SOME PROPERTIES OF SYMPLECTIC RUNGE-KUTTA METHODS

ERNST HAIRER AND PIERRE LEONE

Abstract. We prove that to every rational function $R(z)$ satisfying $R(-z)R(z)=1$, there exists a symplectic Runge-Kutta method with $R(z)$ as stability function. Moreover, we give a surprising relation between the poles of $R(z)$ and the weights of the quadrature formula associated with a symplectic Runge-Kutta method.

1. Introduction

For the numerical solution of $y' = f(y)$ we consider the class of implicit Runge-Kutta methods

$$\begin{aligned} g^{(i)} &= y_0 + h\sum_{j=1}^{s} a_{ij} f\big(g^{(j)}\big), \quad i=1,\dots,s \\ y_1 &= y_0 + h\sum_{i=1}^{s} b_i f\big(g^{(i)}\big), \end{aligned} \tag{1.1}$$

whose theoretical study has started with the seminal work of John Butcher, beginning with [2]. Such methods, applied to a Hamiltonian system, define a symplectic transformation $y_1 = \Phi_h(y_0)$, if the coefficients satisfy (see for example [6, Sect. II.16])

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \qquad \text{for} \quad i,j=1,\dots,s \tag{1.2}$$

(for irreducible methods this condition is also necessary). It is observed by numerical experiments and justified by a backward error analysis that symplectic methods, applied with constant step size h, give a qualitatively correct numerical approximation, and are important for long-time integrations of Hamiltonian systems.

If Φ_h is not symplectic, but conjugate to a symplectic method [8], i.e., there exists a transformation α_h such that $\Psi_h := \alpha_h^{-1} \circ \Phi_h \circ \alpha_h$ is symplectic, then the longtime behaviour is the same for Φ_h and Ψ_h. This follows at once from $\Psi_h^n = \alpha_h^{-1} \circ \Phi_h^n \circ \alpha_h$, so that trajectories of Φ_h and Ψ_h remain close for all times. Assuming that the transformation

Key words and phrases. Symplectic Runge-Kutta methods, W-transformation, poles of stability function, weights of quadrature formula.

α_h is given by a Runge-Kutta method (or a B-series), one sees that the stability function $R(z)$ of conjugate methods is the same. Recall that the stability function of method (1.1) is given by

$$R(z) \;=\; 1 + zb^T(I - zA)^{-1}1\!\!1 \tag{1.3}$$

with $A = (a_{ij})_{i,j=1}^{s}$, $b^T = (b_1, \dots, b_s)$, $1\!\!1 = (1, \dots, 1)^T$, so that we have $y_1 = R(h\lambda)y_0$, when the method is applied to the scalar test equation $y' = \lambda y$. For the linear oscillator $y' = i\omega y$ the method (1.1) becomes $y_1 = R(i\omega h)y_0$, and it is symplectic if and only if $|R(i\omega h)| = 1$ for all $h > 0$. This, however, is equivalent to

$$R(-z)R(z) = 1 \qquad \text{for all } z \in \mathbb{C}\,. \tag{1.4}$$

Consequently, the stability function of a method which is conjugate to a symplectic one, has to satisfy (1.4). It is therefore natural to ask, whether for a given rational function $R(z)$ satisfying (1.4) there exists a symplectic Runge-Kutta method possessing $R(z)$ as stability function. A positive answer to this question is given in Sect. 2, where we construct the method in such a way that its order is the same as that of $R(z)$ approximating $\exp(z)$. The proof is based on the W-transformation [7, Sect. IV.5], which is outlined in an appendix (Sect. 4). As a by-product of the proof we observe that the number of poles of $R(z)$ in the positive half-plane is exactly equal to the number of positive b_i in the method. In Sect. 3 we show that this relationship between poles and weights is true for all symplectic Runge-Kutta methods, for which the degree of the stability function is equal to the number of stages.

2. Construction of Symplectic Methods

Irreducible, rational functions satisfying (1.4) are of the form

$$R(z) = P(z)/P(-z), \tag{2.1}$$

where $P(z)$ is a polynomial. In the following we assume that $P(z)$ and $P(-z)$ have no common zeros.

Theorem 1. *Let the rational function (2.1) satisfy* $R(z) - \exp(z) = \mathcal{O}(z^{p+1})$*, and let* $\deg P = s$*. Then, there exists a symplectic* s*-stage Runge-Kutta method of order* p *which has* $R(z)$ *as stability function.*

Proof. The proof is very similar to the constructive characterization of B-stable Runge-Kutta methods (see [5] and [7, Sect. IV.13]). We outline its ideas, and we emphasize the main differences.

We consider the Cayley transform $\Psi(z)$ of the stability function $R(z)$, defined by

$$R(z) = \frac{1 + \frac{1}{2}\Psi(z)}{1 - \frac{1}{2}\Psi(z)}. \tag{2.2}$$

Since $R(z) = \exp(z) + \mathcal{O}(z^{p+1})$, the continued fraction of $\Psi(z)$ has the form ([7, Theorem IV.13.18])

$$\Psi(z) = \frac{z|}{|1} + \frac{\xi_1^2 z^2|}{|\ 1} + \ldots + \frac{\xi_{k-1}^2 z^2|}{|\ 1} + \xi_k^2 z \Psi_k(z) \tag{2.3}$$

where $k = [(p-1)/2]$, $\xi_j^2 = 1/(4(4j^2-1))$ and $\Psi_k(z) = zg(z)/f(z)$ with $g(0) = f(0) = 1$, $\deg f \le s-k$, and $\deg g \le s-k-1$. The special form (2.1) of the function $R(z)$ implies that $g(z)$ and $f(z)$ are polynomials in z^2. The fact that $P(z)$ and $P(-z)$ have no common zeros implies that also $f(z)$ and $g(z)$ have no common zeros, and that either $\deg f = s-k$ or $\deg g = s-k-1$. Hence, by Lemma 1 below there exists a $(s-k)\times(s-k)$ matrix Q with $q_{11} = 0$, such that $\Psi_k(z) = ze_1^T(I - zQ)^{-1}e_1$ (troughout this article we let $e_1 = (1, 0, \ldots, 0)^T$ with suitable dimension) and

$$\Lambda_k Q + Q^T \Lambda_k = 0, \tag{2.4}$$

where $\Lambda_k = \operatorname{diag}(s-k-n, n)$ with $0 \le n < s-k$. We use the notation $\operatorname{diag}(m, n)$ for the diagonal matrix of dimension $m+n$, for which the first m diagonal entries are $+1$, and the remaining n elements are equal to -1.

We next consider a quadrature formula $(b_i, c_i)_{i=1,\ldots,s}$ of order at least p, where the number of negative weights is equal to n (the number of negative diagonal entries in Λ_k). Such a quadrature formula exists. For example, consider the $(s-n)$-stage Gauss quadrature formula, which has positive weights $b_1, \ldots, b_{s-n}$ and order $2(s-n) \ge 2k+2 \ge p$. Add dummy stages $c_{s-n+1}, \ldots, c_s$ all equal to c_1, choose sufficiently small negative numbers $b_{s-n+1}, \ldots, b_s$, and modify b_1 so that the order remains unchanged.

The rest of the proof is based on the W-transformation. For the convenience of the reader, we have collected its definition and some important properties in an appendix (Sect. 4). In particular, we know from this theory (Lemma 2 below) that there exists a non-singular matrix W satisfying the property $T(k,k)$ with $k = [(p-1)/2]$ and

$$W^T B W = \Lambda,$$

where $B = \operatorname{diag}(b_1, \ldots, b_s)$ and $\Lambda = \operatorname{diag}(s-n, n)$. We then define the matrix Y by (4.1) with Q obtained from the first part of this proof, and we put $A = W(Y + \frac{1}{2}e_1 e_1^T)W^{-1}$. By Theorem 3 (Sect. 4), the Runge-Kutta method with coefficients b_i, a_{ij}, c_j is of order p and has $R(z)$ as stability function. The symplecticity follows from the fact that the matrix $M = BA + A^T B - bb^T = (b_i a_{ij} + b_j a_{ji} - b_i b_j)_{i,j=1,\dots,s}$ satisfies

$$\begin{aligned} W^T M W &= W^T (BA + A^T B - bb^T) W \\ &= W^T B W Y + Y^T W^T B W = \Lambda Y + Y^T \Lambda = 0 \end{aligned}$$

by (2.4) and $W^T b = e_1$. This implies $M = 0$, which is equivalent to the symplecticity condition (1.2). □

Lemma 1. *Let $f(z)$ and $g(z)$ be polynomials in even powers of z, such that $f(0) = 1$, $g(0) = 1$, $\deg f = m$, and either $\deg g = m$ or $\deg g = m - 2$. If $f(z)$ and $g(z)$ have no common zeros, then there exists a matrix Q (of dimension $m+1$ if $\deg g = m$, and of dimension m if $\deg g = m - 2$) such that its first entry satisfies $q_{11} = 0$, that*

$$\frac{g(z)}{f(z)} = e_1^T (I - zQ)^{-1} e_1, \tag{2.5}$$

and that $\Lambda Q + Q^T \Lambda = 0$, where $\Lambda = \mathrm{diag}\,(n_+, n_-)$ with $n_+ \geq 1$.

Proof. Since $f(z)$ and $g(z)$ are polynomials in even powers of z, the expression $f(z)wg(w) + f(w)zg(z)$ vanishes for $w = -z$. We therefore have

$$f(z)wg(w) + f(w)zg(z) = (z + w) \sum_{i,j \geq 1} c_{ij} z^{i-1} w^{j-1}, \tag{2.6}$$

which defines a symmetric matrix C of dimension $m+1$ if $\deg g = m$, and of dimension m if $\deg g = m - 2$. By our assumptions on the polynomials $f(z)$ and $g(z)$ we have $c_{11} = 1$, $c_{12} = 0$, and C is invertible. The invertibility of C follows from [4] or also from the second part of the proof of Theorem 2.

We next decompose C as $C = L^T \Lambda L$, where $Le_1 = e_1$, $\ell_{12} = 0$, and $\Lambda = \mathrm{diag}\,(n_+, n_-)$ with $n_+ \geq 1$. This is possible, because $c_{11} = 1$ and $c_{12} = 0$ (for the computation of C, apply one step of the Cholesky algorithm and continue by diagonalizing a symmetric submatrix). Putting $w = 0$ in (2.6), and using the notation $\vec{z}^T = (1, z, z^2, \dots)$, we get

$$g(z) = \vec{z}^T C e_1 = \vec{z}^T L^T \Lambda L e_1 = \vec{z}^T L^T \Lambda e_1 = \vec{z}^T L^T e_1.$$

We now define the matrix Q by comparing like powers of z in

$$f(z) e_1 = (I - zQ) L \vec{z}.$$

Since $f(z)$ is an even polynomial and $\ell_{12} = 0$, we have $q_{11} = 0$. These relations for $g(z)$ and $f(z)$ imply (2.5). Furthermore, the expression

(2.6) can be written as

$$\begin{aligned}(w+z)\vec{z}^T C\vec{w} &= w\,\vec{z}^T L^T(I-zQ^T)\Lambda L\vec{w} + z\,\vec{z}^T L^T\Lambda(I-wQ)L\vec{w}\\ &= (w+z)\vec{z}^T L^T\Lambda L\vec{w} - wz\,\vec{z}^T L^T(Q^T\Lambda+\Lambda Q)L\vec{w}.\end{aligned}$$

Because of $L^T\Lambda L = C$, this implies that $Q^T\Lambda + \Lambda Q = 0$. □

Remark 1. The analogous theorem for B-stable Runge-Kutta methods (Theorem IV.13.15 of [7]) gives a constructive characterization of *all* B-stable Runge-Kutta methods. This is no longer the case in our situation, because there exist symplectic methods of order p, which do not satisfy $C(k)$ with $k = [(p-1)/2]$. As counter-examples serve composition methods of high order, which are equivalent to diagonally implicit Runge-Kutta methods. They typically only satisfy $C(1)$.

3. Relation between Poles and Weights

If all weights b_i are positive and if the method satisfies the symplecticity condition (1.2), then the method is algebraically stable (Burrage & Butcher [1]), and hence all poles of the stability function $R(z)$ lie in the right half-plane.

For diagonally implicit Runge-Kutta methods satisfying (1.2) we have $a_{ii} = b_i/2$, and the poles of the stability function are at $2/b_i$. Also in this case, the number of positive weights of the quadrature formula is equal to the number of poles of $R(z)$ in the right half-plane. Is this true for all symplectic Runge-Kutta methods?

Theorem 2. *Consider a symplectic s-stage Runge-Kutta method with irreducible stability function, i.e., $R(z) = P(z)/Q(z)$ is irreducible with* $\deg Q = s$. *Then, the number of positive b_i is equal to the number of poles of the stability function $R(z)$ in the right half-plane.*

Proof. With the matrix $S := A - \frac{1}{2}\mathbb{1}\,b^T$ (where $\mathbb{1} = (1,\dots,1)^T$ and $b^T = (b_1,\dots,b_s)$) the symplecticity (1.2) of the Runge-Kutta method can be expressed as

$$BS + S^T B = 0. \tag{3.1}$$

We next write the stability function in terms of the matrix S. An application of the Runge-Kutta method (1.1) to the test equation $y' = \lambda y$ yields $y_1 = y_0 + u$, $g = \mathbb{1}(y_0 + \frac{1}{2}u) + zSg$ (with $z = h\lambda$ and $u = zb^T g$). Inserting $g = (I - zS)^{-1}\mathbb{1}(y_0 + \frac{1}{2}u)$ into $u = zb^T g$ allows one to express u in terms of

$$\Psi(z) = zb^T(I - zS)^{-1}\mathbb{1}.$$

Computing $y_1 = y_0 + u = R(z)y_0$ yields (2.2) for the stability function $R(z)$. Motivated by the computation of Sect. 2, we write $\Psi(z)$ as

$\Psi(z) = zg(z)/f(z)$ where, due to the symplecticity of the method, $f(z)$ and $g(z)$ are polynomials in z^2. We then define the matrix L by the relation

$$f(z)\,\mathbb{1} \;=\; (I - zS)L\vec{z},$$

so that

$$g(z) \;=\; b^T L\vec{z} = \mathbb{1}^T BL\vec{z}.$$

As in the end of the proof of Lemma 1 we compute the expression $f(z)wg(w) + f(w)zg(z)$ and obtain

$$(w+z)\vec{z}^{\,T}L^T BL\vec{w} + wz\,\vec{z}^{\,T}L^T(BS + S^T B)L\vec{w}.$$

Putting $C := L^T BL$, it therefore follows from (3.1) that

$$f(z)wg(w) + f(w)zg(z) \;=\; (z+w)\,\vec{z}^{\,T}C\vec{w}. \tag{3.2}$$

We shall prove that C is non-singular, and that the number of poles of $R(z)$ in the right half-plane is equal to the number of positive eigenvalues of C. By Sylvester's theorem this then proves the statement.

The arguments of the subsequent proof are those of Baiocchi & Crouzeix in their proof on the equivalence of A-stability and G-stability (see [7, Theorem V.6.7]). By (2.2), the poles of $R(z)$ are the values z, for which $\Psi(z) = 2$. We therefore consider the polynomial

$$zg(z) - \lambda f(z), \tag{3.3}$$

which is a polynomial of degree s, and we study its zeros for $\lambda = 2$. If necessary, we slightly perturb the real value λ so that the zeros of (3.3) become distinct, but do not cross the imaginary axis. This is possible, because $f(z)$ and $g(z)$ do not have common zeros. Since $f(z)$ and $g(z)$ are even polynomials, the zeros cannot lie on the imaginary axis.

Let $z_1, \ldots, z_m$ be the distinct zeros of (3.3) which lie in the right half-plane. We get from (3.2) that

$$\vec{z}_k^{\,*}C\vec{z}_l \;=\; \frac{1}{\overline{z}_k + z_l}\Big(f(\overline{z}_k)z_l g(z_l) + f(z_l)\overline{z}_k g(\overline{z}_k)\Big) \tag{3.4}$$

Here, $\vec{z}_k = (1, z_k, z_k^2, \ldots)^T$ and $\vec{z}_k^{\,*}$ is the transposed and complex conjugated vector. We then put

$$\zeta_k = \frac{z_k - 1}{z_k + 1} \qquad \text{so that} \qquad |\zeta_k| < 1,$$

we use the relation

$$\frac{1}{\overline{z}_k + z_l} \;=\; \frac{(1-\overline{\zeta}_k)(1-\zeta_l)}{2(1-\overline{\zeta}_k\zeta_l)},$$

and we expand $(1-\overline{\zeta}_k\zeta_l)^{-1}$ in a geometric series. If we multiply (3.4) by $\overline{v}_k v_l$, and if we sum over $1 \le k \le m$ and $1 \le l \le m$, we get with $v = (v_1, \dots, v_m)^T$ and $V = \sum_{k=1}^m v_k \vec{z}_k$ that

$$V^* C V = \frac{\lambda}{2} \sum_{j\ge 0} \Big| \sum_{k=1}^m v_k \zeta_k^j (1-\zeta_k) f(z_k) \Big|^2 .$$

This expression cannot be zero for $v \ne 0$, because it follows from (3.3) that $f(z_k) \ne 0$ for all k, otherwise $f(z)$ and $g(z)$ would have common zeros. Hence, we have $V^*CV > 0$ for all vectors V lying the subspace spanned by $\vec{z}_1, \dots, \vec{z}_m$.

If we consider the zeros $z_{m+1}, \dots, z_s$ of (3.3) lying in the left half-plan, we have to expand $(1-\overline{\zeta}_k\zeta_l)^{-1} = -\overline{\zeta}_k^{-1}\zeta_l^{-1}(1-\overline{\zeta}_k^{-1}\zeta_l^{-1})^{-1}$ into a geometric series. This creates a negative sign, and we therefore have $V^*CV < 0$ for those vectors V that lie in the subspace spanned by $\vec{z}_{m+1}, \dots, \vec{z}_s$. This proves that C has m positive and $s-m$ negative eigenvalues. $\square$

4. Appendix: W-Transformation

The W-transformation is very useful for the construction of B-stable Runge-Kutta methods. Since B-stability is formally related to symplecticity, this theory turns out to be useful also in our situation. We refer to [7, Sect. IV.5] for the proof of the following results and for more details on this theory.

We recall that a matrix $W = (w_{ij})_{i,j=1,\dots,s}$ is said to have property $T(k,k)$ (with $0 \le k < s$) for a quadrature formula $(b_i, c_i)_{i=1,\dots,s}$, if

- W is non-singular,
- $w_{ij} = P_{j-1}(c_i),\ i = 1,\dots,s,\ j = 1,\dots,k+1,$
- $W^T B W = \operatorname{blockdiag}(I, R),$

where I is the identity matrix of dimension $k+1$, R is an arbitrary symmetric matrix of dimension $s-k-1$, $B = \operatorname{diag}(b_1,\dots,b_s)$, and $P_j(t)$ is the jth shifted Legendre polynomial. The matrix R can be diagonalized by an orthogonal matrix, so that we can always assume that $W^TBW = \Lambda = \operatorname{diag}(s-n, n)$, where $n \le s-k-1$ is the number of negative elements among $b_1, \dots, b_s$.

Lemma 2. *Let the quadrature formula be of order p. Then, there exists a matrix W satisfying property $T(k,k)$ with $k = [(p-1)/2]$.*

This is Theorem IV.5.14 of [7].

Theorem 3. *Let $(b_i, c_i)_{i=1,\dots,s}$ be a quadrature formula of order at least p, let W satisfy $T(k,k)$ with $k = [(p-1)/2]$, and consider*

$$Y = \begin{pmatrix} 0 & -\xi_1 & & & \\ \xi_1 & \ddots & \ddots & & \\ & \ddots & 0 & -\xi_k & \\ & & \xi_k & \multicolumn{2}{|c}{\overline{\quad Q \quad}} \end{pmatrix}, \tag{4.1}$$

where $\xi_j^2 = 1/(4(4j^2-1))$ and Q is a matrix of dimension $s-k$ satisfying $q_{11} = 0$ if p is even (otherwise Q is arbitrary). Then, the Runge-Kutta method with coefficients b_i, a_{ij}, c_j, defined by

$$A = W\big(Y + \frac{1}{2}e_1e_1^T\big)W^{-1},$$

is of order p, and its stability function $R(z)$ is given by (2.2) and (2.3) with $\Psi_k(z) = ze_1^T(I - zQ)^{-1}e_1$.

Proof. By Theorem IV.5.11 of [7], the Runge-Kutta method satisfies the simplifying conditions $C(k)$ and $D(k)$, and it follows from a classical result of Butcher [3] that the method has order p. The statement on the stability function is a consequence of Proposition IV.5.17 and Theorem IV.5.18 on [7]. □

References

[1] K. Burrage and J.C. Butcher, *Stability criteria for implicit Runge-Kutta methods*, SIAM J. Numer. Anal. **16** (1979), 46–57.

[2] J.C. Butcher, *Coefficients for the study of Runge-Kutta integration processes*, J. Austral. Math. Soc. **3** (1963), 185–201.

[3] J.C. Butcher, *Implicit Runge-Kutta processes*, Math. Comput. **18** (1964), 50–64.

[4] T. Eirola and J.M. Sanz-Serna, *Conservation of integrals and symplectic structure in the integration of differential equations by multistep methods*, Numer. Math. **61** (1992), 281–290.

[5] E. Hairer and H. Türke, *The equivalence of B-stability and A-stability*, BIT **24** (1984), 520–528.

[6] E. Hairer, S.P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I. Nonstiff Problems, Second Revised Edition*, Springer-Verlag, Berlin, 1993.

[7] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems, Second Revised Edition*, Springer-Verlag, Berlin, 1996.

[8] D. Stoffer, *On reversible and canonical integrations methods*, Seminar für Angewandte Mathematik, ETH Zürich, Research Report Nr. 88-05, June 1988.

Section de mathématiques, Université de Genève, 2-4 rue du Lièvre, CH-1211 Genève 24, Switzerland

E-mail address, Ernst Hairer: `Ernst.Hairer@math.unige.ch`

E-mail address, Pierre Leone: `Pierre.Leone@math.unige.ch`