Journal of Computational Mathematics, Vol.25, No.6, 2007, 690–696.

NON-EXISTENCE OF CONJUGATE-SYMPLECTIC MULTI-STEP METHODS OF ODD ORDER*

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Abstract

We prove that any linear multi-step method G_1^τ of the form

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H(Z_k)$$

with odd order u ($u \geq 3$) cannot be conjugate to a symplectic method G_2^τ of order w ($w \geq u$) via any generalized linear multi-step method G_3^τ of the form

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H(\sum_{l=0}^{m} \gamma_{kl} Z_l).$$

We also give a necessary condition for this kind of generalized linear multi-step methods to be conjugate-symplectic. We also demonstrate that these results can be easily extended to the case when G_3^τ is a more general operator.

Mathematics subject classification: 65L06.
Key words: Linear multi-step method, Generalized linear multi-step method, Step-transition operator, Infinitesimally symplectic, Conjugate-symplectic.

1. Introduction

For a Hamiltonian system

$$\frac{dZ}{dt} = J^{-1} \nabla H(Z), \quad Z \in \mathbb{R}^{2n}, \tag{1.1}$$

where

$$J = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix},$$

∇ stands for the gradient operator, and $H : \mathbb{R}^{2n} \to \mathbb{R}^1$ is a smooth function (*Hamiltonian*), the symplecticity of any compatible linear m-step method (LMSM)

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H(Z_k) \quad \text{with} \quad \sum_{k=0}^{m} \beta_k \neq 0 \tag{1.2}$$

* Received September 1, 2005; final revised August 15, 2006; accepted December 27, 2006.

can be defined via its step-transition operator (STO) G (also denoted by G^τ): $\mathbb{R}^{2n} \to \mathbb{R}^{2n}$ satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J^{-1} (\nabla H) \circ G^k, \tag{1.3}$$

where G^k stands for k-fold composition of G: $G \circ G \cdots \circ G$.

Definition 1.1. ([4, 7, 12]) *An LMSM* (1.2) *is said to be symplectic for the Hamiltonian system* (1.1) *iff its STO G defined by* (1.3) *is symplectic, i.e.,*

$$\left[\frac{\partial G(Z)}{\partial Z}\right]^\top J \left[\frac{\partial G(Z)}{\partial Z}\right] = J \tag{1.4}$$

for any Hamiltonian function H and any sufficiently small step-size τ*.*

Naturally, one can define an STO for any compatible difference scheme for any ordinarily differential equation and expand the STO as a power series in τ [6, 14]. In particular, the STO G^τ of any LMSM of order s was written as [12]:

$$G^\tau(Z) = \sum_{i=0}^{+\infty} \frac{\tau^i}{i!} Z^{[i]} + aZ^{[s+1]}\tau^{s+1} + \mathcal{O}(\tau^{s+2}), \tag{1.5}$$

where

$$Z^{[0]} = Z, \quad Z^{[1]} = J^{-1}\nabla H(Z), \quad Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]} = Z_z^{[k]} Z^{[1]}$$

for $k = 1, 2, \cdots$, $a \neq 0$ is a real number.

There have been some interesting negative results on the symplecticity of the STOs [7, 12] or even in a weak sense the step-transition mappings [2] for LMSMs. We will concentrate on the conjugate symplecticity of LMSMs and a kind of general linear methods in the sequel.

The following interesting relation was first found by Dahlquist [1] and was introduced to one of the authors (Tang) by Feng [5], and by Scovel [11] in a stimulating discussion on symplectic multistep methods.

For the general ordinary differential equation

$$\frac{dZ}{dt} = f(Z), \quad Z \in \mathbb{R}^p, \tag{1.6}$$

the 2nd-order trapezoidal rule (denoted by $G_{tz}^\tau : Z_0 \to Z_1$)

$$Z_1 = Z_0 + \frac{\tau}{2}[f(Z_1) + f(Z_0)] \tag{1.7}$$

is related to the 2nd-order mid-point rule (denoted by $G_{mp}^\tau : Z_0 \to Z_1$)

$$Z_1 - Z_0 = \tau f\left(\frac{Z_1 + Z_0}{2}\right) \tag{1.8}$$

via the 1st-order Euler-forward scheme (denoted by $G_{ef}^\tau : Z_0 \to Z_1$)

$$Z_1 = Z_0 + \tau f(Z_0). \tag{1.9}$$

More precisely,

$$G_{ef}^{\frac{\tau}{2}} \circ G_{tz}^\tau = G_{mp}^\tau \circ G_{ef}^{\frac{\tau}{2}}. \tag{1.10}$$