G-symplecticity implies conjugate-symplecticity of the underlying one-step method

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Abstract

This note proves that the underlying one-step method of a G-symplectic general linear method is conjugate to a symplectic method. Parasitic solution components are not considered.

1 Introduction

For the numerical solution of differential equations

$$\dot{y} = f(y), \qquad y(0) = y_0 \tag{1}$$

with one-step methods, the long-time behavior is well understood (backward error analysis). In particular, it is known that symplectic methods nearly preserve the energy of Hamiltonian systems over exponentially long times, and they exactly preserve quadratic first integrals of the system.

For multi-value methods, for which the discrete flow evolves in a higher dimensional space, the situation is much more delicate. Inspired by the work of [7] for multistep methods, an extension of symplecticity to general linear methods (an important class of multi-value methods) has been discussed in the thesis [12]. The name G-symplecticity has been proposed in the first edition of [10]. Until now it is an open question whether G-symplecticity has also an impact on the long-time behavior of numerical solutions. This question is addressed in the recent publication [2], which starts with the sentence "The aim of this work is to understand the possible role in the long-term integration of conservative systems of 'G-symplectic' methods".

The present note gives an answer to this question. We prove that G-symplecticity of a general linear method implies conjugate-symplecticity of the underlying one-step method. G-symplecticity does not play a role in the boundedness of parasitic solution components (bounds on parasitic terms are given in [6]). As long as parasitic solution components can be neglected, the numerical solution of a G-symplectic general linear method behaves like that of symplectic one-step method after a global transformation $\chi(y)$ that is $\mathcal{O}(h^p)$ close to the identity (p is the order of the method). Section 2 recalls the frame of multi-value methods, Section 3 discusses the notion of G-symplecticity, and Section 4 presents the main results including proofs.

2 Multi-value methods

This article is concerned with multi-value methods. They are given by a *forward step procedure*

$$Y_{n+1} = (V \otimes I)\, Y_n + h\, \Phi(h, Y_n), \tag{2}$$

a *starting procedure*

$$Y_0 = S_h(y_0), \tag{3}$$

and a *finishing procedure*

$$y_n = F_h(Y_n). \tag{4}$$

The multi-value character of the method is due to the fact that Y_n is a super vector of dimension rd, which contains r vectors of the dimension d of (1). The finishing procedure defines the numerical approximation to the solution of (1). To get an accurate approximation, the starting procedure $S_h(y_0)$ has to be close to the so-called "exact" starting procedure $S_h^*(y_0)$ (typically given as a formal series in powers of the step size h). The main interest of this exact starting procedure is the fact that, for a given forward step procedure and a given finishing procedure, there exist a unique $S_h^*(y_0)$ and a unique (formal) one-step method $\Phi_h^*(y_0)$, such that for $Y_0 = S_h^*(y_0)$ the numerical solution given by (2) and (4) satisfies the one-step relation $y_{n+1} = \Phi_h^*(y_n)$ (see Theorem XV.8.2 of [10]). This one-step method is called *underlying one-step method.* Written out as formulas, the (formal) mappings $S_h^*(y_0)$ and $\Phi_h^*(y)$ are seen to be given by

$$G_h \circ S_h^* = S_h^* \circ \Phi_h^* \qquad \text{and} \qquad F_h \circ S_h^* = \text{identity}, \tag{5}$$

where the forward step procedure is abbreviated as $Y_{n+1} = G_h(Y_n)$. In the following we assume that the matrix V has $\zeta_1 = 1$ as simple eigenvalue with eigenvector v_1, and that it possesses a set of r linearly independent eigenvectors $v_j, j = 1, \ldots, r$ corresponding to eigenvalues ζ_j.

We are mainly interested in general linear methods. For them, the forward step procedure is given by

$$Y_{n+1} = (V \otimes I)Y_n + h(B \otimes I)f(W), \quad W = (U \otimes I)Y_n + h(A \otimes I)f(W),$$

where for a super vector $W = (W_i)_{i=1}^s$ with $W_i \in \mathbb{R}^d$, the super vector $f(W)$ is defined by $f(W) = (f(W_i))_{i=1}^s$. The matrices V, B, U, and A are of dimension $r \times r$, $r \times s$, $s \times r$, and $s \times s$, respectively. The finishing procedure is typically given by $F_h(Y_n) = (d^\mathsf{T} \otimes I)Y_n$ with a vector d satisfying $d^\mathsf{T} v_1 = 1$, but it can also be of the form

$$F_h(Y_n) = (d^\mathsf{T} \otimes I)Y_n + h(e^\mathsf{T} \otimes I)f(W),$$

where the super vector W is given by a formula similar to that in the forward step procedure with possibly different coefficient matrices U and A.

For such methods, the underlying one-step method and the exact starting procedure can be written as formal series in powers of h, and a comparison of like powers of h in (5) yields

$$S_h^*(y) = v_1 \otimes y + h\, s_1 \otimes f(y) + h^2 s_2 \otimes f'(y)f(y) + \mathcal{O}(h^3) \tag{6}$$

which is recognized as a vector of B-series. Here, v_1 is the first eigenvector of V and s_1, s_2 are vectors in $\mathbb{R}^r$. For readers who are not familiar with B-series we suggest to take a quick look at Chapter III of [10].

3 G-symplecticity of multi-value methods

Since the condition for symplecticity is a quadratic first integral of the variational equation, numerical flows that preserve quadratic first integrals are symplectic. A quadratic form $Q(y) = y^{\mathsf{T}}Ey$ with symmetric matrix E is a first integral of $\dot y = f(y)$ if it is preserved along solutions. This is expressed by the condition $y^{\mathsf{T}}Ef(y) = 0$.

Definition 3.1 *Let G be a symmetric matrix satisfying $v_1^{\mathsf{T}}Gv_1 = 1$. The forward step procedure (2) is called* G-symplectic*, if for all quadratic first integrals $Q(y) = y^{\mathsf{T}}Ey$ of $\dot y = f(y)$ the propagation vector satisfies*

$$Y_{n+1}^{\mathsf{T}}(G \otimes E)Y_{n+1} = Y_n^{\mathsf{T}}(G \otimes E)Y_n.$$

The use of a symmetric matrix G in this definition is very natural, because the same matrix also appears in the study of contractivity of multi-value methods for stiff differential equations (G-stability for one-leg methods and algebraic stability for general linear methods).

Lemma 3.2 *A G-symplectic forward step procedure satisfies*

$$V^{\mathsf{T}}GV = G,$$

and it holds $v_i^{\mathsf{T}}Gv_j = 0$ if $\zeta_i\zeta_j \neq 1$.

Proof. Inserting the forward step procedure into the condition of G-symplecticity and putting $h = 0$ proves the relation $V^{\mathsf{T}}GV = G$. Multiplication with v_i^{T} from the left and with v_j from the right yields $v_i^{\mathsf{T}}Gv_j = \zeta_i\zeta_j v_i^{\mathsf{T}}Gv_j$, which proves the second statement. □

It is shown in [7] that all symmetric one-leg methods are G-symplectic. A first example of a G-symplectic general linear method, which is neither a Runge–Kutta method nor a multistep method, is given in [1]. Further examples are presented in [2] and [3].

4 Main result

For linear multistep methods, which constitute an important class of multi-value methods, the following is known: the underlying one-step method cannot be symplectic [13], but for symmetric multistep methods it is conjugate to a symplectic integrator [8]. Can we have a similar result for more general multi-value methods? The results of [9] (see also [4]) strongly indicate that the underlying one-step method of a general linear method cannot be symplectic unless the method can be reduced to a one-step method.

Lemma 4.1 *Consider a multi-value method with underlying one-step method $\Phi_h^*(y)$ and with exact starting procedure $S_h^*(y)$, and let $Q(y) = y^{\mathsf{T}}Ey$ be a first integral of $\dot y = f(y)$. If the method is G-symplectic, then the expression*

$$Q_h(y) = S_h^*(y)^{\mathsf{T}}(G \otimes E)\, S_h^*(y) = y^{\mathsf{T}}E\, y + \mathcal{O}(h^2)$$

is preserved by the underlying one-step method $\Phi_h^*(y)$, i.e., in the sense of formal power series we have $Q_h\big(\Phi_h^*(y)\big) = Q_h(y)$.

Proof. For the choice $Y_n = S_h^*(y)$, condition (5) yields $Y_{n+1} = S_h^*\big(\Phi_h^*(y)\big)$. The definition of G-symplecticity thus implies that $Q_h(y)$ is preserved by the method $\Phi_h^*(y)$. The closeness to $y^\mathsf{T} E y$ follows from (6) and from the fact that $y^\mathsf{T} E f(y) = 0$. □

Theorem 4.2 *Consider a G-symplectic general linear method of order p. Then, for every finishing procedure the underlying one-step method is conjugate-symplectic. More precisely, there exists a change of coordinates $\chi_h(y) = y + \mathcal{O}(h^p)$, such that $\chi_h \circ \Phi_h^* \circ \chi_h^{-1}$ is a symplectic transformation.*

Proof. For general linear methods the underlying one-step method and the components of the exact starting procedure $S_h^*(y)$ can be expressed as B-series. The expression $Q_h(y)$ of Lemma 4.1 is thus precisely of the form that is required for the application of Theorem VI.8.5 of [10], see also [5]. This theorem implies that the underlying one-step method is conjugate to a symplectic method with a change of coordinates $\hat\chi_h$ that is $\mathcal{O}(h^2)$ close to the identity. Once the conjugate-symplecticity is established, an application of Lemma 3.3 of [11] shows the existence of a change of coordinates $z = \chi_h(y)$ satisfying $\chi_h(y) = y + \mathcal{O}(h^p)$, such that in the coordinates z the method is symplectic. □

Let us discuss the impact of this result to the long-time integration of Hamiltonian differential equations:

- Conjugate-sympletcicity of the underlying one-step method means that for $y_{n+1} = \Phi_h^*(y_n)$ the approximations $z_n = \chi_h(y_n)$ behave like that of a symplectic one-step method: The Hamiltonian is preserved up to an error of size $\mathcal{O}(h^p)$ on exponentially long time intervals. For integrable Hamiltonian systems, all action variables are nearly preserved over long times, and the global error increases at most linearly with time. Quadratic first integrals are not exactly preserved, but they are preserved up to $\mathcal{O}(h^p)$ on exponentially long times.

- We emphasize that the present work gives only information on the long-time behavior of the underlying one-step method. Rigorous bounds on parasitic solution components, which are always present in multi-value methods, have recently been obtained in [6]. Unfortunately, G-symplecticity does not seem to have an impact on the boundedness of parasitic components.

The conclusion of the present investigation is that, as long as parasitic components are small and bounded, the numerical solution obtained by a G-symplectic multi-value method has the same behavior as that of a symplectic one-step method after a global change of coordinates that is $\mathcal{O}(h^p)$ close to the identity. This is confirmed by the numerical experiments of [3] and [6].

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