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QUADRATIC INVARIANTS AND SYMPLECTIC STRUCTURE OF GENERAL LINEAR METHODS[*1)]

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Abstract

In this paper, we present some invariants and conservation laws of general linear methods applied to differential equation systems. We show that the quadratic invariants and symplecticity of the systems can be extended to general linear methods by a tensor product, and show that general linear methods with the matrix M=0 inherit in an extended sense the quadratic invariants possessed by the differential equation systems being integrated and preserve in an extended sense the symplectic structure of the phase space in the integration of Hamiltonian systems. These unify and extend existing relevant results on Runge-Kutta methods, linear multistep methods and one-leg methods. Finally, as special cases of general linear methods, we examine multistep Runge-Kutta methods, one-leg methods and linear two-step methods in detail.

Key words: Quadratic invariants, Symplecticity, General linear methods, Hamiltonian systems.

1. Introduction

Investigating whether a numerical method inherits some dynamical properties possessed by the differential equation systems being integrated is an important field of numerical analysis and has received much attention in recent years [1-10,13,16-24,26,27]. See the review articles of Sanz-Serna[9] and Section II.16 of Hairer et. al.[2] for more detail concerning the symplectic methods. Most of the work on canonical integrators has dealt with one-step formulae such as Runge-Kutta methods(RKMs)[2,3,6,7-10,13,18,20-22,24,26] and Runge-Kutta-Nyström methods (RKNMs)[1,2,9,17]. The study of canonical multistep methods has been restricted to linear multistep methods(LMMs) and one-leg methods(OLMs)[2,4,5,16,18,23,27]. Moreover, Cooper[7] has shown that Runge-Kutta methods with algebraic stability matrix M=0 preserve the quadratic invariants of the systems, and Sanz-Serna[10] and Lasagni[6] have shown them to be symplectic when applied to Hamiltonian systems. Eirola and Sanz-Serna[23] have shown that, for symmetric one-leg methods, the quadratic invariants and symplecticity of the systems can be extended to one-leg methods by a tensor product. Eirola[24] demonstrated that all these results follow from a general monotonicity property of these methods for quadratic forms. Bochev and Scovel[18] showed that symplecticity follows from the fact that these methods preserve quadratic integral invariants and are closed under differentiation and restriction to closed subsystems, furthermore pointed out that though general linear methods are closed under both differentiation and restriction to closed subsystems, it is difficult to determine the form of the quadratic invariants to be preserved by general linear methods simultaneously with the conditions on the coefficients of the methods which will guarantee the preservation of these invariants.

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The main purpose of the present paper is to answer the questions from Bochev and Scovel[18] and to unify and extend the existing results in [6,7,10,23] and to investigate under which conditions a general linear method(GLM) is symplectic in an extended sense when applied to Hamiltonian systems of differential equations and under what conditions a GLM inherits the quadratic invariants possessed by the differential equation systems being integrated.

Consider the following system of differential equations on R^{2N}[25]

$$\begin{cases} \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} = f_i(p,q), & i = 1,2,\ldots,N, \\ \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} = g_i(p,q), & i = 1,2,\ldots,N, \end{cases} \tag{1.1}$$

where $H(p,q)$ with

$$p = (p_1, p_2, \cdots, p_N)^T, \quad q = (q_1, q_2, \cdots, q_N)^T$$

is some real valued smooth function on R^{2N}. We call (1.1) a canonical system of differential equations with Hamiltonian H. We can write (1.1) in the vector form

$$\begin{cases} \frac{dp}{dt} = f(p,q), \\ \frac{dq}{dt} = g(p,q), \end{cases} \tag{1.1$'$}$$

where

$$f(p,q) = (f_1(p,q), f_2(p,q), \ldots, f_N(p,q))^T, \quad g(p,q) = (g_1(p,q), g_2(p,q), \ldots, g_N(p,q))^T.$$

Let $p_i = x_i, q_i = x_{i+N}, i = 1,2,\ldots,N,$

$$x = (x_1, x_2, \cdots, x_{2N})^T, \quad \frac{\partial H}{\partial x} = (\frac{\partial H}{\partial x_1}, \frac{\partial H}{\partial x_2}, \ldots, \frac{\partial H}{\partial x_{2N}})^T \in R^{2N}.$$

Then (1.1) follows that

$$\frac{dx}{dt} = J\frac{\partial H}{\partial x} \tag{1.2}$$

with

$$J = [J_{ij}] = \begin{pmatrix} 0 & -I_N \\ I_N & 0 \end{pmatrix}, \tag{1.3}$$

here and in the following text, I_l denotes the $l\times l$ identity matrix, $l = 1,2,\cdots$. The phase space R^{2N} is equipped with a standard symplectic structure defined by the fundamental differential 2-form[21]

$$\omega = \frac{1}{2}Jdx\wedge dx = dp\wedge dq = \sum_{i=1}^{N} dp_i\wedge dq_i,$$

where the symbol $\wedge$ denotes exterior product. Let ψ be a diffeomorphism of R^{2N},

$$x = (p^T, q^T)^T \rightarrow \psi(x) = (\psi_1(x), \psi_2(x), \ldots, \psi_{2N}(x))^T = (\hat{p}^T(p,q), \hat{q}^T(p,q))^T.$$

ψ is called a symplectic transformation if ψ preserves the 2-form ω, i.e.,

$$\sum_{i=1}^{N} d\hat{p}_i\wedge d\hat{q}_i = \sum_{i=1}^{N} dp_i\wedge dq_i. \tag{1.4}$$

This is equivalent to the condition that

$$(\frac{\partial\psi}{\partial x})^T J (\frac{\partial\psi}{\partial x}) \equiv J, \tag{1.5}$$