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Canonical Runge-Kutta methods

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Introduction

In this note we discuss numerical integration schemes for Hamiltonian systems of the form

$$\dot{x} = H_y^T, \quad \dot{y} = -H_x^T,$$

with Hamiltonian $H(x, y, t)$, $x, y \in \mathbb{R}^n$, $t \in \mathbb{R}$. An integration procedure is called canonical, if it generates a globally canonical map (for a definition, see V. I. Arnold [1]) if applied to a Hamiltonian system. The significance of this concept is best illustrated as follows. To integrate a Hamiltonian system with a non-canonical method is as if an undamped system was approximated by a damped system. In both cases the long time behaviour of the exact and the approximate solutions will differ qualitatively. These ideas are described more fully in D. Stoffer [6]. It will be shown in [7] that integration of Hamiltonian systems by a canonical method of order p preserves the energy for times of order exp (const./h) with an error of order h^p, h the step size. In this note we want to characterize *all canonical* Runge-Kutta methods. (For an exhaustive presentation of *RK* methods see e.g. Hairer, Norsett, Wanner [4].) Iselin [5] describes a 3rd order method of R. Ruth which is canonical for Hamiltonians of the form $H(x, y) = U(x) + V(y)$. Feng Kang [2] presents canonical methods of arbitrarily high order which, however, make use of higher order derivatives of the vector field. He also proves that the Implicit Midpoint Rule is canonical. D. Stoffer [6] constructs a canonical method of order 4 which makes use of first order derivatives only.

As usual an s-stage *RK* method is described by its coefficients c_i, b_i, a_{ij}, with i, $j = 1, \ldots, s$, see below. An *RK* method is canonical provided its coefficients satisfy a certain condition, cf. Eq. (1). A well known class of *RK* methods of arbitrary high order are the *RK* methods based on Gaussian quadrature formulas. These methods happen to satisfy the canonicity condition. It also follows that there are *no explicit* canonical *RK* methods.

For substantial help during the preparation of this work I am indebted to D. Stoffer.

Statement of the result

In the following we will deal with differential equations of the form $\dot{z} = f(z, t)$. f is assumed to be sufficiently regular in a suitable domain.

An s-stage *RK* method is given by

$$k_i = f\left(z + h \sum_{j=1}^{s} a_{ij} k_j,\ t + h c_i\right), \quad \bar{z} = z + h \sum_{i=1}^{s} b_i k_i, \quad i \in \{1, \ldots, s\},$$

where $|h| < h_0$ with some $h_0 > 0$. We assume h_0 to be so small that the map $\Phi_h : z \mapsto \bar{z}$ is as close to the identity as needed.

Theorem. The map Φ_h *is globally canonical if*

$$b_i b_j = b_i\, a_{ij} + b_j a_{ij}\,, \qquad i, j \in \{1, \ldots, s\} \tag{1}$$

Furthermore, if a RK method generates a canonical map Φ_h if applied to Hamiltonian systems, then Φ_h is equivalent to a RK method satisfying (1).

Remark. With the definitions

$$B := \operatorname{diag}(b_1, \ldots, b_s)\,,\ A := (a_{ij})_{i,j=1}^{s} \quad \text{and} \quad e := (1, \ldots, 1)^T$$

Eq. (1) becomes

$$BA + A^T B - Bee^T B = 0\,.$$

E. Hairer remarked that for algbraically stable RK methods the quadratic form $BA + A^T B - Bee^T B$ is nonnegative definite. In [3] he gives a characterization of the algebraically stable RK methods which includes the characterization of canonical RK methods as a special case, as follows from the Theorem.

References

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Summary

In the present note we provide a complete characterization of all Runge-Kutta methods which generate a canonical transformation if applied to a Hamiltonian system of ordinary differential equations.

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