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Conjugate symplecticity of second-order linear multi-step methods

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Abstract

We review the two different approaches for symplecticity of linear multi-step methods (LMSM) by Eirola and Sanz-Serna, Ge and Feng, and by Feng and Tang, Hairer and Leone, respectively, and give a numerical example between these two approaches. We prove that in the conjugate relation $G_3^{\lambda\tau} \circ G_1^{\tau} = G_2^{\tau} \circ G_3^{\lambda\tau}$ with G_1^{τ} and G_3^{τ} being LMSMs, if G_2^{τ} is symplectic, then the B-series error expansions of G_1^{τ}, G_2^{τ} and G_3^{τ} of the form $G^{\tau}(Z) = \sum_{i=0}^{+\infty}(\tau^i/i!)Z^{[i]} + \tau^{s+1}A_1 + \tau^{s+2}A_2 + \tau^{s+3}A_3 + \tau^{s+4}A_4 + \mathrm{O}(\tau^{s+5})$ are equal to those of trapezoid, mid-point and Euler forward schemes up to a parameter θ (completely the same when $\theta = 1$), respectively, this also partially solves a problem due to Hairer. In particular we indicate that the second-order symmetric leap-frog scheme $Z_2 = Z_0 + 2\tau J^{-1}\nabla H(Z_1)$ cannot be conjugate-symplectic via another LMSM.

Keywords: Linear multi-step method; Step-transition operator; B-series; Conjugate relation; Symplecticity

1. First approach for symplectic multi-step methods

It is well-known that for a Hamiltonian system

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = J^{-1}\nabla H(Z), \quad Z = [z_1, \ldots, z_{2n}]^{\top} \in \mathbb{R}^{2n}, \tag{1}$$

where $J = [J_{ij}] = \left[\begin{smallmatrix} O_n & I_n \\ -I_n & O_n \end{smallmatrix}\right]$, ∇ stands for the gradient operator, and $H : \mathbb{R}^{2n} \to \mathbb{R}^1$ is a smooth function (*Hamiltonian function*), its phase flow $\{g^t | t \in \mathbb{R}\}$ is a one-parameter group of symplectic transformations [1]. The symplecticity of $g^t : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ means

$$\left[\frac{\partial g^t(Z)}{\partial Z}\right]^{\top} J \left[\frac{\partial g^t(Z)}{\partial Z}\right] = J \tag{2}$$

for any $Z \in \mathbb{R}^{2n}$ and any $t \in \mathbb{R}$.

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It is easy to check that Eq. (2) is equivalent to [6]

$$(g^t)^*\omega = \omega, \tag{3}$$

where $\omega = \frac{1}{2}\sum_{a,b=1}^{2n} J_{ab}\, dz_a \wedge dz_b = \sum_{1\leqslant a<b\leqslant 2n} J_{ab}\, dz_a \wedge dz_b = \sum_{c=1}^{n} dz_c \wedge dz_{n+c}$.

More generally, if J becomes $K(Z)$ where $K(Z) = (K_{ab})$ is an antisymmetric, nondegenerate $2n \times 2n$ matrix satisfying

$$\frac{\partial k_{ab}}{\partial z_c} + \frac{\partial k_{bc}}{\partial z_a} + \frac{\partial k_{ca}}{\partial z_b} = 0, \quad 1 \leqslant a, b, c \leqslant 2n, \tag{4}$$

then (1) becomes the general Hamiltonian system

$$\frac{dZ}{dt} = K^{-1}(Z)\nabla H(Z), \quad Z = [z_1, \ldots, z_{2n}]^\top \in \mathbb{R}^{2n}, \tag{5}$$

and the phase flow $\{\hat{g}^t | t \in \mathbb{R}\}$ of (5) is a one-parameter group of K-symplectic transformations [6,9]:

$$\left[\frac{\partial \hat{g}^t(Z)}{\partial Z}\right]^{\mathrm{T}} K(\hat{g}^t(Z)) \left[\frac{\partial \hat{g}^t(Z)}{\partial Z}\right] = K(Z). \tag{6}$$

Furthermore Eq. (6) is equivalent to

$$(\hat{g}^t)^*\hat{\omega} = \hat{\omega}, \tag{7}$$

where $\hat{\omega} = \frac{1}{2}\sum_{a,b=1}^{2n} K_{ab}\, dz_a \wedge dz_b = \sum_{1\leqslant a<b\leqslant 2n} K_{ab}\, dz_a \wedge dz_b$.

A numerical scheme compatible with (5) is said to be K-symplectic if its step-transition operator $G^\tau : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is a K-symplectic transformation for any stepsize τ. In particular, the mid-point rule $G^\tau_{\mathrm{mp}} : Z \to \widetilde{Z}$ (see [6])

$$Z_1 - Z_0 = \tau J^{-1}\nabla H\left(\frac{Z_1 + Z_0}{2}\right) \tag{8}$$

is a second-order symplectic scheme for the standard Hamiltonian system (1).

The symplecticity of compatible linear m-step method (LMSM) for Hamiltonian system (1)

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1}\nabla H(Z_k), \quad \left(\sum_{k=0}^{m} \beta_k \neq 0\right) \tag{9}$$

is first studied under the consideration of transformations in the higher dimensional manifold $\mathbb{R}^{2mn}$.

For the special case $m = 2$ for example, for the second-order leap-frog scheme

$$Z_2 = Z_0 + 2\tau J^{-1}\nabla H(Z_1), \tag{10}$$

Ge and Feng [11] rewrote (10) into

$$\begin{bmatrix} Z_2 \\ Z_1 \end{bmatrix} = \begin{bmatrix} Z_0 + 2\tau J^{-1}\nabla H(Z_1) \\ Z_1 \end{bmatrix} \tag{11}$$

and showed that the mapping $[Z_1^\top, Z_0^\top]^\top \xrightarrow{\Phi} [Z_2^\top, Z_1^\top]^\top$ preserves the general symplectic structure related to $\begin{bmatrix} O_{2n} & J_{2n} \\ J_{2n} & O_{2n} \end{bmatrix}$.

More generally, Eirola and Sanz-Serna [5] have shown that if one-leg method (see [13,16] for details)

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau J^{-1}\nabla H\left(\sum_{k=0}^{m} \beta_k Z_k\right) \tag{12}$$

is symmetric (i.e., $\alpha_{m-k} = -\alpha_k$, $\beta_{m-k} = \beta_k$, $0 \leqslant k \leqslant m$) and irreducible, then the transformation $(Z_0^\top, \ldots, Z_{m-1}^\top)^\top \longrightarrow (Z_1^\top, \ldots, Z_m^\top)^\top$ in the higher dimensional manifold $\mathbb{R}^{2mn}$ is symplectic with respect to the general structure $\Lambda \otimes J$, where Λ is an $m \times m$ symmetric matrix defined by the coefficients $\alpha_k, \beta_k, 0 \leqslant k \leqslant m$, it is $\begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}$ for the leap-frog scheme (10).