SYMPLECTIC RUNGE-KUTTA METHODS OF HIGH ORDER BASED ON W-TRANSFORMATION*

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Abstract In this paper , characterizations of symmetric and symplectic Runge-Kutta methods based on the W-transformation of Hairer and Wanner are presented. Using these characterizations, we construct two families symplectic (symmetric and algebraically stable or algebraically stable) Runge-Kutta methods of high order. Methods constructed in this way and presented in this paper include and extend the known classes of high order implicit Runge-Kutta methods.

 ${\bf Keywords}~{\rm Runge-Kutta}$ method, symplectic and algebraically stable method, W-transformation.

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1. Introduction

One of Stetter's significant contributions to the study of the numerical solution for ordinary differential equations concerns the existence of asymptotic error expansions in the stepsize for discretization methods (see Gragg [5], Hairer and Lubich [9] and Stetter [15]). This result iterated defect correction techniques for accelerating convergence and laid the foundations for the development of extrapolation. Symmetric methods are of special interest because the asymptotic error expansions occur in even powers of the stepsize h. Stetter [16] first presented an algebraic characterization of symmetry for Runge-Kutta methods. He showed that an s-stage symmetric Runge-Kutta method is generated by a triple (A, b, c) satisfying

$$A + \overline{P}A\overline{P}^{T} = eB^{T}, \qquad \overline{P}b = b, \qquad \overline{P}c = e - c, \qquad (1.1)$$

for some $s \times s$ permutation matrix \overline{P} , where A is an $s \times s$ matrix, b, c are $s \times 1$ vectors of weights and abscissae respectively and $e = (1, 1, ..., 1)^T$.

The design and construction of Symplectic Runge-Kutta methods has been considered by several authors [2–4, 10–12, 17, 18, 20, 21]. In this paper we construct implicit Runge-Kutta methods of high order which are based on certain combinations of the normalized shifted Legendre polynomials. Of particular interest is the

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symplectic property of these methods as well as their order, symmetry and stability properties. These methods are defined in terms of certain simplifying assumptions introduced by Butcher^[2]:

$$B(p): b^{T}c^{k-1} = \frac{1}{k}, \qquad k = 1, \cdots, p,$$

$$C(\eta): Ac^{k-1} = \frac{1}{k}c^{k}, \qquad k = 1, \cdots, \eta,$$

$$D(\zeta): (bc^{k-1})^{T}A = \frac{1}{k}(b^{T} - (bc^{k})T), \qquad k = 1, \cdots, \zeta.$$

Butcher [1] proved the following fundamental theorem:

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

On the other hand it will be seen that the construction of implicit Runge-Kutta methods also relies heavily on the W-transformation proposed by Hairer and Wanner [6, 8]. In particular, the W-transformation facilitates the construction of high order sympletic Runge-Kutta methods. The symplecticness is a characteristic property of geometry possessed by the solution of Hamiltonian systems. A numerical method is called symplectic if, when applied to Hamiltonian problems, it generates numerical solutions that inherit the symplecticness property of the Hamiltonian problems. Sanz-Serna [14] obtained the following result : if the coefficients of an Runge-Kutta method satisfy

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

where

$$B = diag(b_1, b_2, \cdots, b_s),$$

then the method is symplectic. In fact, for an irreducible Runge-Kutta method this condition also is necessary [4].

The paper is organised as follows: In section 2 we recall the W-transformation of Hairer and Wanner and introduce characterizations of symmetric and symplectic methods based on the W-transformation. The properties of the known Gauss and Lobatto IIIA, IIIB, IIIC, IIIE, and IIIS methods are immediately obtained from these characterizations. In section 3 we first construct a four-parameter family of symmetric and symplectic methods based on the combination

$$P(x) = P_s^*(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-3}} \omega P_{s-2}^*(x),$$

where $P_s^*(x)$, $P_{s-2}^*(x)$ are the normalized shifted polynomials of degrees s and s-2 respectively. We give the known symmetric and symplectic implicit RK methods with special choice of parameters and examples of these new methods for 2, 3 and 4 stages, particularly diagonally implicit Runge-Kutta methods for 2 and 3 stages. Secondly, we construct another four-parameters family of symplectic and algebraically stable but non-symmetric methods based on the combination

$$P(x) = P_s^*(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-1}}\omega P_{s-1}^*(x),$$

where $P_s^*(x), P_{s-1}^*(x)$ are the normalized shifted polynomials of degrees s and s-1 respectively. Example of the methods for 2 and 3 stages are given.

2. Characterization of symmetric and symplectic methods

In their study of the algebraic stability of implicit Runge-Kutta methods of high order, Hairer and Wanner [6] 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

$$P_m^*(x) = \sqrt{2m+1} \sum_{i=0}^m (-1)^{m+i} \binom{m}{i} \binom{m+i}{i} x^i, \qquad m = 0, 1, 2, \cdots.$$

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

$$\int_0^1 P_m^*(x) P_n^*(x) dx = \delta_{mn}, \qquad m, n = 0, 1, 2, \cdots.$$

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

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

where $B = diag(b_1, b_2, \dots, b_s)$; thus the (m, n) - th element of X is given by

$$X_{mn} = \sum_{i,j=1}^{s} b_i P_{m-1}^*(c_i) a_{ij} P_{n-1}^*(c_j), \qquad m, n = 1, 2, \dots, s.$$

The matrix X, besides giving a characterization of high-order methods and a convenient way of studying algebraic stability, is also very useful for 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

$$X = W^{T} BAW = \begin{pmatrix} \frac{1}{2} & -\xi_{1} & & \\ \xi_{1} & 0 & -\xi_{2} & \\ & \ddots & \ddots & \ddots & \\ & & \xi_{s-2} & 0 & -\xi_{s-1} \\ & & & \xi_{s-1} & 0 \end{pmatrix} =: X_{G},$$
(2.2)

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where $\xi_l = \frac{1}{2\sqrt{4l^2-1}}$. For other known high order implicit Runge-Kutta methods, the transformation X-matrix is easy to obtain and also has a similar simple form. For example, for the Gauss-Lobatto method^[4] obtained by the X-matrix given by (2.2) with the following exception:

$$X_{s,s-1} = -X_{s-1,s} = \xi_{s-1}\sigma\mu,$$

where $\mu = b^T P_{s-1}^{*2}(c)$, σ is a parameter. In order to give the properties of high order implicit Runge-Kutta methods here we quote some result of [4,8].

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

- 1) W is nonsingular,
- 2) $w_{ij} = P_{j-1}^*(c_i), i = 1, 2, \cdots, s, \quad j = 1, 2, \cdots, \max(\eta, \zeta) + 1,$ 3) $W^T B W = \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix}$ where I is the $(\zeta + 1) \times (\zeta + 1)$ identity matrix; R is an arbitrary matrix of $(s - \zeta - 1) \times (s - \zeta - 1).$

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

Theorem 2.1. Let W satisfy $T(\eta, \zeta)$ for the quadrature formula (b, c), then for an Runge-Kutta method based on (b, c) we have, for the transformation matrix $X = W^T BAW$,

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

From [7, Theorem 8.7] (see also [16,20]), we obtain another criterion for symmetry based on the W-transformation. That theorem says that if the coefficients of an s-stage Runge-Kutta method for some permutation matrix \bar{P} satisfy

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

and

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

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

Theorem 2.2. An s-stage Runge-Kutta 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) Pc = e c for the permutation matrix P,
- b) the transformation matrix X of the method takes the following form

$$X = W^{T} B A W = \begin{pmatrix} \frac{1}{2} & -\xi_{1} & & \\ \xi_{1} & 0 & -\xi_{2} & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 0 & -\xi_{\nu} \\ & & & \xi_{\nu} & |\overline{R_{\nu}} \end{pmatrix}, \text{ where } \nu = \min(\eta, \zeta) \quad (2.3)$$

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

Proof. [4] Since Lemma 2.1 and Theorem 2.1, the transformation matrix X of the method possesses the form of (2.3). By the symmetric property of Legendre polynomials and $\bar{P}c = e - c$ we have

$$\overline{P}P_m^*(c) = (-1)P_m^*(c) \quad for \quad m = 0, 1, \cdots, s-1.$$

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

$$\overline{X}_{mn} = (-1)^{m+n} X_{mn}.$$

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

$$b^T P_m^*(c) = \int_0^1 P_m^*(x) dx = \delta_{m0}, \qquad m = 0, 1, \cdots, s - 1$$

and condition b), then $b^T W = (b^T P_0^*(c), b^T P_1^*(c), \cdots, b^T P_{s-1}^*(c)) = (1, 0, \cdots, 0) = e_1^T$. We have

$$\begin{split} X + \overline{X} &= e_1 e_1^T \Leftrightarrow W^T BAW + W^T \overline{P}^T B \overline{P} \overline{P}^T A \overline{P} W = (b^T W)^T b^T W \\ &\Leftrightarrow W^T BAW + W^T B \overline{P}^T A \overline{P} W = W^T B e b^T W \\ &\Leftrightarrow A + \overline{P}^T A \overline{P} = e b^T \\ &\Leftrightarrow A + \overline{P} A \overline{P}^T = e b^T, \end{split}$$

since W and B are nonsingular.

Since that $A + \overline{P}A\overline{P}^T = eb^T$ and $\overline{P}b = b$ imply $\overline{P}c = e - c$, then the reverse is true.

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

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

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

$$W^T B W > 0$$

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.

Since Theorem 2.2 and condition (2.4) holds, it is easy to show that an irreducible symmetric and algebraically stable method is symplectic (see [8, IV. 13] for details). Hence, the *s*-stage Gauss, Lobatto IIIE, Lobatto IIIS and Lobatto IIISX (which will be given in next section) methods are symplectic. The Gauss, Lobatto IIIE, Lobatto IIIS and Lobatto IIISX methods have stronger stability properties which appear to be unnecessary for the computation of Hamiltonian systems, because an *s*-stage irreducible Runge-Kutta method is symplectic if and only if

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

Combining Lemma 2.1 and Theorem 2.2 with condition (2.5), we immediately obtain:

Theorem 2.3. An s-stage Runge-Kutta method with distinct nodes c_i satisfying $B(p), C(\eta)$ and $D(\zeta)$ with $p \ge s + \zeta$ is symplectic if and only if the transformation matrix X of the method takes the following form:

$$X = W^{T} B A W = \begin{pmatrix} \frac{1}{2} & -\xi_{1} & & \\ \xi_{1} & 0 & -\xi_{2} & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots & \\ & & \ddots & 0 & -\xi_{\nu} \\ & & & \xi_{\nu} & |\overline{R_{\nu}} \end{pmatrix}, \text{ where } \nu = \min(\eta, \zeta) \quad (2.6)$$

having the residue matrix R_{ν} satisfying

$$R_{\nu} + R_{\nu}^T = 0, \qquad (2.7)$$

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

Therefore, the coefficients of symplectic Runge-Kutta methods with high order can easily be generated by

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

and all the weights $b_i \neq 0$; otherwise the symplectic Runge-Kutta method is degenerative. Since $A = A^*B$, we obtain still further

Proposition 2.1. An s-stage irreducible Runge-Kutta 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

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

Proof. [4] Insert $A = A^*B$ into the conditions

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

and

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

respectively.

For the known implicit Runge-Kutta methods with high order (including Lobatto IIISX 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.

The properties (including symmetry, symplecticness and algebraic stability) of known high order implicit Runge-Kutta methods can immediately be obtained by Theorem 2.2 and Theorem 2.3 from Table 1. Although Radau IB and Radau IIB are non-symmetric, they are symplectic and algebraically stable of order 2s-1 from Table 1.

Table 1. Exceptions of transformation matrix A							
Method	$X_{s,s-1}$	$X_{s-1,s}$	$X_{s,s}$	$\overline{P}c = e - c$			
Gauss	ξ_{s-1}	$-\xi_{s-1}$	0	=			
Lobatto IIIA	$\xi_{s-1}\mu$	0	0	=			
Lobatto IIIB	0	$-\xi_{s-1}\mu$	0	=			
Lobatto IIIC	$\xi_{s-1}\mu$	$-\xi_{s-1}\mu$	$\frac{\mu^2}{2(2s-1)}$	=			
Lobatto IIIE	$\xi_{s-1}\mu$	$-\xi_{s-1}\mu$	0	=			
Lobatto IIIS	$\xi_{s-1}\sigma\mu$	$-\xi_{s-1}\sigma\mu$	0	=			
Lobatto IIISX	$\xi_{s-1} \alpha \mu$	$-\xi_{s-1}\beta\mu$	$\frac{\mu^2 \alpha \beta \gamma}{2(2s-1)}$	=			
Radau IA	ξ_{s-1}	$-\xi_{s-1}$	$\frac{1}{4s-1}$	\neq			
Radau IIA	ξ_{s-1}	$-\xi_{s-1}$	$\frac{1}{4s-1}$	\neq			
Radau IB	ξ_{s-1}	$-\xi_{s-1}$	0	\neq			
Radau IIB	ξ_{s-1}	$-\xi_{s-1}$	0	≠			

Table 1. Exceptions of transformation matrix X

3. Construction of high order implicit symplectic methods

3.1. The Gauss-Lobatto methods

In this section, we construct a family of s-stage Implicit Runge-Kutta methods, which are called the Gauss-Lobatto methods, satisfying B(2s-2), C(s-2) and D(s-2), based on the combination

$$P(x) = P_s^*(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-3}}\omega P_{s-2}^*(x),$$

which is symmetric and symplectic, where $P_s^*(x)$ and $P_{s-2}^*(x)$ are the normalized shifted polynomials of degrees s and s-2 respectively. If $\omega < \frac{s-1}{s}$, then P(x) has distinct real roots and the roots satisfy $\bar{P}c = e - c$ (see [8, IV.5] for details). The weights of the Butcher Table are determined by B(2s-2) and satisfy $\bar{P}b = b$. From Lemma 2.1 we can compute a matrix W. Since Theorem 2.1 and Theorem 2.3, we may choose the transformation matrix X as

$$X = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & -\xi_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \xi_{s-2} & 0 & -\xi_{s-1}\mu\beta \\ & & & \xi_{s-1}\mu\alpha & \frac{\mu^2\alpha\beta\gamma}{2(2s-1)} \end{pmatrix}$$

where $\xi_l = \frac{1}{2\sqrt{4l^2-1}}, \ \mu = b^T P_{s-1}^{*2}(c)$ and $\alpha, \beta, \gamma \in \mathbf{R}$. Now since B(2s-2) holds, $W^T B W = diag(1, 1, \cdots, \mu) = J$ and $\mu \neq 0$, hence

$$A = W \widetilde{X} W^T B, \quad \widetilde{X} = J^{-1} X J^{-1},$$

where X is the same matrix as X_G with the exception that

$$x_{s,s-1} = \xi_{s-1}\alpha, \quad x_{s-1,s} = -\xi_{s-1}\beta, \quad x_{s,s} = \frac{\alpha\beta\gamma}{2(2s-1)}$$

Then the four-parameter family of Implicit Runge-Kutta methods with coefficients $A = W \widetilde{X} W^T B$ is symmetric (by Theorem 2.2), symplectic (by Theorem 2.3) and of order at least 2s - 2 (by Theorem 1.1 and Theorem 2.2). In addition, it is also algebraically stable if $W^T B W > 0$. Besides such results with the special chioce of parameters (α, β, γ , and ω), we can obtain:

a) $\omega = 0$ corresponding to *s*-stage Gauss-type method;

- 1) order 2s if $\alpha = \beta = 1$ and $\gamma = 0$,
- 2) order 2s-2 with B(2s), C(s-2), and D(s-2) if $\alpha = \beta \neq 1, \gamma = 0$ and $s \geq 3$,

b) $\omega = -1$ corresponding to s-stage Lobatto-type method with order 2s-2;

- 1) Lobatto IIIA method with B(2s-2), C(s-1) and D(s-1) if $\alpha = 1$ and $\beta = \gamma = 0$,
- 2) Lobatto IIIB method with B(2s-2), C(s-1) and D(s-1) if $\beta = 1$ and $\alpha = \gamma = 0$,
- 3) Lobatto IIIC method with B(2s-2), C(s-1) and D(s-1) if $\alpha = \beta = \gamma = 1$,
- 4) Lobatto IIIE method with B(2s-2), C(s-1) and D(s-1) if $\alpha = \beta = 1$ and $\gamma = 0$,
- 5) Lobatto IIIS method with B(2s-2), C(s-2) and D(s-2) if $\alpha = \beta \neq 1$, $\gamma = 0$ and $s \geq 3$,
- 6) Lobatto IIISX method with B(2s-2), C(s-2) and D(s-2) if $\alpha \neq \beta, \gamma \neq 0$ and $s \geq 3$.

Therefore, we also call this family Implicit Runge-Kutta method the Gauss-Lobatto method as [4]. Its members with 2, 3 and 4 stages are given by the following Butcher Tables 2–4:





where $a = \frac{\sqrt{3(1-2\omega)}}{3}$.



$\frac{\frac{1}{2}}{\frac{1}{2}} - a$	$\frac{\frac{1-a(12a^2-1)(\alpha-\beta)+\frac{1}{4}(12a^2-1)^2\alpha\beta\gamma}{48a^2}}{\frac{1+2a+a\alpha-\frac{1}{4}(12a^2-1)\alpha\beta\gamma}{48a^2}}$	$ (1 - \frac{1}{12a^2})^{\frac{4-8a-4a\beta-(12a^2-1)\alpha\beta\gamma}{8}} \\ (1 - \frac{1}{12a^2})^{\frac{4+\alpha\beta\gamma}{8}} $	$\frac{\frac{1-4a+a(12a^2-1)(\alpha+\beta)+\frac{1}{4}(12a^2-1)^2\alpha\beta\gamma}{48a^2}}{\frac{48a^2}{48a^2}}$
$\frac{1}{2} + a$	$\frac{\frac{1+4a-a(12a^2-1)(\alpha+\beta)+\frac{1}{4}(12a^2-1)^2\alpha\beta\gamma}{48a^2}}{\frac{48a^2}{\frac{1}{24a^2}}}$	$\frac{\left(1-\frac{1}{12a^2}\right)^{\frac{4+8a+4a\beta-(12a^2-1)\alpha\beta\gamma}{8}}}{1-\frac{1}{12a^2}}$	$\frac{\frac{1+a(12a^2-1)(\alpha-\beta)+\frac{1}{4}(12a^2-1)^2\alpha\beta\gamma}{48a^2}}{\frac{48a^2}{\frac{1}{24a^2}}}$

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

 Table 4. Butcher Table of 4-stages Gauss-Lobatto method

$\frac{1}{2} - a$	$\frac{12b^2-1}{24(b^2-a^2)}A_{11}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{12}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{13}$	$\frac{12b^2-1}{24(b^2-a^2)}A_{14}$
$\frac{1}{2} - b$	$\frac{12b^2-1}{24(b^2-a^2)}A_{21}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{22}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{23}$	$\frac{12b^2-1}{24(b^2-a^2)}A_{24}$
$\frac{1}{2} + b$	$\frac{12b^2-1}{24(b^2-a^2)}A_{31}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{32}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{33}$	$\frac{12b^2-1}{24(b^2-a^2)}A_{34}$
$\frac{1}{2} + a$	$\frac{12b^2-1}{24(b^2-a^2)}A_{41}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{42}$	$\frac{12a^2-1}{24(a^2-b^2)}A_{43}$	$\frac{12b^2-1}{24(b^2-a^2)}A_{44}$
	$\frac{12b^2 - 1}{24(b^2 - a^2)}$	$\frac{12a^2 - 1}{24(a^2 - b^2)}$	$\frac{12a^2 - 1}{24(a^2 - b^2)}$	$\tfrac{12b^2 - 1}{24(b^2 - a^2)}$

where
$$a = \frac{\sqrt{525+70}\sqrt{9w^2-10\omega+30-210\omega}}{70}$$
, $b = \frac{\sqrt{525-70}\sqrt{9w^2-10\omega+30-210\omega}}{70}$ and
 $A_{11} = \frac{1}{2} - \frac{(\alpha - \beta)(12a^2 - 1)(20a^3 - 3a)}{2} + \frac{(20a^3 - 3a)^2\alpha\beta\gamma}{2}$,
 $A_{12} = \frac{1}{2} - a + b + \frac{a(12b^2 - 1) - b(12a^2 - 1)}{2} - \frac{\alpha(12b^2 - 1)(20a^3 - 3a) - \beta(12a^2 - 1)(20b^3 - 3b)}{4}$
 $+ \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{2}$,
 $A_{13} = \frac{1}{2} - a - b + \frac{a(12b^2 - 1) + b(12a^2 - 1)}{2} - \frac{\alpha(12b^2 - 1)(20a^3 - 3a) + \beta(12a^2 - 1)(20b^3 - 3b)}{4}$
 $- \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{2}$,
 $A_{14} = \frac{1}{2} - 2a + a(12a^2 - 1) - \frac{(\alpha + \beta)(12a^2 - 1)(20b^3 - 3a)}{2} - \frac{(20a^3 - 3a)^2\alpha\beta\gamma}{2}$,
 $A_{21} = \frac{1}{2} + a - b - \frac{a(12b^2 - 1) - b(12a^2 - 1)}{4} - \frac{\alpha(12a^2 - 1)(20b^3 - 3b) - \beta(12b^2 - 1)(20a^3 - 3a)}{4}$
 $+ \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{4}$,
 $A_{22} = \frac{1}{2} - \frac{(\alpha - \beta)(12b^2 - 1)(20b^3 - 3b)}{4} + \frac{(20b^3 - 3b)^2\alpha\beta\gamma}{2}$,
 $A_{23} = \frac{1}{2} - 2b + b(12b^2 - 1) - \frac{(\alpha + \beta)(12b^2 - 1)(20b^3 - 3b)}{4} - \frac{(20b^3 - 3b)^2\alpha\beta\gamma}{2}$,
 $A_{24} = \frac{1}{2} - a - b + \frac{a(12b^2 - 1) + b(12a^2 - 1)}{2} - \frac{\alpha(12a^2 - 1)(20b^3 - 3b) + \beta(12b^2 - 1)(20a^3 - 3a)}{4}$
 $- \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{2}$,
 $A_{31} = \frac{1}{2} + a + b - \frac{a(12b^2 - 1) + b(12a^2 - 1)}{2} + \frac{\alpha(12a^2 - 1)(20b^3 - 3b) + \beta(12b^2 - 1)(20a^3 - 3a)}{4}$
 $- \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{2}$,
 $A_{34} = \frac{1}{2} - a + b + \frac{a(12b^2 - 1) + b(12a^2 - 1)}{2} + \frac{\alpha(12a^2 - 1)(20b^3 - 3b) - \beta(12b^2 - 1)(20a^3 - 3a)}{4}$
 $+ \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{2}$,
 $A_{41} = \frac{1}{2} + 2a - a(12a^2 - 1) + \frac{(\alpha + \beta)(12a^2 - 1)}{2} + \frac{\alpha(12a^2 - 1)(20b^3 - 3b) - \beta(12b^2 - 1)(20a^3 - 3a)}{4}$
 $+ \frac{(20a^3 - 3a)(20b^3 - 3b)\alpha\beta\gamma}{2}$,
 $A_{41} = \frac{1}{2} + a - b - \frac{a(12b^2 - 1) - b(12a^2 - 1)}{2} + \frac{\alpha(12a^2 - 1)(20a^3 - 3a) - \frac{(20a^3 - 3a)^2\alpha\beta\gamma}{2}$,
 $A_{42} = \frac{1}{2} + a + b - \frac{a(12b^2 - 1) - b(12a^2 - 1)}{2} + \frac{\alpha(12a^2 - 1)(20a^3 - 3a) - (20a^3 - 3a)^2\alpha\beta\gamma}{2}$,
 $A_{43} = \frac{1}{2} + a - b - \frac{a(12b^2 - 1) - b(12a^2 - 1)}{2} + \frac{\alpha(12a^2 - 1)(20a^3 - 3a) - \beta(12a^2 - 1)(20a^3 - 3a)}{2} - \frac{\beta(12a^2 - 1)(20a^3 - 3a)}{2} - \frac{\beta(12a^2 - 1)(20a^$

c) With the special choice of parameters, we can obtain the known implicit Runge-Kutta methods:

1) Gauss methods of order 4 and 6 respectively:

as $\omega = 0$ and $\alpha = \beta = 1, \gamma = 0$.

2) Lobatto IIIA methods of order 4 and 6 respectively:

as $\omega = -1$ and $\alpha = 1, \beta = \gamma = 0$.

3) Lobatto IIIB methods of order 4 and 6 respectively:

as $\omega = -1$ and $\beta = 1, \alpha = \gamma = 0$.

4) Lobatto IIIC methods of order 4 and 6 respectively:

as $\omega = -1$ and $\alpha = \beta = \gamma = 1$.

5) Lobatto IIIE methods of order 4 and 6 respectively:

1

as $\omega = -1$ and $\alpha = \beta = 1, \gamma = 0$.

6) Lobatto IIIS methods of order 4 and 6 respectively:



d) Lobatto IIISX methods of order 4 and 6 respectively:



as $\omega = -1$ and $\alpha \neq \beta, \gamma \neq 0$.

e) Particularly, we can obtain the known diagonally implicit Runge-Kutta (DIRK) methods of order 2 and 4 with some special parameters:

1) DIRK method of order 2:



as $\omega = \frac{1}{8}$, $\alpha = \beta = 1$ and $\gamma = 0$.

2) DIRK method of order 4:

$\frac{1}{2} + a$	$\frac{1}{2} + a$	0	0
$\frac{1}{2}$	1 + 2a	$-(\frac{1}{2}+2a)$	0
$\frac{1}{2}-a$	1 + 2a	-(1+4a)	$\frac{1}{2} + a$
	1 + 2a	-(1+4a)	1 + 2a
21	$-\frac{1}{2}$		

as $\omega = \frac{8+5\cdot 2^{\frac{1}{3}}}{12}$, that is, $a = \frac{2^{\frac{1}{3}}+2^{-\frac{1}{3}}-1}{6}$, $\alpha = \beta = -(\frac{1}{a}+2)$ and $\gamma = 0$.

However, it is impossible that the implicit Runge-Kutta method with B(6), C(2)and D(2) is diagonally by choosing the parameters of ω , α , β and γ . In fact, it is easily shown by satisfying the order condition C(2) or D(2) that symplectic implicit Runge-Kutta methods with B(p), $C(\eta)$ and $D(\zeta)$, when η or $\zeta > 1$, cannot be diagonally [4]. Therefore, we cannot find out symplectic diagonally implicit Runge-Kutta methods of order greater than 4.

3.2. The Gauss-Radau methods

In this section, we construct another family of s-stage Implicit Runge-Kutta methods, which are called the Gauss-Radau methods, satisfying B(2s-1), C(s-1) and D(s-1), based on the combination

$$P(x) = P_s^*(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-1}}\omega P_{s-1}^*(x),$$

which is symplectic but non-symmetric, 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 the P(x) are real and distinct, but $\overline{P}c = e - c$ is not satisfied if $\omega \neq 0$. The weights of the Butcher Table are determined by B(2s-1). For the same reasons of section 3.1, we can also choose the transformation matrix X, which is the same matrix as X_G with the exception that $x_{s,s-1} = \xi_{s-1}\alpha, x_{s-1,s} = -\xi_{s-1}\beta, x_{s,s} = \frac{\alpha\beta\gamma}{4s-1}$. By the Theorem 12.7 of ([8], IV.12.), if $p \geq 2s - 1$, b > 0, the four-parameters family of Implicit Runge-Kutta methods with coefficients

$$A = WXW^TB$$

is symplectic and algebraically stable, and has at least order 2s - 1. Besides such results, with the special chioce of parameters $\omega, \alpha, \beta, \gamma$, we can obtain:

a) s-stage Gauss methods of order 2s with $\omega = 0, \alpha = \beta = 1, \gamma = 0;$

b) s-stage symplectic and algebraically stable Implicit Runge-Kutta methods of order 2s - 1, which satisfy B(2s - 1), C(s - 1) and D(s - 1) and is called Radau IB with $\omega = 1$, $\alpha = \beta = 1$, $\gamma = 0$;

c) s-stage symplectic and algebraically stable Implicit Runge-Kutta methods of order 2s - 1, which satisfy B(2s - 1), C(s - 1) and D(s - 1) and is called Radau IIB with $\omega = -1, \alpha = \beta = 1, \gamma = 0$.

Therefore, we also call this family Implicit Runge-Kutta method the Gauss-Radau method as [4]. Its members with 2 and 3 stages are given by the following Butcher Tables 5–6:



where $a = \sqrt{3 + \omega^2}$.

 Table 6. Butcher Table of 3-stages Gauss-Radau method

c_1	$b_1 A_{11}$	$b_2 A_{12}$	$b_3 A_{13}$
c_2	$b_1 A_{21}$	$b_2 A_{22}$	$b_3 A_{23}$
c_3	$b_1 A_{31}$	$b_2 A_{32}$	$b_3 A_{33}$
	b_1	b_2	b_3

where

$$\begin{split} c_1 &= -M_1 + \frac{5-\omega}{10}, \ c_2 = -M_2 + \frac{5-\omega}{10}, \ c_3 = M_3 + \frac{5-\omega}{10};\\ M_1 &= \frac{\sqrt{\omega^2 + 5}}{5} \sin(\frac{\theta}{3} - \frac{\pi}{6}), \ M_2 = \frac{\sqrt{\omega^2 + 5}}{5} \cos(\frac{\theta}{3}), \ M_3 = \frac{\sqrt{\omega^2 + 5}}{5} \sin(\frac{\theta}{3} + \frac{\pi}{6});\\ \cos\theta &= \frac{\omega(5-\omega^2)}{M}, \ \sin\theta = \frac{5\sqrt{\omega^4 + 2\omega^2 + 5}}{M}, \ M = \sqrt{\omega^6 + 15\omega^4 + 75\omega^2 + 125},\\ b_1 &= \frac{M_2M_3 + \frac{\omega}{10}(M_3 - M_2) - \frac{1}{300}(25 + 3\omega^2)}{(M_1 + M_3)(M_2 - M_1)},\\ b_2 &= \frac{M_1M_3 + \frac{\omega}{10}(M_3 - M_1) - \frac{1}{300}(25 + 3\omega^2)}{(M_2 + M_3)(M_1 - M_2)}, \ b_3 = 1 - b_1 - b_2; \end{split}$$

and

$$\begin{split} A_{11} &= \frac{1}{2} - \frac{1}{4} (\alpha - \beta) (2M_1 + \frac{\omega}{5}) [3(2M_1 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_1 + \frac{\omega}{5})^2 - 1]^2; \\ A_{12} &= \frac{1}{2} - (M_1 - M_2) - \frac{1}{4} \alpha (2M_2 + \frac{\omega}{5}) [3(2M_1 + \frac{\omega}{5})^2 - 1] \\ &\quad + \frac{1}{4} \beta (2M_1 + \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_1 + \frac{\omega}{5})^2 - 1] [3(2M_2 + \frac{\omega}{5})^2 - 1]; \\ A_{13} &= \frac{1}{2} - (M_1 + M_3) + \frac{1}{4} \alpha (2M_3 - \frac{\omega}{5}) [3(2M_1 + \frac{\omega}{5})^2 - 1] \\ &\quad + \frac{1}{4} \beta (2M_1 + \frac{\omega}{5}) [3(2M_3 - \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_1 + \frac{\omega}{5})^2 - 1] [3(2M_3 - \frac{\omega}{5})^2 - 1]; \\ A_{21} &= \frac{1}{2} + (M_1 - M_2) - \frac{1}{4} \alpha (2M_1 + \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] \\ &\quad + \frac{1}{4} \beta (2M_2 + \frac{\omega}{5}) [3(2M_1 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_1 + \frac{\omega}{5})^2 - 1] [3(2M_2 + \frac{\omega}{5})^2 - 1]; \\ A_{22} &= \frac{1}{2} - \frac{1}{4} (\alpha - \beta) (2M_2 + \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_2 + \frac{\omega}{5})^2 - 1]]3(2M_2 + \frac{\omega}{5})^2 - 1]^2; \\ A_{23} &= \frac{1}{2} - (M_2 + M_3) - \frac{1}{4} \alpha (2M_3 - \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] \\ &\quad + \frac{1}{4} \beta (2M_2 + \frac{\omega}{5}) [3(2M_3 - \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_2 + \frac{\omega}{5})^2 - 1] [3(2M_3 - \frac{\omega}{5})^2 - 1]; \\ A_{31} &= \frac{1}{2} + (M_1 + M_3) - \frac{1}{4} \alpha (2M_1 + \frac{\omega}{5}) [3(2M_3 - \frac{\omega}{5})^2 - 1] \\ &\quad - \frac{1}{4} \beta (2M_3 - \frac{\omega}{5}) [3(2M_1 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_1 + \frac{\omega}{5})^2 - 1] [3(2M_3 - \frac{\omega}{5})^2 - 1]; \\ A_{32} &= \frac{1}{2} + (M_2 + M_3) - \frac{1}{4} \alpha (2M_1 + \frac{\omega}{5}) [3(2M_3 - \frac{\omega}{5})^2 - 1] \\ &\quad - \frac{1}{4} \beta (2M_3 - \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_1 + \frac{\omega}{5})^2 - 1] [3(2M_3 - \frac{\omega}{5})^2 - 1]; \\ A_{32} &= \frac{1}{2} + (M_2 + M_3) - \frac{1}{4} \alpha (2M_2 + \frac{\omega}{5}) [3(2M_3 - \frac{\omega}{5})^2 - 1] \\ &\quad - \frac{1}{4} \beta (2M_3 - \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_2 + \frac{\omega}{5})^2 - 1] [3(2M_3 - \frac{\omega}{5})^2 - 1]; \\ &\quad - \frac{1}{4} \beta (2M_3 - \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_2 + \frac{\omega}{5})^2 - 1] [3(2M_3 - \frac{\omega}{5})^2 - 1]; \\ &\quad - \frac{1}{4} \beta (2M_3 - \frac{\omega}{5}) [3(2M_2 + \frac{\omega}{5})^2 - 1] + \frac{5}{44} \alpha \beta \gamma [3(2M_2 + \frac{\omega}{5})^2 - 1$$

$$A_{33} = \frac{1}{2} + \frac{1}{4}(\alpha - \beta)(2M_3 - \frac{\omega}{5})[3(2M_3 - \frac{\omega}{5})^2 - 1] + \frac{5}{44}\alpha\beta\gamma[3(2M_3 - \frac{\omega}{5})^2 - 1]^2.$$

d) The special members of Gauss-Radau methods with 2 and 3 stages, Radau IB and Radau IIB methods, are given by

1) 2-stages Radau IB and Radau IIB methods:

	0	$\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{3}$	$\frac{3}{8}$	$-\frac{1}{24}$
	$\frac{2}{3}$	$\frac{7}{24}$	$\frac{3}{8}$	1	$\frac{7}{8}$	$\frac{1}{8}$
-		$\frac{1}{4}$	$\frac{3}{4}$		$\frac{3}{4}$	$\frac{1}{4}$

2) 3-stages Radau IB and Radau IIB methods:

0	$\frac{1}{18}$	$\frac{-1-\sqrt{6}}{36}$	$\frac{-1+\sqrt{6}}{36}$	4	$\frac{4-\sqrt{6}}{10}$	$\frac{16-\sqrt{6}}{72}$	$\frac{328 - 167\sqrt{6}}{1800}$	$\tfrac{-2+3\sqrt{6}}{450}$
$\frac{6-\sqrt{6}}{10}$	$\tfrac{52+3\sqrt{6}}{450}$	$\frac{16+\sqrt{6}}{72}$	$\tfrac{472-217\sqrt{6}}{1800}$	4	$\frac{4+\sqrt{6}}{10}$	$\frac{328+167\sqrt{6}}{1800}$	$\frac{16+\sqrt{6}}{72}$	$\tfrac{-2-3\sqrt{6}}{450}$
$\frac{6+\sqrt{6}}{10}$	$\tfrac{52-3\sqrt{6}}{450}$	$\frac{472+217\sqrt{6}}{1800}$	$\frac{16-\sqrt{6}}{72}$		1	$\tfrac{17-2\sqrt{6}}{36}$	$\frac{17+2\sqrt{6}}{36}$	$\frac{1}{18}$
	$\frac{1}{9}$	$\frac{16+\sqrt{6}}{36}$	$\frac{16-\sqrt{6}}{36}$			$\frac{16-\sqrt{6}}{36}$	$\frac{16+\sqrt{6}}{36}$	$\frac{1}{9}$

Corollary 3.1 ([4]). For $\omega = 1$ or $\omega = -1$, assume the transformation matrix X be the same matrix as X_G with the difference that

$$X_{s,s-1} = \alpha \xi_{s-1}, \quad X_{s-1,s} = -\beta \xi_{s-1}, \quad X_{s,s} = \frac{1}{4s-1} \alpha \beta \gamma, \qquad \alpha, \beta, \gamma (\neq 0, 1) \in \mathbb{R},$$

we can obtain s-stage ($s \ge 3$) symplectic and algebraically stable Implicit Runge-Kutta 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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