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ON CONJUGATE SYMPLECTICITY OF MULTI-STEP METHODS[*1)]

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Dedicated to Feng Kang on his 80th birthday

Abstract

In this paper, we solve a problem on the existence of conjugate symplecticity of linear multi-step methods (**LMSM**), the negative result is obtained.

Key words: Conjugate symplecticity, Multi-step method

1. Introduction

For an ordinary differential equation

$$\frac{dZ}{dt} = f(Z), \quad Z \in R^p, \tag{1}$$

any compatible linear m-step difference scheme (for simplicity, denoted by **LMSM**):

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

can be characterized by a step-transition operator G (also denoted by G^τ): $R^p \to R^p$ satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k f \circ G^k, \tag{3}$$

where G^k stands for k-time composition of G: $G \circ G \cdots \circ G$ (refer to [1-4]).

The operator G defined by (3) can be represented as a power series in τ with first term equal to identity I. More precisely, it is shown[4] that

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Lemma A. *If scheme (2) is of order s, then the corresponding operator G can be written as the following form:*

$$G(Z) = \sum_{i=0}^{s+1} \tau^i \frac{Z^{[i]}}{i!} + aZ^{[s+1]}\tau^{s+1} + O(\tau^{s+2}), \tag{4}$$

where $Z^{[0]} = Z, Z^{[1]} = f(Z), Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]}, k = 1, 2, \cdots,$ and a is a constant $(\neq 0)$.

Thus, the step-transition operator completely characterizes the multi-step scheme as: $Z_1 = G(Z_0), \cdots, Z_m = G(Z_{m-1}) = G^m(Z_0), \cdots$.

When equation (2) is a hamiltonian system, i.e., $p = 2n$ and $f(Z) = J\nabla H(Z)$, here $J = \begin{bmatrix} 0_n & -I_n \\ I_n & 0_n \end{bmatrix}$, ∇ stands for gradient operator, and $H : R^{2n} \to R^1$ is a (smooth) hamiltonian function, (1), (2) and (3) become

$$\frac{dZ}{dt} = J\nabla H(Z), \quad z \in R^{2n}, \tag{5}$$

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J\nabla H(Z_k) \quad (\sum_{k=0}^{m} \beta_k \neq 0), \tag{6}$$

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ G^k. \tag{7}$$

And one can rewrite

$$\begin{aligned}
Z^{[0]} &= Z, \\
Z^{[1]} &= J\nabla H, \\
Z^{[2]} &= JH_{zz}J\nabla H = Z_z^{[1]} Z^{[1]}, \\
Z^{[3]} &= Z_{z^2}^{[1]} (Z^{[1]})^2 + Z_z^{[1]} Z^{[2]}, \\
Z^{[4]} &= Z_{z^3}^{[1]} (Z^{[1]})^3 + 3Z_{z^2}^{[1]} (Z^{[1]} Z^{[2]}) + Z_z^{[1]} Z^{[3]}, \\
Z^{[5]} &= Z_{z^4}^{[1]} (Z^{[1]})^4 + 6Z_{z^3}^{[1]} \left((Z^{[1]})^2 Z^{[2]} \right) \\
&\quad + 3Z_{z^2}^{[1]} (Z^{[2]})^2 + 4Z_{z^2}^{[1]} (Z^{[1]} Z^{[3]}) + Z_z^{[1]} Z^{[4]},
\end{aligned} \tag{8}$$

or generally,

$$Z^{[s+1]} = \sum_{j=1}^{s} \sum_{l_1+\cdots+l_j=s; l_u \geq 1} d_{l_1 \cdots l_j} J(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]}, \tag{9}$$

where $d_{l_1 \cdots l_j} > 0$ for all $l_1, \cdots, l_j$ and $(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]}$ stands for the multi-linear form

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

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

It is suggested[1],[4] that for hamiltonian systems, the symplecticity of any multi-step method should be defined through its step-transition operator.

Definition 1. *Difference scheme* (6) *is symplectic iff its step-transition operator* G *defined by* (7) *is symplectic, i.e.,*

$$\left[\frac{\partial G(Z)}{\partial Z}\right]^{\top} J \left[\frac{\partial G(Z)}{\partial Z}\right] = J \tag{10}$$

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

In the sense of this definition, it is shown that

Theorem A. *Any linear multi-step difference scheme (with order* $s \geq 1$*) is non-symplectic.*

Moreover, for a sort of generalized multi-step methods (**GMSM**s):

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ (\sum_{l=0}^{m} \gamma_{kl} Z_l) \quad (\sum_{l=0}^{m} \gamma_{kl} = 1, k = 0, \cdots, m) \tag{11}$$

with corresponding step-transition operator G satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ (\sum_{l=0}^{m} \gamma_{kl} G^l), \tag{12}$$

it is established that

Theorem B. *If a* **GMSM** *(with order* $s \geq 1$*) is symplectic, then it must be of order* 2.

And it is conjectured that

Conjecture A. *If a* **GMSM** *(with order* $s \geq 1$*) is symplectic, then it must be equivalent (two* **GMSM***s are said to be equivalent iff they have the same step-transition operator) to the mid-point rule:*

$$Z_{k+1} = Z_k + \tau f\left(\frac{Z_{k+1} + Z_k}{2}\right), \tag{13}$$

which is symplectic with order 2.

For details about the results above, one can see [4]; and for more general results on "*order barriers for symplectic multi-value methods*", one can refer to Hairer and Leone [5].

From McLachlan and Scovel [6], one can find *a review on symplectic multi-step methods.*

In the next section, a new definition of symplecticity (*conjugate symplecticity*) of multi-step methods will be introduced, and a relative problem will be offered.

2. Problem on Conjugate Symplecticity

As an application of Lemma A, we display the following expansions:

For the Euler-forward scheme (denoted by G^τ_{ef})

$$\widetilde{Z} = Z + \tau f(Z), \tag{14}$$

$$\widetilde{Z} = G^\tau_{ef}(Z) = Z + \tau Z^{[1]} + \frac{\tau^2}{2} Z^{[2]} + a\tau^2 Z^{[2]} + O(\tau^3) \tag{15}$$

where $a = -\frac{1}{2}$.

For the Euler-backward scheme (denoted by G^τ_{eb})

$$\widetilde{Z} = Z + \tau f(\widetilde{Z}), \tag{16}$$

$$\widetilde{Z} = G^\tau_{eb}(Z) = Z + \tau Z^{[1]} + \frac{\tau^2}{2} Z^{[2]} + a\tau^2 Z^{[2]} + O(\tau^3) \tag{17}$$

where $a = \frac{1}{2}$.

For the trapezoid rule (denoted by G^τ_{tz})

$$\widetilde{Z} = Z + \frac{\tau}{2}\left[f(\widetilde{Z}) + f(Z)\right], \tag{18}$$

$$\widetilde{Z} = G^\tau_{tz}(Z) = Z + \tau Z^{[1]} + \frac{\tau^2}{2} Z^{[2]} + \frac{\tau^3}{6} Z^{[3]} + a\tau^3 Z^{[3]} + O(\tau^4) \tag{19}$$

where $a = \frac{1}{12}$.

For the mid-point rule (denoted by G^τ_{mp}) (13),

$$\widetilde{Z} = G^\tau_{mp}(Z) = Z + \tau Z^{[1]} + \frac{\tau^2}{2} Z^{[2]} + \frac{\tau^3}{6} Z^{[3]} + \tau^3 A(Z) + O(\tau^4) \tag{20}$$

where $A(Z) = \frac{1}{12} Z^{[1]}_z Z^{[2]} - \frac{1}{24} Z^{[1]}_{z^2} (Z^{[1]})^2$.

For the leap-frog scheme (denoted by G^τ_{lf})

$$\widetilde{Z} = Z_2 = Z_0 + 2\tau f(Z_1), \tag{21}$$

$$\widetilde{Z} = G^\tau_{lf}(Z) = Z + \tau Z^{[1]} + \frac{\tau^2}{2} Z^{[2]} + \frac{\tau^3}{6} Z^{[3]} + a\tau^3 Z^{[3]} + O(\tau^4) \tag{22}$$

where $a = -\frac{1}{12}$.

Now let's introduce another definition:

Definition 2. *Providing three difference schemes G^τ_1, G^τ_2 and G^τ_3 compatible with equation* (1), *G^τ_1 is said to be conjugate to G^τ_2 through G^τ_3 iff their step-transition operators satisfy*

$$G^{\lambda\tau}_3 \circ G^\tau_1 = G^\tau_2 \circ G^{\lambda\tau}_3 \tag{23}$$

for some real number $\lambda \neq 0$ and for any smooth function f and any sufficiently small step-size τ. Here $\circ$ stands for composition of operators.

Let's see an example [7-16][2)]:

$$Z_1 = Z_0 + \frac{\tau}{2}[f(Z_1) + f(Z_0)], \tag{24}$$

then

$$Z_1 = G^{\tau}_{tz}(Z_0); \tag{25}$$

set

$$\xi_1 = Z_1 + \frac{\tau}{2} f(Z_1), \tag{26}$$

and

$$\xi_0 = Z_0 + \frac{\tau}{2} f(Z_0), \tag{27}$$

then

$$\xi_1 = G^{\frac{\tau}{2}}_{ef}(Z_1); \tag{28}$$

$$\xi_0 = G^{\frac{\tau}{2}}_{ef}(Z_0); \tag{29}$$

and

$$\xi_1 + \xi_0 = 2Z_1, \tag{30}$$

and

$$\xi_1 - \xi_0 = \tau f(Z_1) = \tau f(\frac{Z_1 + Z_0}{2}). \tag{31}$$

So

$$\xi_1 = G^{\tau}_{mp}(\xi_0),$$

or

$$G^{\frac{\tau}{2}}_{ef} \circ G^{\tau}_{tz}(Z_0) = G^{\tau}_{mp} \circ G^{\frac{\tau}{2}}_{ef}(Z_0). \tag{32}$$

That is to say, the trapezoid rule G^{τ}_{tz} is conjugate to the mid-point rule G^{τ}_{mp} through the Euler-forward scheme G^{τ}_{ef}.

In the sense of step-transition operator, (32) shows that the trapezoid rule is also symplectic up to a coordinate transformation which is close to the identity. We will call this kind of method *scheme of* **conjugate symplecticity**[3)]. And then, one problem is naturally offered [7-8]:

Is there any other example like the trapezoid rule in the set of linear multi-step schemes?

In the sequel, we'll try to get the answer. And firstly, we'll give several lemmas.

[2)] The author is grateful to Ernst Hairer and the colleagues in Beijing for pointing out some references.

[3)] It is noted[12−13],[15] that Stoffer and Wu also introduced *conjugate canonical method* in their reports [14], [16] respectively.

3. Preliminary Lemmas

Supposing G_1^τ, G_2^τ and G_3^τ are three schemes compatibe with (5), their expressions are

$$G_1^\tau(Z) = \sum_{i=0}^{u+2} \frac{\tau^i Z^{[i]}}{i!} + \tau^{u+1}A(Z) + \tau^{u+2}A_1(Z) + O(\tau^{u+3}), \tag{33.1}$$

$$G_2^\tau(Z) = \sum_{i=0}^{v+2} \frac{\tau^i Z^{[i]}}{i!} + \tau^{v+1}M(Z) + \tau^{v+2}M_1(Z) + O(\tau^{v+3}) \tag{33.2}$$

and

$$G_3^\tau(Z) = \sum_{i=0}^{w+2} \frac{\tau^i Z^{[i]}}{i!} + \tau^{w}B(Z) + \tau^{w+1}B_1(Z) + \tau^{w+2}B_2(Z) + O(\tau^{w+3}) \tag{33.3}$$

respectively (here u, v, $w \geq 2$), then

$$G_3^{\lambda\tau} \circ G_1^\tau = G_2^\tau \circ G_3^{\lambda\tau} \tag{34}$$

means

$$\begin{aligned} &\left[\sum_{i=0}^{w+2} \frac{(\lambda\tau)^i Z^{[i]}}{i!} + (\lambda\tau)^w B(Z) + (\lambda\tau)^{w+1}B_1(Z) + (\lambda\tau)^{w+2}B_2(Z) + O(\tau^{w+2})\right] \\ &\circ \left[\sum_{i=0}^{u+2} \frac{\tau^i Z^{[i]}}{i!} + \tau^{u+1}A(Z) + \tau^{u+2}A_1(Z) + O(\tau^{u+3})\right] \\ &= \left[\sum_{i=0}^{v+2} \frac{\tau^i Z^{[i]}}{i!} + \tau^{v+1}M(Z) + \tau^{v+2}M_1(Z) + O(\tau^{v+3})\right] \\ &\circ \left[\sum_{i=0}^{w+2} \frac{(\lambda\tau)^i Z^{[i]}}{i!} + (\lambda\tau)^w B(Z) + (\lambda\tau)^{w+1}B_1(Z) + (\lambda\tau)^{w+2}B_2(Z) + O(\tau^{w+3})\right]. \end{aligned} \tag{35}$$

At first let's assume $u = v = w$, then we obtain from (35)

$$\lambda^w B_z Z^{[1]} + A = M + \lambda^w Z_z^{[1]} B \tag{36}$$

and

$$\begin{aligned} &\lambda^{w+1}(B_1)_z Z^{[1]} + \tfrac{\lambda^w}{2} B_z Z^{[2]} + \tfrac{\lambda^w}{2} B_{z^2}(Z^{[1]})^2 + \lambda Z_z^{[1]} A + A_1 \\ &= M_1 + \lambda M_z Z^{[1]} + \lambda^{w+1} Z_{z^2}^{[1]} Z^{[1]} B + \tfrac{\lambda^w}{2} Z_z^{[2]} B + \lambda^{w+1} Z_z^{[1]} B_1. \end{aligned} \tag{37}$$

Lemma 1. *Given three schemes with expressions* (33.1–33.3) *and* $u = v = w \geq 2$, *then one necessary condition for scheme* G_1^τ *to be conjugate to* G_2^τ *through* G_3^τ *is that equations* (36) *and* (37) *are satisfied for some real number* $\lambda \neq 0$.

Definition 3. *A transformation* M: $R^{2n} \to R^{2n}$ *is said to be infinitesimal symplectic iff its Jacobian* M_z *satisfies* $M_z^T J + J M_z = \mathbf{0}$.

Lemma 2. *If scheme* G_2^τ *with expression* (33.3) *is symplectic, then* $M(Z)$ *is infinitesimal symplectic.*

Lemma 3. *With the assumptions in* **Lemma 1**, *if* G_2^τ *is symplectic, then* $\lambda^w(B_z Z^{[1]} - Z_z^{[1]} B) + A$ *is infinitesimal symplectic.*

Lemma 4. (see [4]) *Provided* $s \geq 3$, *then* $\sum_{j=1}^{s} \sum_{l_1+\cdots+l_j=s, l_u \geq 1} b_{l_1\cdots l_j}\ J(\nabla H)_{z^j}$ $Z^{[l_1]} \cdots Z^{[l_j]}$ *is infinitesimal symplectic iff* $b_{l_1\cdots l_j} = 0$, *for all* j *and all* $l_1, \cdots, l_j$.

Remark 1. *In* **Lemma 1***, if condition $u = v = w$ changes, then equation (36) will change too. Precisely,*

if $u = v < w$, then (36) changes into

$$A = M; \tag{36.1}$$

if $v = w < u$, then (36) changes into

$$\lambda^w B_z Z^{[1]} = M + \lambda^w Z_z^{[1]} B; \tag{36.2}$$

if $u = w < v$, then (36) changes into

$$\lambda^w B_z Z^{[1]} + A = \lambda^w Z_z^{[1]} B; \tag{36.3}$$

if $u < min\{v, w\}$, then (36) changes into

$$A = 0; \tag{36.4}$$

if $v < min\{u, w\}$, then (36) changes into

$$M = 0; \tag{36.5}$$

if $w < min\{u, v\}$, then (36) changes into

$$\lambda^w B_z Z^{[1]} = \lambda^w Z_z^{[1]} B. \tag{36.6}$$

4. Main Result

Theorem 1. *It is impossible for a LMSM with order $u(\geq 3)$ to be conjugate to a symplectic scheme through another LMSM.*[4)]

Proof. Provided G_1^τ, G_3^τ are LMSMs, and G_2^τ is symplectic.

When $A = aZ^{[u+1]}$ $(a \neq 0)$, $B = bZ^{[u]}$ $(b \neq 0)$ and $u \geq 3$, the case (36) is impossible, according to **Lemma 4**; similarly, any of the cases (36.1-36.6) is also impossible. □

Remark 2. *The result of Theorem 1 is not surely true for $u \leq 2$. In fact when $u = 2$, G_1, G_2 are, for example, the trapezoid rule and the mid-point rule respectively, equation* (36) *becomes*

$$\lambda^w (B_z Z^{[1]} - Z_z^{[1]} B) + \frac{1}{12} Z^{[3]} = \frac{1}{12} Z_z^{[1]} Z^{[2]} - \frac{1}{24} Z_{z^2}^{[1]} (Z^{[1]})^2,$$

we obtain $\lambda^w B = -\frac{1}{8} Z^{[2]}$. If we choose $w = 2$ and $\lambda = \frac{1}{2}$, then $B = -\frac{1}{2} Z^{[2]}$. Here one can recall the example in Section 2.

4) The author would like to thank Clint Scovel for the stimulating discussion right after that this result was obtained in June 1994.

Theorem 1 replies to the question due to Feng [7] and Scovel [8]. The result of theorem 1 shows the non-existence of conjugate symplecticity of **LMSM** (with order ≥ 3), however the author does not hope this is the end of investigation of symplectic multi-step methods. One can get some similar results for **GMSM**, but the proofs would be much more difficult or tedious [17], and it is worth pointing out again (refer to [4]) here that in order to construct symplectic multi-step methods, some novel approach is needed.

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