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CHARACTERIZATIONS OF SYMMETRIC MULTISTEP RUNGE-KUTTA METHODS *1)

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Abstract

Some characterizations for symmetric multistep Runge-Kutta(RK) methods are obtained. Symmetric two-step RK methods with one and two-stages are presented. Numerical examples show that symmetry of multistep RK methods alone is not sufficient for long time integration for reversible Hamiltonian systems. This is an important difference between one-step and multistep symmetric RK methods.

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1. Introduction

It is well known that symmetric one-step methods have similar good long-time behaviours to symplectic methods for reversible Hamiltonian systems. Many researches into symmetric Runge-Kutta methods and symmetric multistep methods have been given (cf.[3-5,7,8,10-14]). More generally, the definition and some properties of symmetric general linear methods (GLMs) are also presented by Hairer, Leone[6], Hairer, Lubich, Wanner[7] and Leone[9] who show that symmetry of linear multistep methods and one-leg methods alone are not sufficient by means of some numerical experiments. In fact, they define the symmetry of a GLM via its underlying one-step method.

Definition 1.1[6,9]**.** *A GLM G_h is symmetric, if there exists a finishing procedure F_h, such that the underlying one-step method Φ_h is symmetric.*

They also give some sufficient conditions under which a GLM(cf.[2,6,9])

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \tag{1.1}$$

is symmetric.

Theorem 1.2[6,9]**.** *If C_{22} is invertible, and there exist the invertible matrix Q satisfying $QS_0 = S_0$ and a permutation matrix P such that*

$$P^{-1}C_{11}P = C_{12}C_{22}^{-1}C_{21} - C_{11}, \tag{1.2a}$$

$$Q^{-1}C_{21}P = C_{22}^{-1}C_{21}, \tag{1.2b}$$

$$P^{-1}C_{12}Q = C_{12}C_{22}^{-1}, \tag{1.2c}$$

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$$Q^{-1}C_{22}Q = C_{22}^{-1}, \tag{1.2d}$$

then the GLM (1.1) is symmetric, where S_0 *is the matrix made up of the eigenvectors of* C_{22} *with eigenvalue 1, i.e.* $C_{22}S_0 = S_0$.

As a special case, a multistep Runge-Kutta method(MRKM) can be written as a GLM (cf. [1,2]) by

$$C_{11} = B = [b_{ij}]\in R^{s\times s}, \quad C_{12} = A = [a_{ij}]\in R^{s\times r}, \tag{1.3a}$$

$$C_{21} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \\ \gamma_1 & \gamma_2 & \dots & \gamma_s \end{pmatrix} \in R^{r\times s}, \quad C_{22} = \begin{pmatrix} 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \\ \alpha_1 & \alpha_2 & \dots & \alpha_r \end{pmatrix} \in R^{r\times r}, \tag{1.3b}$$

where $b_{ij}, a_{ij}, \gamma_i, \alpha_i$ are real constants. Let's set

$$\gamma = (\gamma_1, \gamma_2, \dots, \gamma_s)^T\in R^s, \quad \alpha = (\alpha_1, \alpha_2, \dots, \alpha_r)^T\in R^r.$$

Furthermore, throughout this paper we always assume that

$$\sum_{j=1}^{r} \alpha_i = 1, \quad \sum_{j=1}^{r} a_{ij} = 1, \quad i = 1, 2, \dots, s, \tag{1.4a}$$

$$c_i\neq c_j \ \ for \ i\neq j, \quad \gamma_i\neq 0, \quad i, j = 1, 2, \dots, s, \tag{1.4b}$$

where the relation (1.4a) is the preconsistency condition.

In this paper, some characterizations for symmetric MRKMs are obtained. Symmetric two-step RK methods with one and two-stages are presented. Numerical examples show that symmetry of MRKMs alone is not sufficient for long time integration for reversible Hamiltonian systems. This is an important difference between one-step and multistep symmetric RK methods.

2. Some Characterizations

Theorem 2.1. *If* C_{22} *is invertible and the method (1.3) satisfies*

$$\alpha_1 = 1, \quad \alpha_j = -\alpha_{r+2-j}, \quad j = 2, 3, \cdots, r, \tag{2.1a}$$

$$\gamma_j = \gamma_{s+1-j}, \quad j = 1, 2, \cdots, s, \tag{2.1b}$$

$$b_{i,s+1-j} + b_{s+1-i,j} = a_{i1}\gamma_j, \quad i, j = 1, 2, \cdots, s, \tag{2.1c}$$

$$a_{ij} = a_{i,r+2-j} + a_{i1}\alpha_j, \quad a_{i,r+1} = 0, \quad i = 1, 2, \cdots, s, \quad j = 1, 2, \cdots, r, \tag{2.1d}$$

then this method is symmetric.

Proof. Let

$$P = \begin{bmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \dots & \dots & \dots & \dots \\ 1 & \cdots & 0 & 0 \end{bmatrix} \in R^{s\times s}, \quad Q = \begin{bmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \dots & \dots & \dots & \dots \\ 1 & \cdots & 0 & 0 \end{bmatrix} \in R^{r\times r}.$$

The conclusion follows from Theorem 1.2.

Introduce the following simplifying conditions(cf.[1,9])

$$\begin{array}{lll} B(\eta): & \alpha^T\chi^k = r^k - k\gamma^T c^{k-1}, & k = 1, 2, \cdots, \eta, \\ C(\eta): & A\chi^k = c^k - kBc^{k-1}, & k = 1, 2, \cdots, \eta, \\ D(\eta): & k\gamma^T C^{k-1}B = r^k\gamma^T - \gamma^T C^k, & k = 1, 2, \cdots, \eta, \\ E(\eta): & kA^T diag(\gamma)c^{k-1} = diag(\alpha)(r^k e - \chi^k), & k = 1, 2, \cdots, \eta, \end{array}$$

where $C = diag(c)$,

$$c = (c_1, c_2, \cdots, c_s)^T, \quad \chi = (0, 1, \cdots, r-1)^T,$$

$$e=(1,1,\cdots,1)^T\in R^r,\quad \bar{e}=(1,1,\cdots,1)^T\in R^s$$

and multiplication of vectors is done componentwise.

Theorem 2.2. *Assume that the method (1.3) is symmetric. Let* $a_1=(a_{11},a_{21},\cdots,a_{s1})^T$.

(1) If only $E(1)$ *holds, then* $\gamma^T a_1=r$;

(2) If $E(\eta)(\eta\geq 2)$ *holds, then*

$$\alpha_j=0,\quad a_{ij}=a_{i,r+2-j},\quad i=1,2,\cdots,s,\quad j=2,3,\cdots,r,$$
$$r^k/k=\gamma^T C^{k-1}a_1,\qquad k=1,2,\cdots,\eta;$$

(3) If $D(1)$ *holds, then*

$$2r-\gamma^T a_1=c_j+c_{s+1-j},\quad j=1,2,\cdots,s;$$

(4) If $D(1)$ *and* $E(1)$ *hold, then*

$$c_j+c_{s+1-j}=r,\quad j=1,2,\cdots,s.$$

Proof. (2.1d) yields

$$A(I-\bar{P})=a_1\alpha^T, \tag{2.2}$$

where

$$\bar{P}=\begin{bmatrix}0&0&\cdots&0&0\\0&0&\cdots&0&1\\\cdots&\cdots&\cdots&\cdots&\cdots\\0&1&\cdots&0&0\end{bmatrix}\in R^{r\times r}.$$

Hence

$$\gamma^T A(I-\bar{P})=\gamma^T a_1\alpha^T. \tag{2.3}$$

The conclusion (1) easily follows from (2.3) and $E(1)$. (2.2) yields

$$\gamma^T C^{k-1}A(I-\bar{P})=\gamma^T C^{k-1}a_1\alpha^T,\quad k=1,2,\cdots,\eta. \tag{2.4}$$

(2.4) and $E(\eta)$ yield

$$r^k/k=\gamma^T C^{k-1}a_1,\quad k=1,2,\cdots,\eta, \tag{2.5a}$$

$$\alpha_j(r^k-(j-1)^k-(r-j+1)^k)=0,\quad j=1,2,\cdots,r,\ 1\leq k\leq\eta,\ \eta\geq 2. \tag{2.5b}$$

The conclusion (2) follows from (2.4). (2.1c) yields

$$BP+PB=a_1\gamma^T, \tag{2.6a}$$

$$\gamma^T(BP+PB)=(\gamma^T a_1)\gamma^T. \tag{2.6b}$$

(2.1b) and (2.6b) yields

$$\gamma^T P=\gamma^T,\quad \gamma^T B(I+P)=(\gamma^T a_1)\gamma^T. \tag{2.7}$$

The conclusion (3) follows from D(1) and (2.7). The conclusion (4) follows from the conclusion (1) and (3).

3. Some Examples

In this section, we construct two classes of symmetric MRKMs by using Theorems 2.1 and 2.2.

Example 3.1. Two-step one-stage RK methods (1.3) satisfying $B(2)$ and $C(1)$ are symmetric and of order 2 if

$$b_{11}=a_{11},\quad a_{12}=1-a_{11},\quad \alpha=(1,0)^T,\quad \gamma_1=2,\quad c_1=1.$$

when $a_{11}=0$, it is the leap-frog scheme.

Example 3.2. Two-step two-stage RK methods (1.3) satisfying $B(2)$ and $C(2)$ are symmetric and of order 2 if

$$\alpha = (1,0)^T, \quad \gamma^T = (1,1), \quad c_1 + c_2 = 2,$$

$$a_{21} = a_{11}, \qquad a_{22} = a_{12} = 1 - a_{11},$$

$$b_{21} = a_{11} - b_{12}, \qquad b_{22} = a_{11} - b_{11},$$

$$b_{11} = (c_1^2/2 - c_1c_2 + (c_2 - 1/2)(1 - a_{11}))/(c_1 - c_2),$$

$$b_{12} = (c_1^2/2 + (1/2 - c_1)(1 - a_{11}))/(c_1 - c_2),$$

where $c_1 \neq c_2$. When $b_{11} = b_{22} = a_{11}/2$, $a_{11} = 3(1-c_1)^2$, this class of symmetric MRKMs becomes

$$\alpha = (1,0)^T, \ \gamma^T = (1,1), \ 2\lambda = 3(1-c_1)^2, \ c_2 = 2 - c_1, \tag{3.1a}$$

$$A = \begin{pmatrix} 3(1-c_1)^2 & 1 - 3(1-c_1)^2 \\ 3(1-c_1)^2 & 1 - 3(1-c_1)^2 \end{pmatrix}, \tag{3.1b}$$

$$B = \begin{pmatrix} 3(1-c_1)^2/2 & (c_1-1)(3c_1-1)/2 \\ (1-c_1)(5-3c_1)/2 & 3(1-c_1)^2/2 \end{pmatrix}, \tag{3.1c}$$

where $c_1 \neq 1$ is one parameter. When $c_1c_2 = 2/3$ (i.e. $3(1-c_1)^2 = 1$ or B(3) holds), these symmetric MRKMs is of order 3, but they actually degenerate into two-stage Gauss RK methods with the step-size $2h$.

4. Numerical Experiments

We use the two-step two-stage two-order RK methods (3.1) to solve the following two reversible Hamiltonian equations, and choose $c_1 = 3/2, 1 + \sqrt{3}/6, 1 + \sqrt{6}/6$, i.e. $3(1-c_1)^2 = 3/4, 1/4, 1/2$, respectively.

(1) The mathematical pendulum with a massless rod of length $l = 1$ and mass $m = 1$

$$q'(t) = p, \quad p'(t) = -sin(q), \qquad t \in [tb, te]. \tag{4.1}$$

Its Hamiltonian(energy) is $H(p,q) = p^2/2 - cos(q) = Const.$

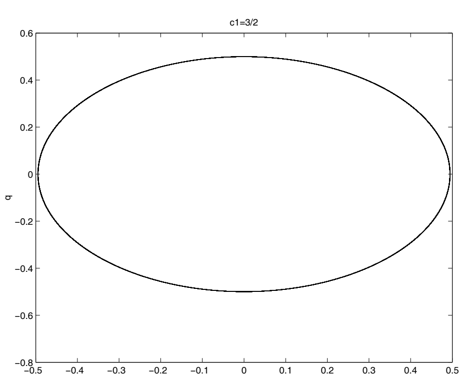
(2) The Kepler problem

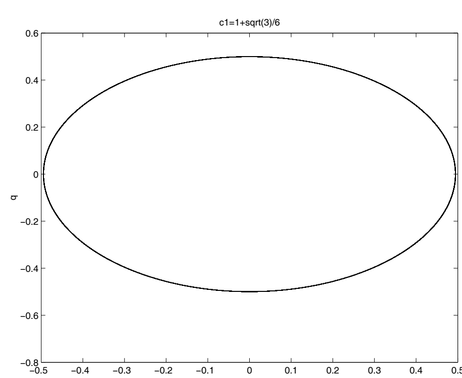
$$q'(t) = H_p(p,q), \quad p'(t) = -H_q(p,q), \qquad t \in [tb, te], \tag{4.2}$$

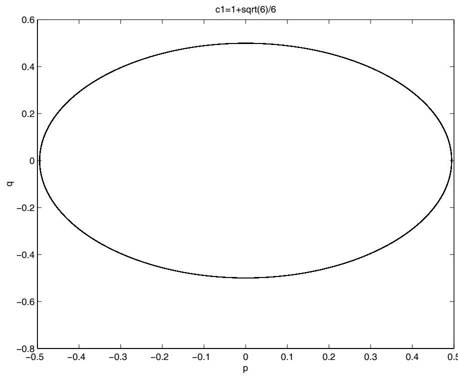
where $q = (q_1, q_2)^T$, $p = (p_1, p_2)^T$, and the Hamiltonian

$$H(p,q) = H(p_1,p_2,q_1,q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} = Const.$$

For the problem (4.1), we consider that $tb = 0, te = 5000$, the step size $h = 0.1$ and the initial conditions $(p(0), q(0)) = (0, 0.5)$. The following figures exhibit the correct qualitative behaviors for long-time integration of the problem (4.1).



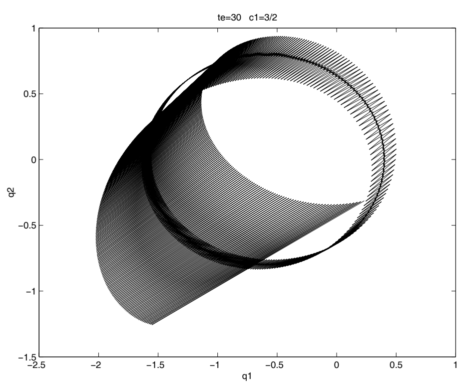


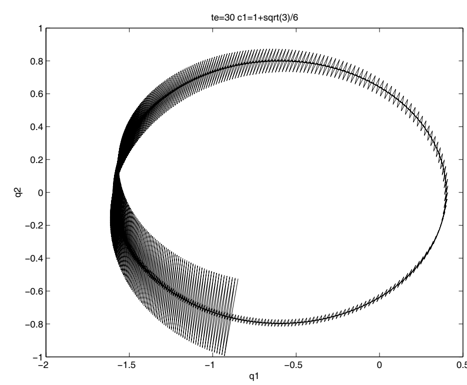


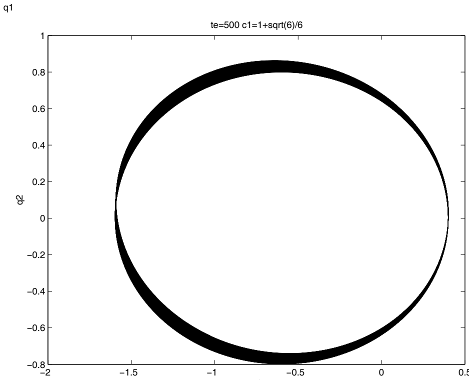
For the problem (4.2), we consider that $tb = 0, te = 30$ or 500, the step size $h = 0.01$ and the initial conditions

$$q_1(0) = 1 - e,\ q_2(0) = 0,\ p_1(0) = 0,\ p_2(0) = \sqrt{\frac{1+e}{1-e}}.$$

Here e is the eccentricity and we choose $e = 0.6$. The following figures exhibit some undesired qualitative behaviors for long-time integration of the problem (4.2).







Therefore, the above numerical examples show that symmetry of multistep RK methods alone is not sufficient for long time integration for reversible Hamiltonian systems.

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