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SYMPLECTIC RK METHODS AND SYMPLECTIC PRK METHODS WITH REAL EIGENVALUES [*1)]

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Abstract

Properties of symplectic Runge-Kutta (RK) methods and symplectic partitioned Runge-Kutta (PRK) methods with real eigenvalues are discussed in this paper. It is shown that an s stage such method can't reach order more than $s+1$. Particularly, we prove that no symplectic RK method with real eigenvalues exists in stage s of order $s+1$ when s is even. But an example constructed by using the **W**-transformation shows that PRK method of this type does not necessarily meet this order barrier. Another useful way other than **W**-transformation to construct symplectic PRK method with real eigenvalues is then presented. Finally, a class of efficient symplectic methods is recommended.

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Key words: Runge-Kutta method, Partitioned Runge-Kutta method, Symplectic, Real eigenvalues.

1. Introduction

A Hamiltonian system

$$\dot{p_i} = -\frac{\partial H}{\partial q_i}, \quad \dot{q_i} = \frac{\partial H}{\partial p_i}, 1 \le i \le d, \tag{1}$$

is a particular instance of the general systems of differential equations

$$\frac{dy}{dt} = F(y), \text{ with } y = [p,q]^T \in \mathbf{R}^{\mathcal{D}}, \mathcal{D} = 2d, \text{ and, } F = J^{-1}\nabla H, \tag{2}$$

where, $J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}$ is the standard symplectic matrix.

When an s stage RK method (A,b,c), i.e. ,

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

applied to system (2), it advances the numerical solution from time t_n to time $t_{n+1} = t_n + h$ through the relation

$$y^{n+1} = y^n + h\sum_{i=1}^{s} b_i F(Y_i), \tag{3}$$

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where the stage vectors Y_i are given by

$$Y_i = y^n + h\sum_{j=1}^{s} a_{ij}F(Y_j), 1 \le i \le s. \tag{4}$$

If the method is implicit, (4) provides a coupled system of $s \times \mathcal{D}$ algebraic equations for the $s \times \mathcal{D}$ components of the stage vectors. The computational cost per step of an implicit RK method is then definitely great, especially if s or $\mathcal{D}$ in large scale, and has become an obstacle to the application of those methods in practice. But a technique due to Butcher and Bickart can remarkably reduce the computation. We simply explain their idea as follows.

First, we introduce the increments

$$Z_i = Y_i - y^n,$$

then (4) can be rewritten as

$$\begin{bmatrix} Z_1 \\ \vdots \\ Z_s \end{bmatrix} = h(A \otimes I) \begin{bmatrix} F(y^n + Z_1) \\ \vdots \\ F(y^n + Z_s) \end{bmatrix}, \tag{5}$$

where the symbol $\otimes$ denotes the Kronecker product.

The simplified Newton iteration for (5) reads

$$(I - hA \otimes J_F)\Delta\mathbf{Z}^{(k)} = -\mathbf{Z}^{(k)} + h(A \otimes I)\mathbf{F}(\mathbf{Z}^{(k)}), \quad \mathbf{Z}^{(k+1)} = \mathbf{Z}^{(k)} + \Delta\mathbf{Z}^{(k)}. \tag{6}$$

Here, $\mathbf{Z}=[Z_1, \cdots, Z_s]$, $\mathbf{F}(\mathbf{Z}) =[F(y^n+Z_1)^T, \cdots, F(y^n+Z^s)^T]^T$, $J_F = \frac{\partial F}{\partial Y}(y^n)$. If A is invertible, then the technique mentioned above is to premultiply (6) by $(hA)^{-1} \otimes I$ and transform A^{-1} into a matrix D with a simpler structure (for instance diagonal, block diagonal, triangular)

$$T^{-1}A^{-1}T = D.$$

In the transformed variables

$$\mathbf{W} = (T^{-1} \otimes I)\mathbf{Z},$$

the iteration (6) reads

$$\begin{cases} (h^{-1}D \otimes I - I \otimes J_F)\Delta\mathbf{W}^{(k)} = -h^{-1}(D \otimes I)\mathbf{W}^{(k)} + (T^{-1} \otimes I)\mathbf{F}((T \otimes I)\mathbf{W}^{(k)}), \\ \mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} + \Delta\mathbf{W}^{(k)}. \end{cases} \tag{7}$$

In the case where D is a diagonal matrix with diagonal entries λ_i, the eigenvalues of A^{-1}, the matrix $(h^{-1}D \otimes I - I \otimes J_F)$ to be factorized is now block diagonal with s blocks $h^{-1}\lambda_i I - J_F$. Hence now it is only necessary to factorize s $\mathcal{D} \times \mathcal{D}$ matrices with an operation count $sO(\mathcal{D}^3)$. This is to be compared with the facterization of an $s\mathcal{D}$-dimensional matrix in (5) with a count $O((s\mathcal{D})^3)$. So it is much computationally efficient if λ_i are all real, i.e. , A has real eigenvalues only. Two particular cases of implicit methods, called SIRK (Singly Implicit Runge-Kutta method) and DIRK (Diagonally Implicit Runge-Kutta method), occur, respectively, when A has an unique non-zero real eigenvalue λ, i.e., $\sigma(A) = \lambda$ and $a_{ij} = 0$ for $i < j$, and they have almost the same efficiency as the multi-step methods. As is known, symplectic RK methods and symplectic PRK methods for non-separable Hamiltonian systems must be implicit. In this paper, we mainly focus on the symplectic RK methods and symplectic PRK methods with real eigenvalues for Hamiltonian system(1). Firstly, we show that an s stage RK&PRK method with real eigenvalues can not reach order more than $s+1$. It is then proved that no symplectic RK method with real eigenvalues exists in stage s of order $s+1$ when s is even. But symplectic PRK methods of this type don't necessarily meet this order barrier, and this is shown by an example constructed by using **W**-transformation. An useful way other than **W**-transformation to construct symplectic PRK methods with real eigenvalues is then presented. The conclusion we make is that, in high order level, composition methods due to Yoshida (see[5]) are of our advantage in consideration of the efficiency for these algorithms. Finally, a class of symplectic efficient methods of low order is recommended.