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CONJUGATE-SYMPLECTICITY OF LINEAR MULTISTEP METHODS*

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Abstract

For the numerical treatment of Hamiltonian differential equations, symplectic integrators are the most suitable choice, and methods that are conjugate to a symplectic integrator share the same good long-time behavior. This note characterizes linear multistep methods whose underlying one-step method is conjugate to a symplectic integrator. The boundedness of parasitic solution components is not addressed.

Mathematics subject classification: 65L06, 65P10.
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1. Main Result

For the numerical integration of $\dot{y} = f(y)$ we consider the linear multistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+j} \;=\; h \sum_{j=0}^{k} \beta_j f(y_{n+j}), \tag{1.1}$$

and we denote its generating polynomials by

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j.$$

We assume throughout this note that the method is consistent (i.e., $\rho(1) = 0$ and $\rho'(1) = \sigma(1) \neq 0$) and irreducible (i.e., $\rho(\zeta)$ and $\sigma(\zeta)$ do not have a common factor).

Since the discrete flow of a multistep method evolves on a product of k copies of the phase space, definitions like that for symplecticity are not straightforward. It was first suggested by Feng Kang [3] (see also [2, pp. 274-283]) to study the symplecticity of a linear multistep method via its *underlying one-step method* (also called step-transition operator). This is a mapping $y \mapsto \Phi_h(y)$, such that the iterates $y_n = \Phi_h^n(y_0)$ satisfy the recursion (1.1). The existence of this underlying one-step method as a formal B-series is discussed in [4, 10], see also [6, Sect. XV.2]. Unfortunately, multistep methods are non symplectic with respect to this definition of symplecticity [9].

A method $\Phi_h(y)$ is called conjugate-symplectic [8] if there exists a transformation $\chi_h(y)$ which is $\mathcal{O}(h)$ close to the identity (and represented by a formal B-series), such that $\chi_h^{-1} \circ \Phi_h \circ \chi_h$ is a (formal) symplectic transformation when $f(y)$ is a Hamiltonian vector field. Although such a method does not need to be symplectic, it shares the long-time behavior of a symplectic integrator because $(\chi_h^{-1} \circ \Phi_h \circ \chi_h)^n = \chi_h^{-1} \circ \Phi_h^n \circ \chi_h$.

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Theorem 1.1. *The underlying one-step method of the linear multistep method* (1.1) *is conjugate-symplectic if and only if* (1.1) *is symmetric, i.e.,* $\alpha_j = -\alpha_{k-j}$ *and* $\beta_j = \beta_{k-j}$ *for all* j.

Since the order of symmetric methods is always even and since we consider arbitrary B-series for the conjugacy mapping χ_h, this provides a new proof for the main result of [7], which states that the underlying one-step method of a method (1.1) with odd order $u \geq 3$ cannot be conjugate to a symplectic method with order $v \geq u$ via any generalized linear multistep method (GLMSM). In that article, a GLMSM denotes a difference formula like (1.1), where $f(y_{n+j})$ is replaced by $f\big(\sum_{l=0}^{k} \gamma_{jl} y_{n+l}\big)$.

In [7] it is furthermore conjectured that if a GLMSM (and in particular also (1.1)) is conjugate-symplectic via another GLMSM, then it must be conjugate to the 2nd order mid-point rule. The requirement on the conjugacy mapping seems very strong, because any B-series for χ_h would imply as well the good long-time behavior of the method. If we relax this requirement and admit arbitrary B-series for χ_h, Theorem 1.1 proves the existence of conjugate-symplectic methods (1.1) of arbitrarily high order.

The proof of Theorem 1.1 is a concatenation of various results that have been proved in a different context by several authors.

2. Proof of Necessity

It suffices to consider the harmonic oscillator which can be written as $\dot{y} = \lambda y$ with $\lambda = \mathrm{i}$ (put $y = p + \mathrm{i}q$). In this situation $\Phi_h(y) = \zeta(\lambda h)y$, where $\zeta = \zeta(z)$ is the solution of

$$\rho(\zeta) - z\,\sigma(\zeta) = 0 \tag{2.1}$$

which is the analytic continuation of $\zeta(0) = 1$. For the harmonic oscillator, conjugate-symplecticity as well as symplecticity and area preservation are equivalent to

$$|\zeta(\mathrm{i}h)|^2 = \zeta(\mathrm{i}h)\zeta(-\mathrm{i}h) = 1.$$

It is proved in [8] and in [3] (see also [2, pp. 274-283]) that this property implies the symmetry of the method (1.1): substituting $-z$ for z and ζ^{-1} for ζ in (2.1) shows that the adjoint mapping $\zeta^*(z) = \zeta(-z)^{-1}$ satisfies the relation $\rho^*(\zeta^*) + z\,\sigma^*(\zeta^*) = 0$ with $\rho^*(\zeta) = \zeta^k \rho(\zeta^{-1})$ and $\sigma^*(\zeta) = \zeta^k \sigma(\zeta^{-1})$. The condition $\zeta(\mathrm{i}h)\zeta(-\mathrm{i}h) = 1$ therefore implies that $\zeta = \zeta(\mathrm{i}h)$ satisfies

$$\rho(\zeta) - \mathrm{i}h\,\sigma(\zeta) = 0, \quad \rho^*(\zeta) + \mathrm{i}h\,\sigma^*(\zeta) = 0$$

for all sufficiently small h. Consequently, we have

$$\rho(\zeta)\,\sigma^*(\zeta) = -\rho^*(\zeta)\,\sigma(\zeta)$$

for $\zeta = \zeta(\mathrm{i}h)$ and, by analytic continuation, for all complex ζ. Since $\rho(\zeta)$ and $\sigma(\zeta)$ do not have common factors, and $\sigma(1) = \sigma^*(1) \neq 0$, this yields $\rho^*(\zeta) = -\rho(\zeta)$ and $\sigma^*(\zeta) = \sigma(\zeta)$ what is equivalent to the symmetry of the method.

3. Proof of Sufficiency

a) The following result has been proved in [5] for multistep methods for second order differential equations and in [6, Sect. XV.4.4] for methods (1.1): if $Q(y)$ is a quadratic first integral of $\dot{y} = f(y)$ and if (1.1) is symmetric, then the underlying one-step method exactly preserves a quantity $\widetilde{Q}(y) = Q(y) + \mathcal{O}(h)$ that can be expressed in terms of elementary differentials.

b) One of the main results in [1] is the following: if, for a problem $\dot{y} = f(y)$ having a quadratic first integral $Q(y)$, a B-series integrator $\Phi_h(y)$ exactly preserves a modified quantity $\widetilde{Q}(y) = Q(y) + \mathcal{O}(h)$, then it is conjugate to a symplectic B-series.

c) A combination of the statements (a) and (b) completes the proof of Theorem 1.1.

4. Comments

Numerical one-step methods that are conjugate-symplectic have the same long-time behaviour as symplectic methods. They nearly conserve the Hamiltonian and quadratic first integrals, and they have an improved error propagation for nearly integrable Hamiltonian systems.

Care has to be taken with multistep methods, because their long-time behavior is not only determined by their underlying one-step method. Also the parasitic solution components have to be got under control (see [4]). A satisfactory long-time analysis is known only for a special class of symmetric multistep methods for problems $\ddot{q} = -\nabla U(q)$ (see [5]).

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