CONSTRUCTION OF HIGH ORDER SYMPLECTIC RUNGE-KUTTA METHODS*1)

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Abstract

Characterizations of symmetric and symplectic Runge-Kutta methods, which are based on the W-transformation of Hairer and Wanner, are presented. Using these characterizations we construct two classes of high order symplectic (symmetric and algebraically stable or algebraically stable) Runge-Kutta methods. They include and extend known classes of high order implicit Runge-Kutta methods.

§1. Introduction

In this paper we construct high order implicit Runge-Kutta methods which are based on certain combinations of the normalized shifted Legendre polynomials. Of particular interest is the symplectic property of these methods as well as their order, symmetry and stability properties. The construction of such methods heavily relies on the following simplifying assumptions of order conditions introduced by Butcher[2]:

$$B(p): b^T c^{k-1} = \frac{1}{k}, \qquad k = 1(1)p,$$
 $C(\eta): Ac^{k-1} = \frac{1}{k}c^k, \qquad k = 1(1)\eta,$ $D(\zeta): (bc^{k-1})^T A = \frac{1}{k}(b^T - (bc^k)^T), \qquad k = 1(1)\zeta$

where A is an $s \times s$ matrix, and b, c are $s \times 1$ vectors of weights and abscissae, respectively. Butcher proved the following fundamental theorem:

Theorem 1.1. If the coefficients A, b, c of an RK method satisfy $B(p), C(\eta), D(\zeta)$ with $p \leq \eta + \zeta + 1$ and $p \leq 2\eta + 2$, then the RK method is of order p.

On the other hand it will be seen that the construction also relies heavily on the W-transformation proposed by Hairer and Wanner^{[6],[8]}. In particular, the W-transformation facilitates more the construction of high order symplectic RK methods. Recently^[4,5] the research of symplectic methods is very active. The symplecticness,

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roughly speaking, is a characteristic property of geometry possessed by the solution of Hamiltonian problems. A numerical method is called symplectic if, when applied to Hamiltonian problems, it generates numerical solutions that inherit the property of symplecticness. Sanz-Serna^[11] obtained the following result: if the coefficients of an RK method satisfy

$$M = BA + A^TB - bb^T = 0,$$

where

$$B = \operatorname{diag}(b_1, \cdots, b_s),$$

then the method is symplectic. In fact, for an irreducible RK method this condition also is necessary^[9]. Up to now it was only found out that symmetric and algebraically stable Gauss, Lobatto III $E^{[10,3]}$, and Lobatto III $S^{[3]}$ methods are symplectic in the class of high order RK methods.

In Section 2 we recall the W-transformation of Hairer and Wanner and present characterizations of symmetric and symplectic methods based on the W-transformation. The properties of known high order RK methods are immediately obtained from these characterizations. In Section 3 we first construct a two-parameter family of symmetric and symplectic methods based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-3}} \alpha P_{s-2}(x),$$

where $P_s(x)$, $P_{s-2}(x)$ are the Legendre polynomials of degrees s and s-2 respectively, and give, with special choice of parameters, known symmetric and algebraically stable methods and examples of these new methods for 2 and 3 stages, particularly diagonally implicit methods for 2 and 3 stages. Then, we construct a one-parameter family of symplectic and algebraically stable methods based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-1}} \alpha P_{s-1}(x),$$

and obtain, with special choice of the parameter, two kinds of new methods which are called Radau I B and Radau II B respectively as new members of the Radau family. Finally, examples of new methods for 2 and 3 stages are given.

§2. Characterization of Symmetric and Symplectic Methods

Hairer and Wanner, in their study of algebraic stability of high order implicit RK methods, introduced a generalized Vandermonde matrix W defined by

$$W = (P_0(c), P_1(c), \cdots, P_{s-1}(c))$$
 (2.1)

where the normalized shifted Legendre polynomials are defined by

$$P_k(x) = \sqrt{2k+1}\sum_{i=0}^k (-1)^{k+i} {k\choose i} {k+i\choose i} x^i, \qquad k=0,1,\cdots.$$

These polynomials form an orthonormal set with respect to integration on [0, 1], that is,

$$\int_0^1 P_k(x)P_l(x)dx = \delta_{kl} \qquad k,l = 0,1,\cdots.$$

For an s-stage RK method generated by (A, b, c) with distinct abscissae they considered the transformation

$$X = W^T B A W$$

where $B = \text{diag } (b_1, \dots, b_s)$; thus the (k, l)-th element of X is given by

$$X_{kl} = \sum_{i,j=1}^{s} b_i P_{k-1}(c_i) a_{ij} P_{l-1}(c_j), \qquad k,l = 1(1)s.$$

From the transformation matrix X they obtained a series of important results which are very useful for studying and constructing symmetric, algebraically stable and symplectic methods. For example, for the Gauss method of order 2s they proved that the transformation matrix X has a special simple form given by

nation matrix
$$X$$
 has a special simple form given by
$$X = W^T B A W = \begin{pmatrix} 1/2 & -\xi_1 \\ \xi_1 & 0 & \ddots \\ & \ddots & & -\xi_{s-2} \\ & & \xi_{s-2} & 0 & -\xi_{s-1} \\ & & & \xi_{s-1} & 0 \end{pmatrix} =: X_G, \tag{2.2}$$

where $\xi_k = \frac{1}{2\sqrt{Ak^2-1}}$. For other known high order RK methods, the X-matrix is easy to obtain and also has a similar simple form. For example, for the Lobatto III E method^[10,3] obtained by the X-matrix is given by (2.2) with the following exception:

$$X_{s,s-1} = -X_{s-1,s} = \xi_{s-1}u,$$

where $u = b^T P_{s-1}^2(c)$. In order to give the properties of high order RK methods here we quote some results of [8].

Definition 2.1. Let η, ζ be given integers between 0 and s-1. We say that an $s \times s$ matrix W satisfies $T(\eta, \zeta)$ for the quadrature formula (b, c) if

- a) W is nonsingular,
- b) $w_{ij} = P_{j-1}(c_i)$, $i = 1, \dots, s$, $j = 1, \dots, \max(\eta, \zeta) + 1$, c) $W^T B W = \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix}$ where I is the $(\zeta + 1) \times (\zeta + 1)$ identity matrix; R is an arbitrary $(s-\zeta-1)\times(s-\zeta-1)$ matrix.

Lemma 2.2. If the quadrature formula has distinct nodes c_i and is of order $p \ge 1$ $s + \zeta$, then W defined by (2.1) has property $T(\eta, \zeta)$.

Theorem 2.3. Let W satisfy $T(\eta,\zeta)$ for the quadrature formula (b,c), then for an RK method based on (b,c) we have, for the transformation matrix $X = W^T B A W$,

- a) the first η columns of X are those of $X_G \iff C(\eta)$,
- b) the first ζ rows of X are those of $X_G \iff D(\zeta)$.

From Theorem 8.7 of [7] (see also [12,13]), we obtain another criterion for symmetry based on the W-transformation. That theorem says that if the coefficients of an s-stage RK method for some permutation matrix \tilde{P} satisfy

$$A + \tilde{P}A\tilde{P}^T = eb^T$$

and

$$\tilde{P}b=b$$
,

where $e = (1, \dots, 1)^T$, then the RK method is symmetric. In fact, if the abscissae of an RK method are ordered in an increasing order, that is, there exist a permutation matrix \tilde{P} whose (i, j)-th element is the Kronecker $\delta_{i, s+1-j}$ such that the conditions above are satisfied, then, by the definition of the symmetric method and Theorem 8.2 of [7], such conditions are also necessary.

Theorem 2.4. An s-stage RK method with distinct nodes c_i and $b_i \neq 0$ satisfying $B(p), C(\eta)$ and $D(\zeta)$ with $p \geq s + \zeta$ is symmetric if and only if

- a) $\widetilde{P}c = e c$ for the permutation matrix \widetilde{P} ,
- b) the transformation matrix X of the method takes the following form

$$X = W^{T}BAW = \begin{pmatrix} 1/2 & -\xi_{1} & & & \\ \xi_{1} & \ddots & \ddots & & \\ & \ddots & 0 & -\xi_{\nu} & \\ & & \xi_{\nu} & \hline & R_{\nu} \end{pmatrix}, \quad where \quad \nu = \min(\eta, \zeta) \qquad (2.3)$$

having the residue matrix R_{ν} whose (k,l)-th element $r_{kl}=0$ if k+l is even. (If B is singular the Theorem is still true).

Proof. By Lemma 2.2 and Theorem 2.3 the transformation matrix X of the method possesses the form of (2.3). If $\tilde{P}c = e - c$, then by the symmetric property of Legendre polynomials we have

$$\tilde{P}P_k(c) = (-1)^k P_k(c)$$
 for $k = 0(1)s - 1$.

Let $\widetilde{X} = (\widetilde{P}W)^T BA(\widetilde{P}W)$ (the technique of the proof is borrowed from [3]). It then follows that

$$\widetilde{X}_{kl} = (-1)^{k+l} X_{kl}.$$

On the other hand, since B(s) holds and $\widetilde{P}c = e - c$, we have $\widetilde{P}b = b$ or $\widetilde{P}^TB\widetilde{P} = B$. Furthermore, since

$$b^T P_k(c) = \int_0^1 P_k(x) dx = \delta_{k0}, \qquad k = 0(1)s - 1,$$

then $b^TW = (b^TP_0(c), b^TP_1(c), ..., b^TP_{s-1}(c)) = (1, 0, ..., 0) = e_1^T$, by condition b). We have

$$X + \widetilde{X} = e_1 e_1^T$$

$$\Leftrightarrow W^{T}BAW + W^{T}\tilde{P}^{T}B\tilde{P}\tilde{P}^{T}A\tilde{P}W = (b^{T}W)^{T}b^{T}W$$

$$\iff W^{T}BAW + W^{T}B\tilde{P}^{T}A\tilde{P}W = W^{T}Beb^{T}W$$

$$\iff A + \tilde{P}^{T}A\tilde{P} = eb^{T}$$

$$\iff A + \tilde{P}A\tilde{P}^{T} = eb^{T},$$

since W and B are nonsingular.

The reverse is easy to obtain by noting that $A + \tilde{P}A\tilde{P}^T = eb^T$ and $\tilde{P}b = b$ imply $\tilde{P}c = e - c$.

Now we recall the definition [1] that an irreducible RK method is called algebraically stable if B>0 and

$$M = BA + A^TB - bb^T \ge 0.$$

If we consider the W-transformation of Hairer and Wanner, an equivalent condition

$$W^TBW > 0$$

and

$$W^{T}MW = W^{T}BAW + W^{T}A^{T}BW - W^{T}bb^{T}W$$

= $X + X^{T} - e_{1}e_{1}^{T} \ge 0$ (2.4)

is obtained.

It is easy from Theorem 2.4 and condition (2.4) (see [8], IV. 13 for details) to show that an irreducible symmetric and algebraically stable method is symplectic. Hence the s-stage Gauss, Lobatto III E and Lobatto III S methods are symplectic. The Gauss, Lobatto III E and III S methods have stronger stability properties which appear to be unnecessary for the computation of Hamiltonian problems, because an s-stage irreducible RK method is symplectic if and only if

$$W^T M W = X + X^T - e_1 e_1^T = 0. (2.5)$$

Combining condition (2.5) with Lemma 2.2 and Theorem 2.3. We immediately obtain Theorem 2.5. An s-stage RK method with distinct nodes c_i satisfying $B(p), C(\eta)$ and $D(\zeta)$ with $p \geq s + \zeta$ is symplectic if and only if the transformation matrix X of the method takes the following form:

having the residue matrix R_{ν} satisfying

$$R_{\nu} + R_{\nu}^{T} = 0 \quad , \tag{2.7}$$

namely, R_{ν} is a skew-symmetric matrix.

Therefore, the coefficients of symplectic RK methods with high order can easily be generated by

$$A = WXW^TB = A^*B,$$

and all the weights $b_i \neq 0$; otherwise the symplectic RK method is degenerative. Then we obtain still further from $A = A^*B$

Proposition 2.6. An s-stage irreducible RK method is symplectic if and only if the matrix $A^* = AB^{-1}$ satisfies

$$A^* + A^{*T} - ee^T = 0.$$

Furthermore, if the method is symmetric, then there are still

$$A^* - \widetilde{P}A^{*T}\widetilde{P}^T = 0$$
 and $\widetilde{P}b = b$.

Proof. Insert $A = A^*B$ into the conditions

$$BA + A^TB - bb^T = 0$$

and

$$A + \widetilde{P}A\widetilde{P}^T = eb^T$$

respectively.

For the known implicit RK methods with high order (including Radau I B and Radau II B which will be given in the next section), their transformation matrix X is the same matrix as X_G with the exceptions given by Table 1.

Table 1

Method	$X_{s,s-1}$	$X_{s-1,s}$	$X_{s,s}$	$\widetilde{P}c = e - c$
Gauss	ξ_{s-1}	$-\xi_{s-1}$	0	=
Lobatto III A	$\xi_{s-1}u$	0	0	= .
Lobatto III B	0	$-\xi_{s-1}u$	0	
Lobatto III C	$ \xi_{s-1}u $	$-\xi_{s-1}u$	$\left \frac{u^2}{2(2s-1)}\right $	=
Lobatto III E	$ \xi_{s-1}u $	$-\xi_{s-1}u$	0	<u>=</u>
Lobatto III S	$\xi_{s-1}\sigma u$	$-\xi_{s-1}\sigma u$	0	_
Radau I A	ξ_{s-1}	$-\xi_{s-1}$	$\frac{1}{4s-1}$	≠
Radau II A	ξ_{s-1}	$-\xi_{s-1}$	$\frac{1}{4s-1}$	/
Radau I B	ξ_{s-1}	$-\xi_{s-1}$	0	≠
Radau II B	ξ_{s-1}	$-\xi_{s-1}$	0	≠
				1

The properties (including symmetry, algebraic stability and symplecticness) of known high order implicit RK metods are immediately obtained by Theorem 2.4 and Theorem 2.5 from Table 1. Radau I B and Radau II B are non-symmetric, but are algebraically stable and symplectic, and of order 2s-1 from Table 1.

§3. The Construction of Symplectic RK Methods

We first construct a family of s-stage IRK methods satisfying B(2s-2), C(s-2) and D(s-2), based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-3}} \alpha P_{s-2}(x)$$
,

which is symmetric and symplectic, where $P_s(x)$ and P_{s-2} are the normalized shifted polynomials of degrees s and s-2 respectively. If $\alpha < (s-1)/s$, then the roots of M(x) are real, distinct and satisfy $\tilde{P}c = e - c$, and the weights are determined by B(2s-2) (see[8] IV.5. for details). From Lemma 2.2 we can compute a matrix W. Then by Theorem 2.3 and Theorem 2.5 we may choose the transformation matrix X as

where $\xi_k=\frac{1}{2\sqrt{4k^2-1}},\ u=b^TP_{s-1}^2(c)$ and $\sigma\in I\!\!R$. Now since $W^TBW=$ diag $(1,\cdots,1,u)=J$ and $u\neq 0$, hence $A=W\overline{X}W^TB,\,\overline{X}=J^{-1}XJ^{-1},$ where \overline{X} is the same matrix as X_G with the exception that

$$\overline{x}_{ss-1} = -\overline{x}_{s-1s} = \xi_{s-1}\sigma.$$

Then the two-parameter family of IRK methods with coefficients $A = W\overline{X}W^TB$ is symmetric (by Theorem 2.4), symplectic (by Theorem 2.5) and of order at least 2s - 2 (by Theorem 1.1 and Theorem 2.4). In addition, it is still algebraically stable if $W^TBW > 0$. Besides such results with the special choice of parameters (α and σ) we can obtain:

- a) $\alpha = 0$ corresponding to s-stage Gauss-type method;
 - 1) order 2s if $\sigma = 1$,
 - 2) order 2s-2 with B(2s), C(s-2) and D(s-2) if $\sigma \neq 1$ and $s \geq 3$;
- b) $\alpha = -1$ correspoding to s-stage Lobatto-type method with order 2s 2;
 - 1) Lobatto III E method with B(2s-2), C(s-1), and D(s-1) if $\sigma=1$,
- 2) Lobatto III S method with B(2s-2), C(s-2) and D(s-2) if $\sigma \neq 1$ and $s \geq 3$.

Therefore, we call the family the Gauss-Lobatto method. Its members with 2 and 3 stages are given by

where
$$a = \frac{\sqrt{3(1-2\alpha)}}{3}$$
, and
$$\frac{1/2-a}{2} = \frac{\frac{1}{48a^2}}{\frac{1}{24a^2}} = \frac{(1-\frac{1}{12a^2})\left[1/2-(1+\sigma/2)a\right]}{\frac{1}{2}\left[\frac{1/2-2a+(12a^2-1)a\sigma}{24a^2}\right]} = \frac{\frac{1}{2}\left[\frac{1/2+(1+\sigma/2)a}{24a^2}\right]}{\frac{1}{24a^2}} = \frac{\frac{1}{2}(1-\frac{1}{12a^2})}{\frac{1}{24a^2}} = \frac{\frac{1}{48a^2}}{\frac{1}{24a^2}} = \frac{\frac{1}{24a^2}}{\frac{1}{24a^2}} = \frac{\frac{1}{24a^2}}{(1-\frac{1}{12a^2})\left[1/2+(1+\sigma/2)a\right]} = \frac{\frac{1}{48a^2}}{\frac{1}{24a^2}} = \frac{\frac{1}{24a^2}}{\frac{1}{24a^2}} = \frac{\frac{$$

where
$$a=\frac{\sqrt{5(3-2\alpha)}}{10}$$
.

c) Particularly, with the special choice of parameters we can obtain DIRK methods of order 2 and 4 respectively:

as $\alpha = 1/8$ and $\sigma = 1$ as $a = (2^{1/3} + 2^{-1/3} - 1)/6$ and $\sigma = -(2 + 1/a)$.

But it is impossible to choose α and σ such that the RK method with B(6), C(2) and D(2) is diagonally implicit. In fact it is easily shown by satisfying the order condition C(2) or D(2) that symplectic RK method with B(p), $C(\eta)$ and $D(\zeta)$, when η or $\zeta > 1$, cannot be diagonally implicit. Therefore, according to what was described in this section, order greater than 4 symplectic DIRK methods cannot be found out.

Secondly, we construct a family of s-stage IRK methods satisfying B(2s-1), C(s-1) and D(s-1), based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-1}}\alpha P_{s-1}(x),$$

which is symplectic, where $P_s(x)$ and $P_{s-1}(x)$ are the normalized shifted polynomials of degrees s and s-1 respectively. Now the roots of M(x) are real and distinct, but there exist no $\widetilde{P}c=e-c$ if $\alpha\neq 0$. The weights are determined by B(2s-1). For the same reasons we may choose the transformation matrix X as $X=X_G$. Since $p\geq 2s-1$ by Theorem 12.7 of ([8], IV.12.), b>0, the one-parameter family of IRK methods with coefficients

$$A = WX_GW^TB$$

is symplectic and algebraically stable, and has at least order 2s - 1. Besides such results, with the special choice of parameter α we still obtain:

a) s-stage Gauss method of order 2s if $\alpha = 0$;

- b) s-stage symplectic and algebraically stable IRK method of order 2s-1 satisfying B(2s-1), C(s-1) and D(s-1), called Radau I B if $\alpha=1$;
- c) s-stage symplectic and algebraically stable IRK method of order 2s-1 satisfying B(2s-1)C(s-1) and D(s-1) called Radau II B if $\alpha=-1$.

Therefore, we call the family Gauss-Radau method. Furtheremore, since the stability function of RK methods depends only on the transformation matrix X (here $X = X_G$ and $W^TBW = I$) and not on the underlying quadrature formula (see [8] p.89), all s-stage Gauss-Radau methods possess an identical stability function. Its members with 2 and 3 stages are given by

$$egin{array}{c|c} 3-a-lpha & \dfrac{a-lpha}{4a} & \dfrac{(1/2-a/3)(a+lpha)}{2a} \ \dfrac{3+a-lpha}{6} & \dfrac{(1/2+a/3)(a+lpha)}{2a} & \dfrac{a+lpha}{4a} \ \dfrac{a-lpha}{2a} & \dfrac{a+lpha}{2a} \end{array}$$

where $a = \sqrt{3 + \alpha^2}$, and

where
$$C_1 = -X_1 + (5 - \alpha)/10$$
, $C_2 = X_2 + (5 - \alpha)/10$, $C_3 = -X_3 + (5 - \alpha)/10$;
$$b_1 = \frac{X_2X_3 + \alpha(X_2 - X_3)/10 + (25 + 3\alpha^2)/300}{(X_3 - X_1)(X_1 + X_2)},$$
$$b_2 = \frac{X_1X_3 + \alpha(X_1 + X_3)/10 + (25 + 3\alpha^2)/300}{(X_3 + X_2)(X_1 + X_2)},$$
$$b_3 = 1 - b_1 - b_2 \; ; \quad \omega_{12} = (X_1 + X_2)[6X_1X_2 + 3\alpha(X_2 - X_1)/5 - (3\alpha^2 + 75)/50];$$
$$\omega_{23} = (X_2 + X_3)[6X_2X_3 + 3\alpha(X_2 - X_3)/5 - (3\alpha^2 + 75)/50] \; ;$$
$$\omega_{13} = (X_1 - X_3)[6X_1X_3 + 3\alpha(X_1 + X_3)/5 + (3\alpha^2 + 75)/50] \; ;$$
$$X_1 = \frac{1}{5}K^{\frac{1}{3}}\sin\left(\frac{\pi}{6} + \frac{\theta}{3}\right), \quad X_2 = \frac{1}{5}K^{\frac{1}{3}}\cos\left(\frac{\theta}{3}\right), \quad X_3 = \frac{1}{5}K^{\frac{1}{3}}\sin\left(\frac{\pi}{6} - \frac{\theta}{3}\right) \; ;$$
$$\cos\theta = \alpha(5 - \alpha^2)/K, \quad \sin\theta = 5(\alpha^4 + 2\alpha^2 + 5)^{1/2}/K \; ;$$
$$K = (\alpha^6 + 15\alpha^4 + 75\alpha^2 + 125)^{1/2}.$$

Its special members with 2 and 3 stages, Radau I B and Radau II B methods, are given by

and

respectively.

Corollary 3.1. For $\alpha = 1$ and $\alpha = -1$, let the transformation matrix X be the same matrix as X_G with the exception that

$$X_{ss-1} = -X_{s-1s} = \xi_{s-1}\sigma, \qquad \sigma(\neq 0, 1) \in \mathbb{R},$$

we can obtain s-stage $(s \ge 3)$ symplectic and algebraically stable IRK methods of order 2s-3 satisfying B(2s-1), C(s-2) and D(s-2), called Radau-type I and II methods respectively.

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