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A note on symplecticity of step-transition mappings for multi-step methods

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Abstract

We prove that for a linear multi-step method $\sum_{k=0}^{m}\alpha_k Z_k=\tau\sum_{k=0}^{m}\beta_k f(Z_k)$, even though the mappings $Z_0 \to Z_1, \ldots, Z_{m-2} \to Z_{m-1}$ are chosen to be symplectic, $Z_{m-1} \to Z_m$ will be non-symplectic. Similarly, there is an interesting result for a sort of general linear methods.

Keywords: Linear multi-step method; Infinitesimally symplectic; Symplecticity; General linear method

1. Introduction

For an ordinary differential equation

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = f(Z), \quad Z \in \mathbb{R}^p, \tag{1}$$

any compatible linear m-step difference scheme

$$\sum_{k=0}^{m}\alpha_k Z_k = \tau\sum_{k=0}^{m}\beta_k f(Z_k) \quad \left(\sum_{k=0}^{m}\beta_k \neq 0\right) \tag{2}$$

is of order s if and only if (refer to [6])

$$\sum_{k=0}^{m}\alpha_k = 0, \quad \sum_{k=0}^{m}\alpha_k k^l = l\sum_{k=0}^{m}\beta_k k^{l-1}, \quad 1 \leqslant l \leqslant s, \quad \sum_{k=0}^{m}\alpha_k k^{s+1} \neq (s+1)\sum_{k=0}^{m}\beta_k k^s. \tag{3}$$

When Eq. (1) is a hamiltonian system, i.e., $p=2n$ and $f(Z)=J\nabla H(Z)$, here

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

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∇ stands for gradient operator, and $H : \mathbb{R}^{2n} \to \mathbb{R}^1$ is a (smooth) hamiltonian function, people have studied the symplecticity of scheme (2).

Definition 1 (*refer to [1]*). A transformation $T : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is called canonical or symplectic if

$$\left[\frac{\partial T(Z)}{\partial Z}\right]^{\mathrm{T}} J \left[\frac{\partial T(Z)}{\partial Z}\right] \equiv J. \tag{4}$$

Eirola and Sanz-Serna [2], Ge and Feng [3] have shown respectively that under some condition on the coefficients in (2), the transformation $(Z_0^{\mathrm{T}}, \ldots, Z_{m-1}^{\mathrm{T}})^{\mathrm{T}} \longrightarrow (Z_1^{\mathrm{T}}, \ldots, Z_m^{\mathrm{T}})^{\mathrm{T}}$ in the higher dimensional manifold $\mathbb{R}^{2mn}$ is symplectic with respect to some more general structure.

On the other hand, Hairer and Leone [4], Tang [9] have got the negative result for the step-transition operator (underlying one-step method) $G : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ G^k \tag{5}$$

to be symplectic (in the sense of Definition 1).

From Hairer et al. [5], MacKay [7], McLachlan and Scovel [8], one can find *reviews on symplectic multi-step methods*.

In this note, we study mappings from $\mathbb{R}^{2n}$ to $\mathbb{R}^{2n}$ for linear multi-step method (2) for hamiltonian system. Let us see what happens to Z_m if we choose $Z_0, \ldots, Z_{m-1}$ such that $Z_i \to Z_{i+1} (0 \leqslant i \leqslant m-2)$ is symplectic. We will also consider the case for a sort of general linear methods:

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k f\left(\sum_{l=0}^{m} \gamma_{kl} Z_l\right) \quad \left(\sum_{l=0}^{m} \gamma_{kl} = 1, k = 0, \ldots, m\right). \tag{6}$$

2. Main results

Theorem 1. *For any linear multi-step method* (2) *with* $\alpha_m \neq 0$ *of order s for hamiltonian system, if we choose* $Z_0, \ldots, Z_{m-1}$ *such that mappings* $Z_i \to Z_{i+1} (0 \leqslant i \leqslant m-2)$ *are symplectic, then mapping* $Z_{m-1} \to Z_m$ *will be non-symplectic.*

In order to prove Theorem 1, we introduce the following Definition 2 and Lemma 1:

Definition 2. A transformation M: $\mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is said to be infinitesimally symplectic iff its Jacobian M_z satisfies $M_z^{\mathrm{T}} J + J M_z = 0$.

Lemma 1 (*see [9]*). *For* $k \geqslant 2$, $Z^{[k]}$ *cannot be infinitesimally symplectic. Provided* $s \geqslant 3$, *then* $\sum_{j=1}^{s} \sum_{\substack{l_1+\cdots+l_j=s \\ l_u \geqslant 1}} b_{l_1 \cdots l_j} J(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]}$ *is infinitesimally symplectic iff* $b_{l_1 \cdots l_j} = 0$, *for all j and all* $l_1, \ldots, l_j$.

Here we use the notation $Z^{[0]} = Z$, $Z^{[1]} = f(Z)$, $Z^{[k+1]} = (\partial Z^{[k]}/\partial Z) Z^{[1]} = Z_z^{[k]} Z^{[1]}$ for $k = 1, 2, \ldots$. And $(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]}$ stands for the multi-linear form

$$\sum_{1 \leqslant t_1, \ldots, t_j \leqslant 2n} \frac{\partial^j (\nabla H)}{\partial Z_{(t_1)} \cdots \partial Z_{(t_j)}} Z_{(t_1)}^{[l_1]} \cdots Z_{(t_j)}^{[l_j]},$$

$Z_{(t_u)}^{[l_u]}$ stands for the t_uth component of the $2n$-dim vector $Z^{[i_u]}$.

Proof of Theorem 1. Setting $Z = Z_0$, according to the order condition we can only choose

$$Z_k = \sum_{i=0}^{+\infty} \frac{k^i \tau^i}{i!} Z^{[i]} + \tau^{s+1} \Theta_k(Z) + \mathrm{O}(\tau^{s+2}), \quad 1 \leqslant k \leqslant m-1, \tag{7}$$

and then we also have

$$Z_m = \sum_{i=0}^{+\infty} \frac{m^i \tau^i}{i!} Z^{[i]} + \tau^{s+1} \Theta_m(Z) + \mathrm{O}(\tau^{s+2}). \tag{8}$$

It follows that

$$\left[\frac{\partial Z_k}{\partial Z}\right]^{\mathrm{T}} J \left[\frac{\partial Z_k}{\partial Z}\right] = J + \tau^{s+1} \left\{ \left[\frac{\partial \Theta_k}{\partial Z}\right]^{\mathrm{T}} J + J \left[\frac{\partial \Theta_k}{\partial Z}\right] \right\} + \mathrm{O}(\tau^{s+2}) \tag{9}$$

for $1 \leqslant k \leqslant m$.

Since the composition of any two symplectic transformations is symplectic, $Z_i \to Z_{i+1} (0 \leqslant i \leqslant m-2)$ is symplectic means $Z_0 \to Z_{i+1} (0 \leqslant i \leqslant m-2)$ is symplectic. Therefore,

$$\left[\frac{\partial \Theta_k}{\partial Z}\right]^{\mathrm{T}} J + J \left[\frac{\partial \Theta_k}{\partial Z}\right] = 0, \quad 1 \leqslant k \leqslant m-1, \tag{10}$$

that is to say Θ_k is infinitesimally symplectic for $1 \leqslant k \leqslant m-1$.

Substituting (7) and (8) into (2) and comparing the terms of τ^{s+1} on both sides we obtain

$$\Theta_m(Z) = \sum_{k=0}^{m-1} \delta_k \Theta_k(Z) + \delta_m Z^{[s+1]}, \tag{11}$$

where $\delta_k = -\alpha_k/\alpha_m$ for $1 \leqslant k \leqslant m-1$ and $\delta_m = \sum_{k=0}^{m} k^s [(s+1)\beta_k - k\alpha_k]/[\alpha_m (s+1)!] \neq 0$.

According to Lemma 1, we easily conclude from (10), (11) that Θ_m cannot be infinitesimally symplectic. Thus, we know from (9) that $Z \to Z_m$ (and then $Z_{m-1} \to Z_m$) is non-symplectic. □

For general linear methods in form (6), we establish the following:

Theorem 2. *For any general linear method* (6) *with* $\alpha_m \neq 0$ *of order* s *for hamiltonian system*, *if we choose* $Z_0, \ldots, Z_{m-1}$ *such that the symplecticity of mappings* $Z_i \to Z_{i+1} (0 \leqslant i \leqslant m-2)$ *results in the symplecticity of mapping* $Z_{m-1} \to Z_m$, *then* $s = 2$.

Proof of Theorem 2. Setting $Z = Z_0$, similarly we also have (7), (8), (9) and (10). Substituting (7) and (8) into (6) and comparing the terms of τ^{s+1} on both sides we obtain

$$\Theta_m(Z) = \sum_{k=0}^{m-1} \delta_k \Theta_k(Z) + \sum_{j=1}^{s} \sum_{\substack{t_1+\cdots+t_j=s \\ 1 \leqslant t_u \leqslant s}} \lambda_{t_1 \cdots t_j} J(\nabla H)_{z^j} Z^{[t_1]} \cdots Z^{[t_j]}, \tag{12}$$

where $\delta_k = -\alpha_k/\alpha_m$ for $1 \leqslant k \leqslant m-1$, $\lambda_{t_1 \cdots t_j} = \rho_{t_1 \cdots t_j}/\alpha_m$ and each $\rho_{t_1 \cdots t_j}$ is a polynomial in α_i $(1 \leqslant i \leqslant m-1)$, β_j $(1 \leqslant j \leqslant m)$ and γ_{kl} $(1 \leqslant k, l \leqslant m)$. According to the order condition, $\lambda_{t_1 \cdots t_j}$ is not always null for $t_1 + \cdots + t_j = s$, $1 \leqslant t_u \leqslant s$.

According to Lemma 1, for $s \geqslant 3$ we conclude from (10), (12) that Θ_m cannot be infinitesimally symplectic. One can easily check the same situation for $s = 1$. Thus, we know from (9) that $Z \to Z_m$ (and then $Z_{m-1} \to Z_m$) is non-symplectic unless $s = 2$. □

3. Concluding remark

The results of Theorems 1 and 2 show the difficulty of getting a series of stringent symplectic step-transition mappings for the linear multi-step methods (and some sort of general linear methods). One should try constructing of symplectic multi-step methods in a weaker sense.

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