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EXPANSIONS OF STEP-TRANSITION OPERATORS OF MULTI-STEP METHODS AND ORDER BARRIERS FOR DAHLQUIST PAIRS *1)

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Abstract

Using least parameters, we expand the step-transition operator of any linear multi-step method (LMSM) up to $O(\tau^{s+5})$ with order $s = 1$ and rewrite the expansion of the step-transition operator for $s = 2$ (obtained by the second author in a former paper). 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 being an LMSM, (1) the order of G_2 can not be higher than that of G_1; (2) if G_3 is also an LMSM and G_2 is a symplectic B-series, then the orders of G_1, G_2 and G_3 must be 2, 2 and 1 respectively.

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1. Introduction

For an ordinarily differential equation (ODE)

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

any compatible linear m-step difference scheme (DS)

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

can be characterized by a step-transition operator (STO) (also called underlying one-step method) G (also denoted by G^τ): $\mathbb{R}^p \to \mathbb{R}^p$ 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 [2,3,5,6,7]). This operator G^τ can be represented as a power series in τ with first term equal to the identity I. More

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precisely, one can expand[9] the STO $G^\tau(Z)$ of any linear multi-step method (LMSM)[2] of form (2) with order $s \geq 2$ up to $O(\tau^{s+5})$:

$$G^\tau(Z) = \sum_{i=0}^{+\infty} \frac{\tau^i}{i!} Z^{[i]} + \tau^{s+1}A(Z) + \tau^{s+2}B(Z) + \tau^{s+3}C(Z) + \tau^{s+4}D(Z) + O(\tau^{s+5}) \qquad (4)$$

(where $Z^{[0]} = Z$, $Z^{[1]} = f(Z)$, $Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]} = Z_z^{[k]} Z^{[1]}$ for $k = 1, 2, \cdots$) with complete formulae for calculation of $A(Z)$, $B(Z)$, $C(Z)$ and $D(Z)$.

Thus, the STO G^τ satisfying equation (3) completely characterizes the LMSM (2) as: $Z_1 = G^\tau(Z_0), \cdots, Z_m = G^\tau(Z_{m-1}) = [G^\tau]^m(Z_0), \cdots$.

When equation (1) is a hamiltonian system, i.e., $p = 2n$ and $f(Z) = J\nabla H(Z)$, 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, (1), (2) and (3) become

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

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

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

and we can rewrite

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

and generally,

$$Z^{[r+1]} = \sum_{j=1}^{r} \sum_{i_1+i_2+\cdots+i_j=r; i_u \geq 1} \frac{r!}{j!} \frac{\Omega(i_1, i_2, \cdots, i_j)}{i_1! i_2! \cdots i_j!} J(\nabla H)_{z^j} Z^{[i_1]} Z^{[i_2]} \cdots Z^{[i_j]}$$

where $i_1 \leq i_2 \leq \cdots \leq i_j$, $\Omega(i_1, i_2, \cdots, i_j)$ is the number of all different permutations of $\{i_1, i_2, \cdots, i_j\}$, and $(\nabla H)_{z^j} Z^{[i_1]} Z^{[i_2]} \cdots Z^{[i_j]}$ stands for the multi-linear form

$$\sum_{1 \leq t_1, \cdots, t_j \leq 2n} \frac{\partial^j (\nabla H)}{\partial Z_{(t_1)} \cdots \partial Z_{(t_j)}} Z_{(t_1)}^{[i_1]} \cdots Z_{(t_j)}^{[i_j]},$$

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

The expansion of STO (4) has been used to study the symplecticity of LMSM (refer to [3], [7]), and also the symplecticity of Dahlquist pair (refer to [8]).

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[2]) More generally, one can use an STO to characterize any DS compatible with ODE (1), and obviously the STO can be written in form (4).