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Symplectic Runge-Kutta Methods from the Viewpoint of Symmetry

By

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Abstract

The Weinstein generating function is introduced in order to represent a symplectic mapping, and it is shown that the representation is closely related to a certain symplectic Runge-Kutta method. Furthermore, the symmetry property is characterized by means of the generating function, and in relation to the symmetry, several stabilities intrinsic to linearly symplectic Runge-Kutta methods are studied.

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Introduction

A frequent use has been made of symplectic integrators (abbreviated to SIA's) in such fields as nuclear physics, celestial mechanics and so on. Since Sanz-Serna showed that certain Runge-Kutta (abbreviated to RK) methods give symplectic mappings when integrating a Hamiltonian system [7], many aspects of symplectic RK methods have been studied. It is widely known that a symplectic mapping is expressed locally in terms of a generating function, and symplectic RK methods are studied from this viewpoint, too. Almost any symplectic mapping can be represented by use of another kind of generating function discovered by Weinstein [9], though it is rather unfamiliar. This representation is motiviated by construction of a nonlinearlization of Cayley transformation in linear algebra, and the transformation was tried to use for numerical integration of linear Hamiltonian systems in cinjunction with Padé approximation [3]. One purpose of this paper is to study a numerical use of the representation.

On the other hand, attention is paid to a time-reversible method which may be considered as an inheritance of properties intrinsic to a flow of a dynamical system. In RK methods, symmetric ones are familiar in that they possess reversibility, and the methods not only possess a few excellent properties on stabilities but also are related to linear symplecticity. The second purpose of this paper is show the reversible methods are linearly symplectic, that is, they give symplectic mappings when the systems to integrate are confined to linear Hamiltonian systems with constant coeffients.

The contents of this paper are arranged as follows. The next section is devoted to introduction of the representation of a symplectic mapping in terms of a Weinstein generating function, and the reversibility of an SIA is considered related to the function. Section 2 deals with RK methods subject to $R(z)R(-z) = 1$ which is a necessary and sufficient condition to be linearly symplectic. Furthermore, our attention is paid to algebraiccaly stable and symmetric methods from a viewpoint of symplecticity. A few remarks are mentioned in the final section.

1. Weinstein generating function and reversibility

In this section, we review the representation of a symplectic mapping by use of the Weinstein generating function, and study its relation with numerical integration.

We start by designating a conservative Hamiltonian system with N degrees of freedom expressed as

$$\frac{dx}{dt} = J \cdot \operatorname{grad} H(x), \quad \text{where } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{1}$$

Here, x is an R^{2N}-valued variable. We assume that the phase space D is an Euclidean space R^{2N} or its subdomain, and the functions and mappings on D are differentiable up to a necessary order throughout the paper. Furthermore, the symbols n and h are used to represent the step number and the step size, respectively.

Now, let us review Cayley transformation wellknown in linear algebra, for the representation which we are concerned with can be considered as its nonlinearlization in a sense.

Definition 1. *We define two sets G_{-1} and g_1 of $2N$-dimensional matrices and two mappings $\sigma : g_1 \to G_{-1}$ and $\tau : G_{-1} \to g_1$ as follows.*

$$\begin{aligned} G_{-1} &= \{P \in Sp(2N, R) \mid \det(I + P) \neq 0\}, \\ g_1 &= \{Q \in sp(2N, R) \mid \det(I - Q) \neq 0\}, \\ \sigma(Q) = (I + Q)(I - Q)^{-1}, &\quad \tau(P) = -(I - P)(I + P). \end{aligned} \tag{2}$$

The following theorem is obvious, and its proof is omitted.

Theorem 1. *Both σ and τ are bijections, and the one is the inverse of the other.*

We remark that the above theorem holds even if $Sp(2N, R)$ and $sp(2N, R)$ in Definition 1 are replaced with any linear Lie group composed of all matrices P subject to $P^T KP = K, K$ being an arbitrary nonsingular matrix, and its Lie algebra, respectively. Also, we refer to a pioneering work where $\sigma(Q)$ is tried to utilize for integration of a linear Hamiltonian system in conjunction with the Padé approximation [3].

Let us think of a symplectic mapping on D

$$y = \phi(x). \tag{3}$$

If we denote by P the Jacobian matrix $\partial\phi/\partial x$, then P belongs to $Sp(2N,\ R)$. We put

$$z = (\phi(x) + x)/2, \tag{4}$$

and assume that P does not have an eigenvalue -1. Then, x becomes a function of z at least locally, and we can introduce an R^{2N}-valued function T of z by

$$T(z) = \frac{\phi(x(z)) - x(z)}{2}. \tag{5}$$

Thereby, the mapping (3) is represented in such a manner as

$$y = z + T(z), \qquad x = z - T(z), \tag{6}$$

z being an intermediate parameter defined by (4). If Q means the Jacobian matrix $\partial T/\partial z$, it follows from $P \in G_{-1}$ that $Q = \tau(P)$ and $Q \in g_1$.

Theorem 2. *If the Jacobian matrix of a symplectic mapping given by* (3) *does not have an eigenvalue -1, the mapping is expressed in terms of a function S as*

$$y = z + J \cdot grad\ S(z), \qquad x = z - J \cdot grad\ S(z) \tag{7a}$$

at least locally, where z is an intermediate parameter.

Proof. Since $Q \in g_1$, is satisfied the integrability condition for T in (5) to be expressed as $J \cdot \mathrm{grad}\ S$.

Definition 2. *The function S in* (7a) *is called the Weinstein generating function.*

As is seen from this theorem, almost every symplectic mapping can be represented in the form (7a). The representation itself can be used as a numerical scheme to integrate (1) by putting $y = x_{n+1}$ and $x = x_n$. For the numerical use, the consistency is ensured, if and only if

$$S(z) = \frac{h}{2}H(z) + o(h) \tag{7b}$$

holds up to a difference of a constant. Since the Jacobian matrix of an arbitrary SIA is near to the identity matrix when $h > 0$ is suffciently small, every SIA can be expressed as (7) in principle. In particular, our attention is concentrated on the case that

$$grad\ S \quad is\ odd\ with\ resepct\ to\ h. \tag{8}$$

Concerning (7), we define two mappings indicating the step size explicitly.

$$\phi_h : x \mapsto y, \qquad \psi_{h/2} : z \mapsto y.$$

It is easy to prove that (8) leads to (9) and the resulting equation comes to (10), where

$$\phi_h = \psi_{h/2} \circ \psi_{-h/2}^{-1}, \tag{9}$$

$$\phi_{-h} = \phi_h^{-1}. \tag{10}$$

Hereafter, a scheme ϕ_h is called reversible if the property (10) holds good for an arbitrary small $h > 0$. We can see immediately that the property (8) follows from the reversibility, and accordingly, we have

Theorem 3. *With resepct to an SIA ϕ_h, the following three assertions are equivalent to one another.*

1. *An SIA is reversible.*
2. *grad S is odd with regard to h, S denoting the Weinstein generating function.*
3. *ϕ_h is a composition of a forward scheme and its backward version.*

This theorem is a characeristic of reversibility in terms of the Weinstein generating function. With resepect to (9), it is often the case that though ψ_h is a scheme of a low order, ϕ_h is of a higher order, and further ψ_h is not necessarily determined from ϕ_h uniquely. The simplest scheme among those given by (7) is the one obtained by $S = h \cdot H/2$, which is nothing but the implicit midpoint scheme, that is, the one-stage Gauss-Legendre method.

2. RK methods subject to R(z)R(-z)=1 and symplecticity

This section deals with RK methods subject to $R(z)R(-z) = 1$ and their symplectic properties on the basis of reversibility.

As is well known, the whole of RK methods forms a group with composition of mappings being the product operation. If ψ_h stands for a mapping obtained by applying an irreducible RK method $\frac{A}{b^T}$ (Stetter tableau) to a system of ordinary differential equations, the mapping $\psi_{h/2} \circ \psi_{-h/2}^{-1}$ is realized by a single RK method $\begin{array}{cc} (-A+eb^T)/2 & 0 \\ eb^T/2 & A/2 \\ \hline b^T/2 & b^T/2 \end{array}$. Here, e means the vector $(1, \cdots, 1)^T$ and the resulting Stetter tableau may happen to be reducible. On the contrary, an RK method is called symmetric [8], if it is reversible when applied to any arbitrary ordinary differential equation. It is already known that a symmetric RK method is decomposable as in (9) by means of RK methods. The following theorem is a slight modification of those proposed in [8, §3.2].

Theorem 4. *An irreducible RK method given by $\frac{A}{b^T}$ is symmetric, if and only if there is a permutation matrix P such that*

$$A + PAP^{-1} = eb^T, \qquad Pb = b. \tag{11}$$

These equations are reexpressed in terms of elements as $a_{ij} + a_{\sigma(i)\sigma(j)} = b_j = b_{\sigma(j)}$, where σ denotes the permutation. Under (11), ψ_h in (9) is realized by an RK method determined by $\frac{eb^T - 2A}{b^T}$.

Let us illustrate two-stage symmetric RK methods.

Example 1 (Two-stage symmetric RK methods). *Put $P = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, and all symmteric RK methods subject to B(1) condition turn out to form a two-parameter family given by*

$$\begin{array}{cc} 1/4+\alpha & 1/4-\beta \\ 1/4+\beta & 1/4-\alpha \\ \hline 1/2 & 1/2 \end{array} \quad (\alpha \text{ and } \beta \text{ are arb. parameters}). \tag{12}$$

Each method is of order two or four, whereas ψ_h in Theorem 4 is always of order one and is given by $\begin{array}{cc} -2\alpha & 2\beta \\ -2\beta & 2\alpha \\ \hline 1/2 & 1/2 \end{array}$. With resepect to stabilities, the above method is

$$A\text{-stable when } |\alpha| \le |\beta| \; ; \qquad \text{algebraically stable when } \alpha = 0.$$

Furthermore, the family contains such known methods as

1. $\alpha = 0, \quad \beta = \sqrt{3}/6$	*Gauss-Legendre method.*
2. $\alpha = -1/4, \quad \beta = 1/4$	*Lobatto IIIA method.*
3. $\alpha = 1/4, \quad \beta = 1/4$	*Lobatto IIIB method.*
4. $\alpha + \beta = 1/2$	*Symmetric Lobatto method.*

Now, we intend to consider a relation between symmetric methods and simplecticity. Sanz-Serna proved that $M = 0$ is a condition for an RK method to give a symplectic mapping when integrating an arbitrary Hamiltonian system [7]. However, the symmetry property treated now is independent of $M = 0$ and a symmetric RK method does not always yield a symplectic mapping in numerical integration of a nonlinear Hamiltonian system.

Definition 3. *An RK method is called linearly symplectic, if its stability function $R(z)$ satisfies*

$$R(z)R(-z) = 1. \tag{13}$$

Equation (13) is a necessary and sufficient condition that an RK method gives a linearly symplectic mapping when applied to any linear Hamiltonian system with constant coefficients [4]. A symmetric RK method does satisfy (13), though M does not necessarily vanish [5]. Of course, any RK method subject to $M = 0$ is linearly symplectic. In Fig.1, we show the relations among the three kinds of RK methods.

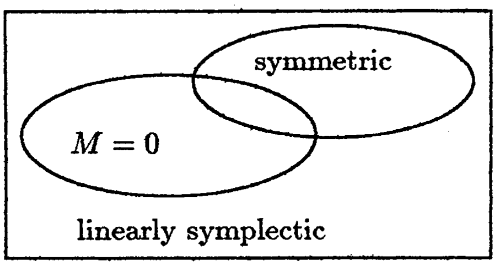

Figure 1: Relations among three kinds of RK methods

The two subsets are true ones, and there is no inclusion relation between them. As for their dynamical properties, we can enumerate interesting items.

1. linearly symplectic RK method.
   (a) It gives a linearly symplectic mapping for any linear Hamiltonian system.
   (b) It is reversible for any linear system with constant coefficients.
   (c) It inherits at most quadratic first integrals admitted by any linear system with constant coefficients [6].
2. Symmetric RK method.
   (a) It is reversible for any system of ordinary differential equations.
3. RK method subject to $M = 0$.
   (a) It gives a symplectic mapping for every Hamiltonian system.
   (b) It inherits at most quadratic first integrals admitted by any system of ordinary differential equations [1].

The three properties intrinsic to linearly symplectic methods are propagated separately according as the systems to integrate are enlarged to nonlinear ones. We are allowed to mention that symmetric RK methods subject to $M = 0$, the intersection of the two subsets, inherit the original three properties. In the case of two-stage methods, the one-parameter family $\begin{array}{cc} 1/4 & 1/4-\beta \\ 1/4+\beta & 1/4 \\ \hline 1/2 & 1/2 \end{array}$ is in comformity, where β is an arbitrary constant. The subsequent theorem fits this family.

Theorem 5. *An algebraically stable and symmetric RK method satisfies $M = 0$.*

Proof. Since $PMP^{-1} = -M$ follows from (11), the eigenvalues of M come in individual pairs $\{\lambda, -\lambda\}$. Therefore, in order that M is non-negative definite, M must vanish.

As is seen in Example 1, though every two-stage RK method which is symmetric and subject to $M = 0$ is algebraically stable, algebraic stability is not possessed automatically when the stage number exceeds two. However, for each fixed stage number, the whole of algebraically stable and symmetric methods forms a family including the Gauss-Legendre method, and there exist methods with tractable parameters in the family.

In the remainder, we intend to study a few excellent features intrinsic to (linear) symplectic RK methods. Among the methods satisfying (13), our attention should be paid to those such that

$$R(z) \text{ has no pole in the left-half plane.} \tag{14}$$

According to [5], the conditions of (13) and (14) lead to the followings:

$$\text{When } Re(z) < 0, \ |R(z)| < 1; \tag{15a}$$

$$\text{When } Re(z) = 0, \ |R(z)| = 1; \tag{15b}$$

$$\text{When } Re(z) > 0, \ |R(z)| > 1. \tag{15c}$$

The first property (15a) means A-stablility, and therefore, (14) is necessary and sufficient for a linearly symplectic method to be A-stable. In addition to A-stability, the remaining two properties (15b) and (15c) bless the method with a few good dynamical properties related to integration of an arbitrary linear system with constant coeffients [5].

1. If a true solution converges to the origin, the corresponding numerical solution also converges for any $h > 0$. On the contrary, any divergent solution is reproduced numerically in a similar manner.

2. For the system of two variables, every elliptic orbit is reproduced accurately for any $h > 0$.

As far as linear systems are treated, there seems to be little difference between A-stability and algebraic stability. In dealing wth nonlinear systems, however, algebraic stability plays an important role. Let us show a dynamical property possessed by an RK method subject to $M = 0$ and $b > 0$. In the sequel, $f(x)$, $<,>$, and $\|\cdot\|$ denote $J \cdot \text{grad } H(x)$, the Euclidean inner product, and the corresponding norm, respectively. Then, for two numerical solutions $\{\tilde{x}_n\}$ and $\{x_n\}$, it holds that

$$\|\tilde{x}_{n+1} - x_{n+1}\|^2 = \|\tilde{x}_n - x_n\|^2 + 2h \sum_i b_i < f(\tilde{\xi}_i) - f(\xi_i),\ \tilde{\xi}_i - \xi_i >, \qquad (16)$$

where $\tilde{\xi}_i = \tilde{x}_n + h \sum_j a_{ij} f(\tilde{\xi}_j)$ and $\xi_i = x_n + h \sum_j a_{ij} f(\xi_j)$. Since a Hamiltonian system preserves volume, it is not dissipative at all and the notion of B-stability is not effective. However, there is a domain D_1 where the signature of $< f(x) - f(y),\ x - y >$ remains constant, x and y being arbitrary points in D_1. Roughly speaking, Equation (16) indicates that in the domain, if two solutions of (1) come up to each other as time passes, numerical solutions behave in a similar way, and if the distance of two solutions grows longer, a similar circumstance is reproduced numerically. This is ensured if all of $\tilde{\xi}_i$ and ξ_i are contained in D_1 in a strict sense.

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