Journal of Computational and Applied Mathematics 313 (2017) 486–498

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

G-symplectic second derivative general linear methods for Hamiltonian problems

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A R T I C L E   I N F O

Article history:
Received 20 April 2016
Received in revised form 22 September 2016

Keywords:
Hamiltonian problems
General linear methods
Second derivative methods
G-symplecticity
Parasitism

A B S T R A C T

It is our purpose to design second derivative general linear methods (SGLMs) for solving Hamiltonian problems. To do this, we explore G-symplectic SGLMs which preserve a generalization of quadratic invariants along the long-time integration. We find sufficient conditions on the coefficients matrices of the methods which ensure G-symplecticity and control parasitism. We construct such methods up to order 4. Numerical experiments of the constructed methods on the well-known Hamiltonian problems indicate ability of the methods in solving Hamiltonian problems over long-time integration.

1. Introduction

The purpose of this paper is derivation of conservative second derivative methods for the numerical integration of Hamiltonian problems

$$\begin{cases} \dot{p} = -\nabla_q H(p, q), \\ \dot{q} = \nabla_p H(p, q), \end{cases} \tag{1}$$

where $H : \mathbb{R}^{2d} \to \mathbb{R}$ is the Hamiltonian or energy of the system as a function of generalized momenta $p = [p_1 \quad p_2 \quad \cdots \quad p_d]^T \in \mathbb{R}^d$ and generalized coordinates $q = [q_1 \quad q_2 \quad \cdots \quad q_d]^T \in \mathbb{R}^d$. Such systems have the remarkable properties that the energy is preserved along the solutions and the system has a geometric structure called symplecticity. In general, symplecticity means that the sum of the areas of the projections of an oriented two-dimensional surface in phase space onto coordinate planes (p_i, q_i), $i = 1, 2, \ldots, d$, is unchanged under the flow of a Hamiltonian system [1]. This implies volume preservation and for systems with one degree of freedom it is equivalent to area preservation.

Numerical integrators exactly inheriting such properties are called geometric numerical integrators. Symplectic numerical methods belong to the family of geometric numerical integrators methods, which are used for long term integration of Hamiltonian systems. Moreover, these methods are able to preserve of Hamiltonian along the numerical solution without any drift and exactly preserve quadratic first integrals of the system. Symplectic one-step methods were first studied by de Vogelaere [2], Ruth [3] and Feng [4]. Also, Sanz-Serna [5] investigated symplectic Runge–Kutta methods. For Runge–Kutta methods $[A, b^T, c]$ to be symplectic, the matrix

$$M = \text{diag}(b)A + A^T \text{diag}(b) - bb^T,$$

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http://dx.doi.org/10.1016/j.cam.2016.10.011
0377-0427/

must be zero matrix [1,6,5]. These conditions imply that an irreducible symplectic Runge–Kutta method is necessarily implicit, although for separable Hamiltonian problems originating from a system of second order differential equations, there exist explicit symplectic integrators, such as Runge–Kutta–Nyström and partitioned Runge–Kutta methods [7,8].

The multistep methods are non-symplectic due to multivalue nature. As a more general result for multivalue methods, Butcher and Hewitt [9] proved that general linear methods (GLMs) with more than a single input and output value cannot be genuine symplectic. However multivalue methods, and in general GLMs, can be equipped by an extension of symplecticity, known as G-symplecticity, see [1,10]. Although G-symplectic GLMs do not exactly conserve the quadratic invariants, they preserve a generalization of quadratic invariants, indeed, they have approximately symplectic behaviour [11]. Also, there is a strong relation between G-symplectic and symplectic maps, which is discussed in [12]. It is proved in [12] that a G-symplectic method of order p has the same behaviour of a symplectic one-step method after a global change of coordinates and the Hamiltonian is preserved up to an error of size $O(h^p)$ on exponentially long time intervals.

The GLM

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right],$$

with r and s respectively as the number of input and stage values, is G-symplectic if the nonlinear stability matrix

$$M = \left[\begin{array}{c|c} DA + A^T D - B^T GB & DU - B^T GV \\ \hline U^T D - V^T GB & G - V^T GV \end{array}\right], \tag{2}$$

be zero matrix where G is a positive semi-definite symmetric $r \times r$ matrix and D is a $s \times s$ diagonal matrix [10,13–15]. Unfortunately, G-symplecticity of a multivalue numerical method, such as GLMs, is not good enough for a long-time behaviour. Since these methods introduce parasitic corruption, this phenomenon hinders their ability to produce qualitatively correct numerical results. So, it is necessary to get under control the parasitic solution components. Recently, some G-symplectic GLMs with zero parasitic growth factors have been constructed which have excellent near conservation of invariants over long time intervals [10,13–19].

On the other hand, to construct methods with higher order and extensive stability region, some efficient second derivative methods within the class of linear multistep methods [20,21] and Runge–Kutta methods [22,23] have been introduced. Also, the second derivative general linear methods (SGLMs), as an extension of GLMs, for unifying framework of the second derivative methods were introduced by Butcher and Hojjati in [24] and were investigated more by Abdi and Hojjati in [25–28]. In comparison with GLMs, an SGLM has more free parameters which can be used to achieved better properties such as higher order and wider region of absolute stability. Nevertheless, it has been shown that the computational cost is usually lower [28].

We are interested in SGLMs for long time integration of differential equation systems having quadratic invariants. SGLMs are multivalue in nature so, as GLMs, we cannot expect for symplectic behaviour or the true conservation of quadratic invariants. However, we aim to investigate if these methods can be G-symplectic. To do this, we seek conditions of G-symplecticity for SGLMs by making some relations between the coefficients matrices of the methods, which is the topic discussed in Section 2. The multivalue nature of these methods contributes to the corruption of numerical solution by the parasitic solution components [15]. So, in Section 3, we find sufficient conditions on the coefficient matrices of the methods for bounded parasitic components. Some examples of G-symplectic SGLMs with bounded parasitic components are presented in Section 4. Numerical experiments are shown in Section 5 and compared with those of an existing G-symplectic GLM and a symplectic Runge–Kutta method.

2. G-symplectic SGLMs

Consider the system of differential equations

$$\begin{aligned} y'(x) &= f(y(x)), \quad x \in [x_0, x_N] \\ y(x_0) &= y_0, \end{aligned} \tag{3}$$

with $f : \mathbb{R}^d \to \mathbb{R}^d$ and $(\mathbb{R}^d, \langle \cdot, \cdot \rangle)$ as an inner-product space, which has the property

$$\langle f(y), Qy \rangle = 0, \tag{4}$$

for all y. Here, Q is a symmetric matrix so that (4) is equivalent to the statement that $\langle y(x), Qy(x) \rangle$ is a quadratic invariant of (3) which is preserved along solutions.

Since the symplecticity means that variational equation conserve quadratic invariants [7], numerical flows that preserve quadratic invariants are symplectic.

We are going to study methods in class of the SGLMs which their introduced numerical approximations to $y(x)$ respect this invariance. We recall that an SGLM of order p and stage order q for solving (3) makes use of r input and output values, and s stage values and stage first and second derivative values. The collection of quantities imported at the start of step number n and the quantities exported at the end of this step will be denoted as $y^{[n-1]} = [y_i^{[n-1]}]_{i=1}^r$ and $y^{[n]} = [y_i^{[n]}]_{i=1}^r$ respectively. Denoting $Y^{[n]} = [Y_i^{[n]}]_{i=1}^s$ as an approximation of stage order q to the vector $y(x_{n-1}+ch) = [y(x_{n-1}+c_ih)]_{i=1}^s$ and the vectors