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On Inheritance of Quadratic First Integral of Linear System via Runge–Kutta Methods

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Abstract

This paper deals with a condition for any quadratic homogeneous first integral of an arbitrary linear system with constant coefficients to be conserved by a discrete system obtained by applying Runge–Kutta methods.

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1 Introduction

It is often the case that physical or chemical dynamical systems possess conservative quantities. For example, any Hamiltonian particle system admits an energy integral, and some chemical reactance systems leave invariant the total mass and so on. In numerical computation of these systems, nothing can be better than that first integrals of the original system are inherited as conservatives of the discretized ones.

As for the problem, it is usually impossible that all first integrals are inherited. It has been proved, however, that every first integral linear homogeneous in dependent coordinates is conserved by an arbitrary Runge-Kutta method (hereafter abbreviated to RK method) [5]. Moreover, RK methods subject to a condition $M = 0$ inherit all first integrals at most quadratic in dependent coordinates [1]. These facts have led to a prediction that an arbitrary RK method cannot inherit first integrals other than at most quadratic ones. In pursuing this problem, the contents of this paper have been obtained, which are an addition to a result in [1] in a sense. The object of this paper is to verify that as far as differential equations are confined to linear ones with constant coefficients, all quadratic first integrals are inherited under a condition weaker than $M = 0$.

The next section deals with a new condition described above. In § 3, it is shown that the condition is truely weaker than $M = 0$ by illustrating a few RK methods.

2 Condition of R(z)R(-z)=1

This section treats a condition for all quadratic first integrals admitted by any linear system to be conserved by a discrete system which an RK method yields.

Let us consider a linear system on $\boldsymbol{R}^N$ given by

$$\frac{dx}{dt} = Ax, \quad x \in \boldsymbol{R}^N, \tag{1}$$

where A denotes a nontrivial matrix of order N. A quadratic form

$$f(x) = \frac{1}{2}\, {}^t xSx, \quad {}^tS = S \tag{2}$$

is a first integral of (1), if and only if

$${}^tAS + SA = 0 \tag{3}$$

holds good, where the superfix t stands for matrix transpose. This equation is due to $df/dt =^t x({}^tAS + SA)x/2$. From now on, we call a first integral expressed as the above a quadratic first integral (abbreviated to QFI).

Now, choose an arbitrary RK method and discretize (1) thereby. Then, we have the following recurrence, n denoting the step number,

$$x_{n+1} = R(hA)x_n, \quad n = 0,\ 1,\ \cdots, \tag{4}$$

where $R(z)$ is a stability function [2]. $R(z)$ is a polynomial or a rational function according as the method is explicit or (semi)implicit, and therefore it is holomorphic.

Lemma 2.1 *The QFI given by (2) is inherited by (4) as an invariant, if and only if*

$$S \cdot \{R(-hA)R(hA) - I\} = 0 \tag{5}$$

holds good, where I is a unit matrix.

Proof. The equation $f(x_{n+1}) = f(x_n)$ is equivalent to ${}^tR(hA)SR(hA) = S$. Due to (3), we have $({}^tA)^nS = S(-A)^n$ for an arbitrary nonnegative integer n. Then, it results that ${}^tR(hA)S = SR(-hA)$, since $R(z)$ is a holomorphic function. This completes the proof.

The following is a direct result of the lemma.

Theorem 2.1 *If the stability function satisfies*

$$R(z)R(-z) = 1, \tag{6}$$

then every QFI of any linear system (1) is inherited.

Proof. Since $R(-hA)R(hA) - I = 0$ holds under the supposition, (5) is satisfied irrespective of S.

The next step is to show that the reverse of the above theorem is true. That is,

Lemma 2.2 *If the stability function satisfies*

$$R(z)R(-z) \neq 1, \tag{7}$$

the energy integral of that linear Hamiltonian system is not inherited by the discrete system (4), at least one of the eigenvalues of whose Hamiltonian matrix is not equal to 0.

Proof. Let A be a Hamiltonian matrix and N be even. Then, as is well known, (1) admits an energy integral expressed as (2) with $S = J^{-1}A$, J being $\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$. If we reexpress (5) by means of the Jordan normal form of A, a diagonal component of the resulting equation should satisfy

$$a \cdot \{R(-ha)R(ha) - 1\} = 0, \tag{8}$$

where a is an eigenvalue of A. Since a nonzero a can be selected by supposition, Equation (8) is not satisfied for (almost) all $h > 0$, for (7) is true and $R(z)$ is holomorphic.

Combining Theorem 2.1 and the above lemma, we have obtained the conclusion of this section.

Theorem 2.2 *Every QFI of any linear system given by (1) is inherited by the discrete system (4), if and only if the stability function of the RK method satisfies (6).*

We close this section by remarking that the equation (6) has been familiar in that a symplectic mapping is obtained when any RK method subject to the condition is applied to a linear Hamiltonian system [3], and that closed orbits are reproduced numerically under the condition [4] and so on.

3 Relation between three conditions

In this section, we make clear the relations between three conditions related to inheritance of QFIs.

Let us define three sets of RK methods by the followings.

$\Gamma = \{$ RK methods subject to $R(z)R(-z) = 1\}$,

$\Gamma_1 = \{$ RK methods subject to $M = 0\}$,

$\Gamma_2 = \{$ symmetric RK methods $\}$. [6]

In the above, any RK method subject to $M = 0$ inherits all QFIs of an arbitrary autonomous system of ordinary differential equations [1]. In this sense, the condition (6) is weaker than $M = 0$. We intend to make clear the relations among the three.

Lemma 3.1 *Γ_1 and Γ_2 are true subsets of Γ.*

Proof. It is already proved in [4] that Γ_1 and Γ_2 are included in Γ. The method given by the following Stetter tableau

$$\begin{array}{cc} 3/4 & 0 \\ 0 & -1/4 \\ \hline 3/4 & 1/4 \end{array}$$

satisfies (2), whereas it is neither symmetric nor subject to $M = 0$.

Lemma 3.2 $\Gamma_1 \cap \Gamma_2 \neq \phi, \quad \Gamma_1 \setminus \Gamma_2 \neq \phi, \quad \Gamma_2 \setminus \Gamma_1 \neq \phi.$

Proof. Let us think of two methods given by

$$\begin{array}{cc} 3/8 & 3/16 \\ 3/16 & 1/8 \\ \hline 3/4 & 1/4 \end{array}, \quad \text{and} \quad \begin{array}{cc} 3/4 & 1/4 \\ 1/4 & -1/4 \\ \hline 1/2 & 1/2 \end{array}.$$

It is easy to see that the former method belongs to $\Gamma_1 \setminus \Gamma_2$ and the latter one belongs to $\Gamma_2 \setminus \Gamma_1$. Moreover, Gauss-Legendre methods both satisfy $M = 0$ and are symmetric.

According to these two lemmas, we have found that as far as differential equations are confined to linear ones with constant coeffients, a wider class of RK methods than what is specified in [1] inherits all QFIs.

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