

Symmetric-Adjoint and Symplectic-Adjoint Runge-Kutta Methods and Their Applications

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Abstract. Symmetric and symplectic methods are classical notions in the theory of numerical methods for solving ordinary differential equations. They can generate numerical flows that respectively preserve the symmetry and symplecticity of the continuous flows in the phase space. This article is mainly concerned with the symmetric-adjoint and symplectic-adjoint Runge-Kutta methods as well as their applications. It is a continuation and an extension of the study in [14], where the authors introduced the notion of symplectic-adjoint method of a Runge-Kutta method and provided a simple way to construct symplectic partitioned Runge-Kutta methods via the symplectic-adjoint method. In this paper, we provide a more comprehensive and systematic study on the properties of the symmetric-adjoint and symplectic-adjoint Runge-Kutta methods. These properties reveal some intrinsic connections among some classical Runge-Kutta methods. Moreover, those properties can be used to significantly simplify the order conditions and hence can be applied to the construction of high-order Runge-Kutta methods. As a specific and illustrating application, we construct a novel class of explicit Runge-Kutta methods of stage 6 and order 5. Finally, with the help of symplectic-adjoint method, we thereby obtain a new simple proof of the nonexistence of explicit Runge-Kutta method with stage 5 and order 5.

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1. Introduction

In his book *Institutionum calculi integralis* in 1768 [12], Euler introduced a first-order numerical procedure for solving ordinary differential equations (ODEs), which

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is nowadays known as the Euler method. It is the most basic explicit method for the numerical integration of initial value problems for ODEs of the form

$$y'(t) = f(t, y), \quad y(t_0) = y_0. \quad (1.1)$$

More than 100 years later around 1900, the German mathematicians Runge and Kutta developed the nowadays known Runge-Kutta methods. The Runge-Kutta methods are a family of iterative methods for the numerical integration of (1.1), and they include the Euler method as a simple and special case. Choosing a step-size $h \in \mathbb{R}_+$, an s -stage Runge-Kutta method takes the following form:

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i, \quad (1.2)$$

where

$$k_i = f\left(t_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j\right), \quad i = 1, \dots, s, \quad (1.3)$$

the coefficients $a_{ij}, i, j = 1, \dots, s, b_1, b_2, \dots, b_s, c_1, c_2, \dots, c_s$ are real numbers, and (2.1) holds. The matrix $\mathbf{A} = (a_{ij})_{i,j=1}^s$ is called the Runge-Kutta matrix, while $\mathbf{b} = (b_i)_{i=1}^s$ and $\mathbf{c} = (c_i)_{i=1}^s$ are known as the weighting and nodal vectors, respectively. These data are usually arranged in a mnemonic device, known as a Butcher tableau (after Butcher),

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} = \frac{\mathbf{c}}{\mathbf{b}^T} \mathbf{A}. \quad (1.4)$$

The study of Runge-Kutta methods has a long and colourful history. In this paper, we are concerned with several classical notions in the theory of Runge-Kutta methods including symmetric method, symplectic method, adjoint method, and explicit/implicit method. Symmetric-adjoint method was originated by Scherer [27] and Butcher [6] who proposed the notion of reflected Runge-Kutta methods and in [16, 17], this class of Runge-Kutta methods is referred to as the adjoint methods, and their properties were studied. In [14], motivated by the symmetric-adjoint method, we introduced the notion of symplectic-adjoint method of a Runge-Kutta method. Some interesting properties about the symplectic-adjoint methods were presented in [14]. This article is a continuation as well as an extension of the study in [14]. First, we present the properties of the symmetric-adjoint and symplectic-adjoint Runge-Kutta methods in a more comprehensive and systematic way. Using those properties, we reveal some intrinsic connections among some classical Runge-Kutta methods including the Lobatto-type and Radau-type methods. Moreover, we show that those properties can be used to significantly simplify the order conditions and hence can be applied to the construction