{\lambda(t_1)}{\lambda(t_{i+1})} y_1$$

Clearly, then, if $h^{-1} << |\lambda(t_{i+1})| << |\lambda(t_1)|$ we get a large increase in the numerical approximation, while the exact solution actually decreases.

Note that the midpoint and the trapezoidal schemes are both symmetric and A-stable. They also have very similar properties for nonstiff problems. Their different behaviour for (2) has been observed before. In fact, it is known (Burrage and Butcher [8]) that all collocation schemes at Gauss points satisfy (4) for the test equation (2), while all collocation schemes at Lobatto points do not. This is because collocation at Gaussian points leads to Runge-Kutta schemes which are *algebraically stable* whereas collocation at Lobatto points leads to schemes which are not algebraically stable, see Burrage and Butcher [8], Hairer and Wanner [11].

At this point one might wonder about the practical importance, for stiff boundary value ODEs, of this additional stability concept. Let us therefore consider a numerical example.

Example 1 (Kreiss, Nichols and Brown [12])

Consider

$$\epsilon y'' = t y' + 1/2\, y \qquad -1 \le t \le 1 \tag{5a}$$

$$y(-1) = 1, \qquad y(1) = 2\,. \tag{5b}$$

The solution is

$$y(t) = e^{-(t+1)/\epsilon} + 2e^{(t-1)/\epsilon} + O(\epsilon)$$

so, there are boundary layers at the ends, but $y(t)$ is smooth near the turning point $t = 0$. The numerical error propagates from the boundaries to the middle of the interval [-1,1], see Ascher [2].

We now rewrite (5a) as a first order system

$$\epsilon y' = ty + z \tag{5c}$$

$$z' = -1/2\, y \tag{5d}$$

and apply collocation at k Gauss points and at k+1 Lobatto points, see Ascher and Weiss [5], Ascher [1]. The meshes are determined as follows. For a given error tolerance δ, layer meshes are constructed as described in [5, eqns. (3.46)-(3.48)]. These are dense meshes which cover the boundary layer regions. They are then overlayed by a uniform mesh with $h = .2$ to create a mesh on the whole interval [-1,1]. The resulting number of mesh points is listed in the table below under N. The maximum error in y away from the layers (but including sampling at t=0) is listed under e. We take $\epsilon = 10^{-6} \equiv .1\text{-}5$ and use the notation $.a-b$ for $.a * 10^{-b}$.

k	scheme	δ	N	e
1	Gauss (midpoint)	.1-1	24	.14-1
2	Lobatto (trapez.)	.1-1	24	.10+2
3	Gauss	.1-5	28	.19-5
4	Lobatto	.1-5	28	.59-1

Table 1 - Numerical results for (5) with $\epsilon = .1\text{-}5$

Clearly, the Gauss schemes give better results

□

The above example motivates us to look for symmetric, algebraically stable schemes. (In § 2 we define these terms more precisely.) It turns out that the class of symmetric, algebraically stable Runge-Kutta schemes is much smaller than the class of symmetric, A-stable schemes. In particular, for continuous piecewise polynomial collocation schemes (see, e.g. [4, §3]) we obtain in §2 that

> The only symmetric, algebraically stable collocation schemes are those based on Gauss points.

If we consider symmetric, algebraically stable Runge-Kutta schemes which are not necessarily equivalent to collocation, then more schemes qualify. The basic motivation for considering these is that collocation at Gauss points gives a fully implicit method. So, the hope is to find a scheme which allows a cheaper implementation (even after taking into account a lower accuracy) without giving up desired properties. In §3 we first give some characterization of the class of symmetric, algebraically stable Runge-Kutta schemes and then show that some recent suggestions for a cheaper implementation do not yield schemes in this class.

The result that highest order collocation schemes are also the most stable symmetric ones is somewhat counter-intuitive. But we recall that for very stiff problems these schemes suffer an order reduction (see Ascher and Weiss [4,5] and references therein). In §4 we discuss this property. We have not found any other symmetric, algebraically stable scheme which has a better reduced order than that of the corresponding Gauss scheme.

We conclude that the best Runge-Kutta schemes known to us, which are symmetric and algebraically stable, are those equivalent to collocation at Gaussian points.

2. Symmetric, algebraically stable schemes

A *k-stage Runge-Kutta* scheme is given by k(k+2) coefficients

$$\mathbf{c} = (c_1, \ldots, c_k)^T, \qquad \mathbf{b} = (b_1, \ldots, b_k)^T, \tag{6}$$

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1k} \\ \vdots & & \vdots \\ a_{k1} & \cdots & a_{kk} \end{bmatrix}$$

where $0 \leq c_1 \leq \cdots \leq c_k \leq 1$ and $\sum_{l=1}^{k} a_{jl} = c_j$, $1 \leq j \leq k$. Then, for a first order system of n ODEs

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \qquad 0 \leq t \leq 1 \tag{7}$$

an approximating mesh function $\{\mathbf{y}_i\}_{i=1}^{N+1}$ is determined on a mesh (3) by requiring that the boundary conditions associated with (7) be satisfied, and that

$$\mathbf{y}_{i+1} = \mathbf{y}_i + \sum_{l=1}^{k} b_l \mathbf{K}_l, \qquad 1 \leq i \leq N \tag{8a}$$

$$\mathbf{K}_j = h_i \mathbf{f}(t_{ij}, \mathbf{y}_i + \sum_{l=1}^{k} a_{jl} \mathbf{K}_l) \qquad 1 \leq j \leq k \tag{8b}$$

$$t_{ij} = t_i + h_i c_j \qquad 1 \leq j \leq k \tag{8c}$$

(the dependence of $\mathbf{K}_j$ on i has been suppressed.)

The scheme (8) is called *symmetric* if it remains invariant under a change in the direction of integration, from t to $1-t$. This implies, without loss of generality (cf Scherer and Turke [14]), that

$$c_l = 1 - c_{k+1-l} \qquad 1 \leq l \leq k \tag{9a}$$

$$a_{k+1-j,k+1-l} + a_{jl} = b_l = b_{k+1-l} \qquad 1 \leq j, l \leq k \tag{9b}$$

In matrix-vector notation we may write (9) as

$$\mathbf{c} + E\mathbf{c} = \mathbf{1}, \qquad \mathbf{b} = E\mathbf{b} \tag{10a}$$

$$EAE + A = \mathbf{1}\,\mathbf{b}^T \tag{10b}$$

where

$$E = \begin{pmatrix} 0 & & 1 \\ & 1 & \\ 1 & \cdot & 0 \end{pmatrix} \qquad 1 = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \qquad B = \begin{pmatrix} b_1 & & & 0 \\ & b_2 & & \\ & & \cdot & \\ 0 & & & b_k \end{pmatrix} \tag{10c}$$

(Note that $E^T = E^{-1} = E$).

Consider next the $k \times k$ matrix $M = (m_{jl})$ defined by

$$M = BA + A^T B - \mathbf{b}\, \mathbf{b}^T \tag{11a}$$

i.e.,

$$m_{jl} = b_j a_{jl} + b_l a_{lj} - b_j b_l \qquad 1 \le j, l \le k \tag{11b}$$

The scheme (8) is called *algebraically stable* if $B \ge 0$ and $M \ge 0$. Burrage and Butcher [8] show that algebraically stable schemes are AN-stable (i.e. they satisfy (4) for the test equation (2)) and BN-stable (i.e. they retain dissipativity for nonlinear problems). The converse is also true in general, if the c_j are distinct. In particular, algebraic stability is necessary for AN-stability in this case.

We will assume throughout this paper that $B > 0$. If some $b_j = 0$ then $M \ge 0$ implies that the j-th row and column of M are identically zero, and the scheme becomes reducible.

Let us now consider schemes which possess the two properties of interest.

Lemma 1

A symmetric Runge-Kutta scheme is algebraically stable if and only if

$$M = 0$$

Proof: Trivially, if $M=0$ then M is positive semidefinite, hence the scheme is algebraically stable. To show the other direction, note that by (10b)

$$EME = -M$$

So

$$M \geq 0 \Rightarrow EME = E^{-1}ME \geq 0 \Rightarrow -M \geq 0 \Rightarrow M = 0$$

□

Now, the coefficients a_{jl} and b_l, $1 \leq l \leq k$, can be viewed as quadrature weights for integrations on $[0,c_j]$ and $[0,1]$, respectively. Consider their precision, letting $\mathbf{P}_q$ denote the class of polynomials of order q (degree $< q$) on a suitable domain. Following Butcher [9] we define properties $\mathbf{B}(q)$, $\mathbf{C}(q)$ and $\mathbf{D}(q)$ depending on a positive parameter q as follows.

$$\mathbf{C}(q): \quad \sum_{l=1}^{k} a_{jl}\, p(c_l) = \int_0^{c_j} p(s)ds \qquad all\ p \in \mathbf{P}_q,\ 1 \leq j \leq k$$

$$\mathbf{B}(q): \quad \sum_{l=1}^{k} b_l\, p(c_l) = \int_0^{1} p(s)ds \qquad all\ p \in \mathbf{P}_q$$

Clearly these properties can be defined in terms of the monomials $p(s) = s^{r-1}$, $1 \leq r \leq q$, alone. Similarly define

$$\mathbf{D}(q): \quad \sum_{j=1}^{k} b_j\, c_j^{r-1} a_{jl} = b_l(1-c_l^r)/r \qquad 1 \leq l \leq k,\ 1 \leq r \leq q.$$

Let us paraphrase some of Butcher's results [9]:

Theorem 1

(a) If $\mathbf{C}(\xi)$, $\mathbf{D}(\eta)$ and $\mathbf{B}(\xi+\eta)$ then the method is of (nonstiff) order $\xi+\eta$.

(b) If the method is of (nonstiff) order $\xi+\eta$ then $\mathbf{B}(\xi+\eta)$. If, in addition, the points c_j are distinct, then $\mathbf{C}(\xi)$ and $\mathbf{D}(\eta)$.

□

Let now c_j be distinct. It is well-known (see, e.g. [4]) that collocation at the points t_{ij} of (8c) by a continuous piecewise polynomial function of order k+1 yields a Runge-Kutta scheme (8). In fact, the following lemma is easy to prove

Lemma 2

With c_j distinct, the Runge-Kutta scheme is a collocation method if and only if $\mathbf{B}(k)$ and $\mathbf{C}(k)$.

Proof: This follows from the facts that, on one hand, when starting from collocation, the a_{jl} and b_l are integrals of the k-th order Lagrange interpolating polynomials and that, on the other hand, the conditions $\mathbf{B}(k)$ and $\mathbf{C}(k)$ determine the coefficients (6) uniquely for given points $\mathbf{c}$.

$\square$

Suppose now that $\mathbf{B}(q)$ and $\mathbf{C}(q)$ hold for some integer q, $1 \leq q \leq k$. Let us multiply (11b) by c_j^{r-1}, $1 \leq r \leq q$, and sum on j. The right hand side yields, by $\mathbf{B}(q)$, $\mathbf{C}(q)$,

$$\sum_{j=1}^{k} b_j c_j^{r-1} a_{jl} + b_l \sum_{j=1}^{k} a_{lj} c_j^{r-1} - b_l \sum_{j=1}^{k} b_j c_j^{r-1} =$$

$$= \sum_{j=1}^{k} b_j c_j^{r-1} a_{jl} + (c_l^r - 1) b_l / r$$

Hence, if $M=0$ then $\mathbf{D}(q)$. Also, if $q=k$ then $\mathbf{D}(k)$ implies $M=0$.

Further, let us now multiply (11b) by $c_j^{r-1} c_l^{s-1}$, $1 \leq r, s \leq q$, and sum on j and l. When $M=0$ we obtain

$$0 = \sum_{j=1}^{k} b_j c_j^{r-1} \sum_{l=1}^{k} a_{jl} c_l^{s-1} + \sum_{l=1}^{k} b_l c_l^{s-1} \sum_{j=1}^{k} a_{lj} c_j^{r-1} - \sum_{j=1}^{k} b_j c_j^{r-1} \sum_{l=1}^{k} b_l c_l^{s-1}$$

Using $\mathbf{C}(q)$ and $\mathbf{B}(q)$ this gives

$$0 = \frac{1}{s} \sum_{j=1}^{k} b_j c_j^{r+s-1} + \frac{1}{r} \sum_{l=1}^{k} b_l c_l^{r+s-1} - \frac{1}{rs}$$

so,

$$\sum_{j=1}^{k} b_j c_j^{r+s-1} = \frac{1}{r+s} .$$

The last equality means $\mathbf{B}(2q)$. By theorem 1, therefore, the method must be of order at least $2q$ in general and precisely $2q$ if the c_j are distinct. In particular, for collocation $q=k$ by lemma 2, so the method must be of order $2k$ and only collocation at Gauss points achieves that. We have proved

Theorem 2

Let the k-stage Runge-Kutta scheme (8) be symmetric and satisfy $\mathbf{B}(q)$ and $\mathbf{C}(q)$ for some positive integer $q \le k$. Then the following holds:

(a) If the scheme is algebraically stable then $\mathbf{D}(q)$.

(b) If the scheme is algebraically stable then it is of order at least $2q$; the order is precisely $2q$ if the points c_j are distinct.

(c) If $q=k$ then the converse to (a),(b) holds as well, i.e. either $\mathbf{B}(k)$, $\mathbf{C}(k)$, $\mathbf{D}(k)$ or $\mathbf{B}(2k)$, $\mathbf{C}(k)$ imply algebraic stability.

(d) A symmetric algebraically stable collocation scheme has to be at Gaussian points.

$\square$

The uniqueness result for collocation at Gaussian points follows also from a result in Burrage [7].

3. Further considerations

We address ourselves first to the question, what Runge-Kutta schemes (8) are there, which are symmetric and algebraically stable, and are not equivalent to collocation at Gaussian points. We know that these cannot be collocation schemes.

Following Hairer and Wanner [11] we define the $k \times k$ matrices W and X such that

$$W^T B W = I \qquad i.e. \qquad W^{-1} = W^T B \tag{12a}$$

and

$$X = W^{-1} A W = W^T B A W \tag{12b}$$

It follows [11] that

$$W^T M W = X + X^T - \mathbf{e}\,\mathbf{e}^T, \qquad \mathbf{e} := (1,0,\ldots,0)^T = W^T \mathbf{b}$$

If $M = 0$ then

$$X + X^T = \mathbf{e}\,\mathbf{e}^T \tag{13a}$$

so, in our case, X is skew-symmetric with the exception

$$x_{11} = \frac{1}{2}. \tag{13b}$$

Moreover, if we multiply (10b) from the left by $W^T B$ and from the right by W, we obtain

$$DXD + X = \mathbf{e}\,\mathbf{e}^T \tag{13c}$$

$$D := W^T B E W = diag\,(1,-1,1,-1,\ldots) \tag{13d}$$

Thus

$$x_{jl} = 0 \qquad all \ \ | \, j - l \, | \ \ even \, , \ except \ \ j = l = 1. \tag{13e}$$

Let us now assume that a symmetric, algebraically stable Runge-Kutta scheme satisfies $\mathbf{B}(2q)$, $\mathbf{C}(q)$, $\mathbf{D}(q)$ for some q, $1 \le q \le k$. Hairer and Wanner [11] show that in this case the elements of the first $q-1$ rows and columns of X are all zeros except for x_{11}, given by (13b), and the first super- and sub-diagonals, given by

$$x_{j+1,j} = -x_{j,j+1} = \frac{1}{2\sqrt{4j^2-1}}, \quad 1 \le j \le q-1. \tag{14}$$

Let $\hat{X}$ be the $(k+1-q)\times(k+1-q)$ lower right block of X. By (13), $\hat{X}$ is skew-symmetric (with the exception (13b) which is relevant when $q=1$), and satisfies (13e).

In particular, taking $q = k-1$, we obtain a one parameter family of schemes with

$$\hat{X} = \begin{pmatrix} 0 & -\alpha \\ \alpha & 0 \end{pmatrix} \tag{15a}$$

while $q = k-2$ gives a two-parameter family

$$\hat{X} = \begin{pmatrix} 0 & -\alpha & 0 \\ \alpha & 0 & -\beta \\ 0 & \beta & 0 \end{pmatrix} \tag{15b}$$

Example 2: k=2, q=1

Here

$$X = \begin{pmatrix} 1/2 & -\alpha \\ \alpha & 0 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}, \quad W = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

so the scheme is given by **b** and

$$\mathbf{c} = \begin{pmatrix} 1/2-\alpha \\ 1/2+\alpha \end{pmatrix}, \qquad A = \begin{pmatrix} 1/4 & 1/4-\alpha \\ 1/4+\alpha & 1/4 \end{pmatrix}, \qquad 0 \le \alpha \le 1/2.$$

Two interesting choices of α are $\alpha = 1/4$, giving a singly diagonally implicit Runge-Kutta scheme,

$$\mathbf{c} = \begin{pmatrix} 1/4 \\ 3/4 \end{pmatrix}, \qquad A = \begin{pmatrix} 1/4 & 0 \\ 1/2 & 1/4 \end{pmatrix}$$

and $\alpha = 0$, giving a scheme with a singular matrix A,

$$\mathbf{c} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}, \qquad A = \begin{pmatrix} 1/4 & 1/4 \\ 1/4 & 1/4 \end{pmatrix}.$$

The latter scheme is nothing but an unusual way of writing the midpoint scheme $\mathbf{c} = A = 1/2$, $\mathbf{b} = 1$. Indeed, the other schemes in this class (except for $\alpha = \frac{\sqrt{3}}{6}$ which gives $q = k = 2$, see (14) for $j = 1$) are similar in stability and accuracy properties to the midpoint scheme (which is the 1-stage Gauss collocation scheme), and are inferior to it on efficiency grounds.

$\square$

Collocation at Gauss points is well-known to be equivalent to a family of Runge-Kutta schemes with highest order of (nonstiff) accuracy for a given number of stages k. However, these schemes also have the well-known disadvantage of being fully implicit. Thus, in (8b) there are nk nonlinear equations to be solved, with a full $nk \times nk$ Jacobian matrix, for each i, $1 \leq i \leq N$. This is too expensive for initial value problems, where $\mathbf{y}_i$ is known when (8b) is solved and the accuracy to which the $\mathbf{K}_j$ are needed depends on the overall tolerance desired. Hence, other schemes have been proposed. Particularly popular are diagonally implicit schemes, where

$$a_{jl} = 0 \qquad\qquad l > j. \tag{16}$$

(The explicit schemes, where $a_{jl} = 0$, $l \geq j$, are hopeless for stiff problems.)

For boundary value problems, the situation is somewhat different. Firstly, the variables $\mathbf{y}_i$, $\mathbf{y}_{i+1}$, and $\mathbf{K}_j$ of (8) are equally unknown, so if a Newton iteration is executed for the mesh values $\mathbf{y}_i$, no more than one inner iteration is done for (8b). Secondly, using (8a) to eliminate $\mathbf{K}_k$ in (8b) yields only $n(k-1)$ equations for the local elimination (inevitably depending on $\mathbf{y}_i$ and on $\mathbf{y}_{i+1}$).

Still, more efficient schemes are desired. In addition to diagonally implicit schemes, an idea more suitable for BVPs is to use $\mathbf{y}_i$, $\mathbf{y}_{i+1}$, $\mathbf{K}_1 = h_i \mathbf{f}(t_i, \mathbf{y}_i)$ and $\mathbf{K}_k = h_i \mathbf{f}(t_{i+1}, \mathbf{y}_{i+1})$ and make the other stages explicitly dependent on these values, see van Bokhoven [6], Gupta [10], Muir [13]. We now examine such schemes, when they are required to be symmetric and algebraically stable.

Consider first a diagonally implicit scheme, i.e. assume that (16) is satisfied. Then from (9b)

$$a_{kl} = b_l \quad 1 \leq l \leq k\text{-}1, \quad a_{kk} = b_k - c_1, \; a_{11} = c_1$$

Trying to check for **C** (2) (assuming **B** (2)), we obtain

$$\frac{(1-c_1)^2}{2} = \int_0^{1-c_1} s \; ds = \sum_{l=1}^{k} a_{kl} \, c_l = \sum_{l=1}^{k} b_l \, c_l - c_1 c_k = \frac{1}{2} - c_1(1-c_1)$$

This holds only when $c_1 = 0$. But then $a_{11} = 0$. Now, for an algebraically stable scheme, by (11b), $m_{jj} = b_j\,(2a_{jj} - b_j\,) = 0$, so

$$a_{jj} = 1/2 \; b_j \neq 0, \qquad 1 \leq j \leq k. \tag{17}$$

Thus, no symmetric algebraically stable diagonally implicit scheme can satisfy more than **C** (1) if **B** (2). (That **C** (1), **B** (2) can be achieved we have seen in example 2 with $\alpha = 1/4$.) Also, since $M = 0$, we cannot have here more than **D** (1), because **D** (2) $\Rightarrow$**C** (2).

In general, a diagonally implicit scheme which satisfies $B > 0$ and $M = 0$ must satisfy (16), (17), and therefore

$$a_{jl} = b_l \qquad j > l. \tag{18}$$

Hence,

$$c_j = \sum_{l=1}^{k} a_{jl} = \sum_{l=1}^{j-1} b_l + 1/2 \; b_j < \sum_{l=1}^{j} b_l < c_{j+1}$$

i.e. the points c_j are distinct. By theorem 1(b) we then obtain

Theorem 3

A symmetric, algebraically stable, diagonally implicit scheme is of order at most 2.

□

Next, consider a scheme using $\mathbf{K}_1 = h_i \, \mathbf{f} \; (t_i \, , \mathbf{y}_i\,)$. This means $a_{1l} = 0, \; 1 \leq l \leq k$. In particular, $a_{11} = 0$ and (17) is again violated. Note also that a scheme using $\mathbf{K}_k = h_i \, \mathbf{f} \; (t_{i+1}, \mathbf{y}_{i+1})$ must use, by symmetry, $\mathbf{K}_1 = h_i \, \mathbf{f} \; (t_i \, , \mathbf{y}_i\,)$ and again cannot be algebraically stable. In particular, collocation based on Lobatto points is not algebraically stable.

The schemes studied in [6,10,13] are written as (8) with

$$a_{jl} = \alpha_{jl} + \theta_j b_l \qquad 1 \le j, l \le k, \tag{19a}$$

$$\alpha_{jl} = 0 \qquad l \ge j. \tag{19b}$$

Now, if such a scheme is required to satisfy $M=0$ then, by (17),

$$\theta_j = 1/2 \qquad 1 \le j \le k.$$

Moreover, setting $m_{jl} = 0$ for $j > l$ we obtain

$$b_j \, (\alpha_{jl} + 1/2 \, b_l) + b_l \, (0 + 1/2 \, b_j) - b_j \, b_l = 0,$$

so $\alpha_{jl} = 0$. The only interesting scheme remaining in this class is again the midpoint scheme.

4. Order reduction

In Ascher and Weiss [4,5], Ascher [1], it is shown that when solving very stiff boundary value problems involving different time scales, there is a reduction in the superconvergence order of Gaussian collocation schemes. No such order reduction is present for collocation with Lobatto or Radau points.

To investigate the question of order reduction, it is sufficient to consider the ODE

$$\epsilon y' = \lambda y + \phi(t), \qquad 0 < t < 1 \tag{20}$$

with λ a constant of moderate size and $\phi(t)$ a smooth inhomogeneity, as $\epsilon \to 0$. We write the corresponding numerical scheme (8) as

$$\epsilon h_i^{-1}(y_{ij} - y_i) = \sum_{l=1}^{k} \lambda a_{jl} y_{il} + g_{ij}, \qquad 1 \le j \le k \tag{21a}$$

$$\epsilon h_i^{-1}(y_{i+1} - y_i) = \sum_{l=1}^{k} \lambda b_l y_{il} + g_{i,k+1} \tag{21b}$$

and restrict consideration to symmetric, A-stable schemes with A nonsingular.

Eliminating $y_{i1}, \ldots, y_{ik}$ from (21a) and substituting in (21b), we obtain

$$y_{i+1} = \gamma(\zeta_i) y_i + \psi_i, \qquad 1 \le i \le N \tag{22a}$$

$$\gamma(\zeta) = 1 + \mathbf{b}^T(\zeta^{-1} I - A)^{-1}\mathbf{1}, \qquad \zeta_i = \frac{\lambda h_i}{\epsilon} \tag{22b}$$

$$\psi_i = \epsilon^{-1} h_i [g_{i,k+1} + \mathbf{b}^T(\zeta_i^{-1} I - A)^{-1} \mathbf{g}_i], \qquad \mathbf{g}_i = (g_{i1}, \ldots, g_{ik})^T. \tag{22c}$$

From (22a),

$$y_{i+1} = [\prod_{l=1}^{i} \gamma(\zeta_l)] y_1 + \sum_{j=1}^{i} [\prod_{l=j+1}^{i} \gamma(\zeta_l)] \psi_j \qquad 1 \le i \le N. \tag{23}$$

Now, letting $\epsilon \to 0$ in (22b) we obtain

$$\gamma(\zeta) \to 1 - \mathbf{b}^T A^{-1} \mathbf{1} \equiv \gamma_\infty \tag{24}$$

Denoting

$$\mathbf{x}^T := \mathbf{b}^T A^{-1} \tag{25}$$

we obtain, upon multiplying (10b) by $\mathbf{x} + E\mathbf{x}$, that

$$Ex = (\sum_{l=1}^{k} z_l - 1)x$$

i.e. $(\sum_{l=1}^{k} z_l - 1)$, x are an eigenpair of E. There follow two possibilities:

(a) $\sum_{l=1}^{k} z_l - 1 = 1 \Rightarrow \gamma_\infty = -1;\ z_{k+1-j} = z_j, 1 \leq j \leq k$

(b) $\sum_{l=1}^{k} z_l - 1 = -1 \Rightarrow \gamma_\infty = 1;\ z_{k+1-j} = -z_j,\ 1 \leq j \leq k.$

Setting $\epsilon = 0$ in (23) yields

$$y_{i+1} = \begin{cases} y_1 + \sum_{j=1}^{i} \psi_j & \gamma_\infty = 1 \\ (-1)^i y_1 + \sum_{j=1}^{i} (-1)^{i-j} \psi_j & \gamma_\infty = -1 \end{cases} \tag{26}$$

which shows the marginal stability, in the limit, of symmetric Runge-Kutta schemes with nonsingular A.

Next, consider the error $e_i := y_i - y(t_i)$, $e_{ij} := y_{ij} - y(t_{ij})$. If a scheme satisfies $\mathbf{C}(q)$, $\mathbf{B}(2q)$, $q \leq k$, then the difference equations (21) are satisfied for the error with the inhomogeneities

$$g_{i,k+1} = \epsilon O(h_i^{2q}), \quad g_{ij} = \epsilon O(h_i^{q}), \quad 1 \leq j \leq k. \tag{27}$$

The functions in (27) vary smoothly with i. Assuming that $|e_1|$ is very small (see [4,5,1] for error control in boundary layers), we obtain from (26)

Theorem 4

Let e_i be the error at mesh point t_i when approximating (20) for $\epsilon \to 0$ by a symmetric Runge-Kutta scheme with a nonsingular coefficient matrix. Assume $|e_1| \leq const\ h^{q+1}$. Then

$$e_i = O(h^q) \qquad 1 \leq i \leq N. \tag{28a}$$

Furthermore, if $\gamma_\infty = -1$ and $h_{i+1} = h_i(1+O(h_i))$ for all i odd *or* all i even, then

$$e_i = O(h^{q+1}) \qquad 1 \le i \le N. \tag{28b}$$

$\square$

The error estimates (28) are sharp for collocation at Gaussian points (where q=k and (28b) holds for k odd) and are of a significantly lower order than the nonstiff order 2k. In contrast, no such order reduction occurs with collocation at Radau or Lobatto points [4]. For these schemes $a_{kl} = b_l, 1 \le l \le k$, hence $g_{ik} = g_{i,k+1}$. Furthermore, for the Radau schemes (which are nonsymmetric with $\gamma_\infty = 0$) $\mathbf{x}^T = (0,...,0,1)$, and for the Lobatto points (which are symmetric, with $\gamma_\infty = \pm 1$) $x_j = 0,\ j \neq 1,k$. Indeed, with the latter two families of schemes the error for (20) at mesh points vanishes, and the usual superconvergence order shows up only when adding slow solution components to the BVP under investigation (cf [1,4]). However, as noted before, Lobatto schemes are not algebraically stable, essentially for the same reason that allows superconvergence order to be retained; namely, $a_{kk} = b_k$ implies $a_{11} = 0$, violating (17).

Theorem 4 basically says that the additional accuracy at mesh points due to higher accuracy $\mathbf{B}(2q)$ is lost. What we have is the error estimate obtainable from $\mathbf{C}(q)$, $\mathbf{B}(q)$. The question remains, whether it is possible to find a symmetric, algebraically stable scheme with $q > \frac{k}{2}$, so that its nonstiff order is >k, with a reduced order also exceeding k. The answer is conjectured to be negative.

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