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A Note on the Generating Function Method

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Abstract. The generating function method plays an important role in the construction of symplectic methods and closely depends on different generating functions. The three typical generating functions are widely applied in practical computations. This paper follows the general framework of the generating function method proposed by Feng Kang to produce a simple generating function with parameterized coordinates. This new generating function is more practical and covers the three typical ones by fixing the parameter to specific values. The relationship between symplectic transformation and new generating function and the Hamilton-Jacobi equation are discussed. A new family of arbitrary high-order symplectic methods with free parameter is obtained. Through the composition of the obtained low-order symplectic method, we derive another new class of any high-order symmetric symplectic methods with free parameter. These parametric symplectic methods will have more freedom of adjustment to design integrators which preserve energy or non-quadratic invariants. Computational examples illustrate the effectiveness of the proposed methods.

AMS subject classifications: 65L05, 65P10, 70H15, 70H20

Key words: Hamiltonian systems, generating function methods, symplectic methods.

1 Introduction

All real physical processes with negligible dissipation could be represented in the appropriate Hamiltonian form. We consider canonical Hamiltonian systems with n degrees of freedom in the form

$$\dot{y}=J_{2n}^{-1}\nabla H(y),\quad J_{2n}=\begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix},\quad y=(p,q)^T\in\mathbb{R}^{2n}, \tag{1.1}$$

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where I_n is the identity matrix of dimension n and $p,q \in \mathbb{R}^n$ generally describe the momenta and position of (1.1). One of the most widely studied properties of (1.1) is the symplecticity along the exact flows. For the numerical integration of such systems, the prominent works include the construction and research of symplectic methods. The basic idea is that the numerical integrator is devised to conserve the symplectic conservation law of (1.1) at each time step.

For the beginning of these studies, the concept of symplectic methods was first introduced in the pioneering work of De Vogelaere [6] and affirmed to be a very robust framework for the accurate, efficient and long-time integration of Hamiltonian systems (see the monographs [1,8,11,13,21]). The conservation property of symplectic methods bring fame to excellent qualitative behaviour and stability which can be explained in terms of backward error analysis [2,11,19]. These advantages make the foundational work of symplectic methods have a rapid development period [7, 9, 10, 12, 16, 18, 20, 24, 28]. Feng [7] innovatively defined symplectic methods by proving that the step-transition operator characterizing a numerical integrator is symplectic, and established the relationship between symplectic methods and generating functions in [9] to present a general approach called generating function method for constructing symplectic methods. The generating function method depends on various generating functions, and the three typical generating functions are widely applied in numerical simulations [4, 8, 11, 14, 15, 17, 26, 29]. Since Hamiltonian systems can be naturally partitioned into the variables p and q, partitioned Runge-Kutta (RK) methods received extensive attentions, which generalized standard RK methods. The symplectic members of RK methods were first identified by Lasagni [12] and Sanz-Serna [20], and symplectic partitioned RK methods appeared in Sanz-Serna [21] and Sun [24]. Yoshida [28] and Qin [18] obtained the construction of higher order symplectic methods by composition. For more details on the development of symplectic methods, please refer to references on Lie-Poisson integrators [10] and variational integrators [16].

In this paper, our aim is to discuss the generating function method. The generating function is the solution of Hamilton-Jacobi equations and can be directly connected to any symplectic map [9, 11, 23]. It is theoretically possible to find such a function to generate a given symplectic transformation. The generating function method and the symplectic (partitioned) RK methods are two different frameworks for constructing symplectic algorithms of Hamiltonian systems. Since any symplectic (partitioned) RK method corresponds to a generating function of explicit form and thereby can be derived from the framework of generating function methods (see the monograph [8,11]), in this sense, the generating function method is more general than the symplectic (partitioned) RK methods. However, the generating function is not unique [11]. By choosing appropriate coordinates, any symplectic transformation can be generated by various generating functions. This means that we can construct symplectic integrators in a variety of ways. By defining the fractional transformations in [9], the relationship between symplectic maps and gradient maps was given, and a bridge was established between symplectic maps and generating functions. Under the research of Hamilton-Jacobi theory, the generating function