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THE STEP-TRANSITION OPERATORS FOR MULTI-STEP METHODS OF ODE'S*1)

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Abstract

In this paper, we propose a new definition of symplectic multistep methods. This definition differs from the old ones in that it is given via the one step method defined directly on M which is corresponding to the m step scheme defined on M while the old definitions are given out by defining a corresponding one step method on $M \times M \times \cdots \times M = M^m$ with a set of new variables. The new definition gives out a steptransition operator $g : M \longrightarrow M$. Under our new definition, the Leap-frog method is symplectic only for linear Hamiltonian systems. The transition operator g will be constructed via continued fractions and rational approximations.

Key words: Multi-step methods, Explike and loglike function, Fractional and rational approximation, Simplecticity of LMM, Nonexistence of SLMM.

1. Introduction

The disadvantage of symplectic methods in using the information from past time steps leads to their needing more function evaluation than nonsymplectic methods. This disadvantage can be overcome if one could construct symplectic multi-step methods. But the first problem should be solved is to give out the definition of symplectic multi-step method. Until now, a popular idea is that an m-step method on M may be written as a one-step method on M^m. In paper [2, 7], the authors have investigated the circumstance under which a difference scheme can preserve the product symplectic structure on M^m. In this paper, a completely different criterion is given because the induced one-step method corresponding to the original multi-step method is defined, it gives out a transition operator $g : M \longrightarrow M$.

Consider the autonomous ODE's on R^n

$$\frac{dz}{dt} = a(z), \tag{1.1}$$

where $z = (z_1, \cdots, z_n)$ and $a(z) = (a_1(z), \cdots, a_n(z))$ is a smooth vector field on R^n defining the system. For equation (1.1), we define a linear m step method (LMM) in standard form by

$$\sum_{j=0}^{m} \alpha_j z_j = \tau \sum_{j=0}^{m} \beta_j a_j, \tag{1.2}$$

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where α_j and β_j are constants subject to the conditions

$$\alpha_m = 1, \quad |\alpha_0| + |\beta_0| \neq 0.$$

If $m = 1$, we call (1.2) a one step method. In other cases, we call it a multi-step method. Here linearity means the right hand of (1.2) linearly dependent on the value of $a(z)$ on integral points. For the compatibility of (1.2) with equation (1.1), it must at least of order one and thus satisfies

1°. $\alpha_1 + \alpha_2 + \cdots + \alpha_m = 0$.

2°. $\beta_0 + \beta_2 + \cdots + \beta_m = \sum_{j=0}^{m} j\alpha_j \neq 0$.

LMM method (1.2) has two characteristic polynomials

$$\zeta(\lambda) = \sum_{i=0}^{m} \alpha_i \lambda^i, \quad \sigma(\lambda) = \sum_{i=0}^{m} \beta_i \lambda^i. \tag{1.3}$$

Equation (1.2) can be written as

$$\zeta(E) y_n = \tau a(\sigma(E) y_n). \tag{1.4}$$

In section 2, we will study symplectic multi-step methods for linear Hamiltonian systems. We will give a new definition via transition operators which are corresponding to the multi-step methods. We will point out that if these operators are of exponential forms and their reverse maps are of Log forms then the original multi-step method are symplectic. In section 3, we will use continued fractions and rational approximations to approximate the transition operators. In section 4, we show that for non-linear Hamiltonian systems, there exists no symplectic multi-step methods in the sense of our new definition. Numerical examples are also presented.

2. Symplectic LMM for Linear Hamiltonian Systems

First we consider a linear Hamiltonian system

$$\frac{dz}{dt} = az, \tag{2.1}$$

where a is an infinitesimal $n \times n$ symplectic matrix. Its phase flow is $z(t) = \exp(ta) z_0$. The LMM for (2.1) is

$$\alpha_m z_m + \cdots + \alpha_1 z_1 + \alpha_0 z_0 = \tau a(\beta_m z_m + \cdots + \beta_1 z_1 + \beta_0 z_0). \tag{2.2}$$

Our goal is to find a matrix g, i.e., a linear transformation $g : R^{2n} \longrightarrow R^{2n}$ which can satisfy (2.2)

$$\alpha_m g^m(z_0) + \cdots + \alpha_1 g(z_0) + \alpha_0 z_0 = \tau a(\beta_m g^m(z_0) + \cdots + \beta_1 g(z_0) + \beta_0 z_0). \tag{2.3}$$

Such a map g exists for sufficiently small τ and can be represented by continued fractions and rational approximations. We call this transformation is step transition operator.