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MULTIPLICATIVE EXTRAPOLATION METHOD FOR CONSTRUCTING HIGHER ORDER SCHEMES FOR ORDINARY DIFFERENTIAL EQUATIONS

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Abstract

In this paper, we develop a new technique called multiplicative extrapolation method which is used to construct higher order schemes for ordinary differential equations. We call it a new method because we only see additive extrapolation method before. This new method has a great advantage over additive extrapolation method because it keeps group property. If this method is used to construct higher order schemes from lower symplectic schemes, the higher order ones are also symplectic. First we introduce the concept of adjoint methods and some of their properties. We show that there is a self-adjoint scheme corresponding to every method. With this self-adjoint scheme of lower order, we can construct higher order schemes by multiplicative extrapolation method, which can be used to construct even much higher order schemes. Obviously this constructing process can be continued to get methods of arbitrary even order.

Introduction

When we construct a higher order scheme for systems of ordinary differential equations:

$$y' = f(y) \tag{1}$$

(where $y = y(x)$, and x is a variable), we often use the "Taylor series expanding" method, but sometimes this method is very tedious when it is applied to get higher order schemes. There is another method: Lie series, it is the method we use in this paper. J.Dragt, F.Neri, and Stanly Steinberg have done a lot of work in developing this method. For details, one can refer to [4,6,8]. We just apply this method to our problem, and do not need to compute out the exact terms of the "Lie series" of a scheme: we just use the form of them. Thus the deduction becomes simple when this Lie series method is applied to multiplicative extrapolating method as we will show later.

In section 1, we will give the definition of adjoint methods, self-adjoint methods and some properties of them. Section 2 is about the multiplicative extrapolation method.

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This paper is a summary of a pre-print one, all the proofs and other details omitted here are given in that paper.

Notice: all the functions considered in this paper are supposed to be analytic.

1. Adjoint Method And Self-adjoint Method

We know every one-step difference scheme can be written as follows:

$$y_{n+1} = s(\tau)y_n \tag{2}$$

where $s(\tau)$ is the operator corresponding to the difference scheme, and τ is the step length.

Definition 1.1. *An operator $s^*(\tau)$ is called the adjoint operator of $s(\tau)$, if*

$$s^*(-\tau)s(\tau) = I \tag{3.1}$$

$$s(\tau)s^*(-\tau) = I \tag{3.2}$$

are satisfied.

We rewrite (2) in the form:

$$y_{n+1} = y_n + \tau\Phi(x, y_n, \tau) \tag{4}$$

here

$$\begin{cases} y_{n+1} = y_\tau(x_n + \tau) \\ y_n = y_\tau(x_n) \end{cases} \tag{5}$$

and $\Phi(x, y_n, \tau)$ is the increment function corresponding to the scheme (2).

Definition 1.2. *A scheme $y_{n+1} = y_n + \tau\Phi^*(x, y_n, \tau)$ is the adjoint of (4) if*

$$B = A - \tau\Phi(x + \tau, A, -\tau) \tag{6.1}$$

$$A = B + \tau\Phi^*(x, B, \tau) \tag{6.2}$$

are satisfied.

Theorem 1.3. *The definitions 1.1 and 1.2 are equivalent.*

Definition 1.4. *We call an operator $s(\tau)$ is self-adjoint, if $s^*(\tau) = s(\tau)$.*

Theorem 1.5. *For any operator $s(\tau)$, $s^*(\tau)s(\tau)$ (or $s(\tau)s^*(\tau)$) is a self-adjoint operator.*

Theorem 1.6. *The symmetric composition $s_1(\tau)s_2(\tau)s_1(\tau)$ of self-adjoint operators $s_1(\tau)$, $s_2(\tau)$ is a self-adjoint operator.*

2. Multiplicative Extrapolation Method for Constructing of Higher Order Integrators

Denote $f = [f_1, f_2, \cdots, f_n]^T, g = [g_1, g_2, \cdots, g_n]^T, D = [\frac{d}{dy_1}, \frac{d}{dy_2}, \cdots, \frac{d}{dy_n}]^T$ where $f_1, f_2, \cdots, f_n$ and $g_1, g_2, \cdots, g_n$ are scalar functions. Let

$$L_f = f^T D = \sum_{i=1}^{n} f_i \frac{\partial}{\partial y_i} \tag{7}$$

be a first order differential operator. The action of L_f on a scalar function φ yields:

$$L_f\varphi = (\sum_{i=1}^{n} f_i \frac{\partial}{\partial y_i})\varphi = f^T D\varphi(y).$$

Definition 2.1. *The commutator of two first order differential operators L_f and L_g is given by*

$$[L_f, L_g] = L_f L_g - L_g L_f. \tag{8}$$

The commutator of the two operators is still a first order differential operator. We can prove that for this kind of commutator the total of the first order differential operators form a Lie algebra.

Definition 2.2. *A Lie series is an exponential of a first order linear differential operator,*

$$e^{tL_f} = \sum_{n=0}^{\infty} \frac{t^n L_f^n}{n!}. \tag{9}$$

The action of a Lie series on a scalar function $\varphi(y)$ is given by:

$$\begin{aligned} e^{tL_f}\varphi(y) &= \sum_{k=0}^{\infty} \frac{t^k L_f^k}{k!}\varphi(y) = \sum_{k=0}^{\infty} \frac{t^k}{k!}(f^T(y)D)^k\varphi(y) \\ &= \varphi(y) + tf^T(y)(D\varphi(y)) + \frac{t^2}{2} f^T(y)D(f^T(y)D\varphi(y)) + \cdots. \end{aligned} \tag{10}$$

We give several properties of Lie series. All of them can be proved as in [4]. Let:

$$f = [f_1(y), f_2(y), \cdots, f_n(y)]^T, g = [g_1(y), g_2(y), \cdots, g_n(y)]^T$$
$$\text{and} \quad e^{tf^T D} g = [e^{tf^T D} g_1, e^{tf^T D} g_2, \cdots, e^{tf^T D} g_n]^T.$$

(1) Composition:

$$e^{tL_f} g(y) = g(e^{tL_f} y) \tag{11}$$

(2)Product preservation:

$$e^{tL_f}(pq) = (e^{tL_f}p)(e^{tL_f}q) \tag{12}$$

where $p(y), q(y)$ are scalar functions.

(3)Non-commuting exponential identities: *Since the total of first order differential operators we defined form a Lie algebra, we have the Baker-Campbell-Hausdroff formula:*

$$e^{tL_f} e^{tL_g} = e^{t(L_f+L_g)+t^2 w_2 + t^3 w_3 + \cdots} \tag{13}$$

where

$$\begin{aligned} w_2 &= \frac{1}{2}[L_f, L_g] \\ w_3 &= \frac{1}{12}[[L_f, L_g], L_f] + \frac{1}{12}[[L_f, L_g], L_g] \\ w_4 &= \frac{1}{24}[L_f[L_g[L_g, L_f]]], \quad \cdots\cdots \end{aligned}$$

(4)Differential equation property: *If* $y(t) = e^{tf^T D}y, y = y(0)$, *then* $y'(t) = f(y(t))$.

From property (4), we know the solution of (1) can be represented in the form $y(t) = e^{tL_f}y(0)$, we hope that the operator of a scheme can also be represented in this form. In [6], Dragt and Finn showed us the relation between a one parameter family of symplectic transformations and a Hamiltonian system. From their work we get:

Lemma 2.3. *The action of any operator $s(\tau)$ on an initial value $y(0)$ can be represented formally in the form of the solution of some ODE problem.*

This is just the general case of the conclusion of Dragt and Finn when we deal with non-Hamiltonian systems and use non- symplectic schemes.

Since $s(\tau)$ may not form a one parameter group, the corresponding ODE problem may be time-dependent, but we still can get the formal exponential representation of $s(\tau)$ as follows[1]:

$$s(\tau) = exp(\tau A + \tau^2 B + \tau^3 C + \tau^4 D + \tau^5 E + \cdots)$$

and the sequence

$$\tau A + \tau^2 B + \tau^3 C + \tau^4 D + \tau^5 E + \cdots$$

may not be convergent, where $A, B, C, D, E, \cdots$ are first order differential operators. However, we still can get:

Lemma 2.4. *Every operator $s(\tau)$ has an exponential representation.*

Now using Lemma 2.4, we can get an important result[2].

Theorem 2.5. *Every self-adjoint operator has an even order of accuracy.*

Corollary 2.6. Let $s(\tau)$ be a self-adjoint operator of order 2n, then the operator $s(c_1\tau)s(c_2\tau)s(c_1\tau)$, with c_1, c_2 satisfying:

$$2c_1^{2n+1} + c_2^{2n+1} = 0, \quad 2c_1 + c_2 = 1 \quad (when \quad n = 1, c_1 = \frac{1}{2 - 2^{\frac{1}{3}}}, \quad c_2 = \frac{-2^{\frac{1}{3}}}{2 - 2^{\frac{1}{3}}})$$

is of order $2n + 2$.

We say the operator $s(c_1\tau)s(c_2\tau)s(c_1\tau)$ is constructed from the operators $s(c_i\tau)(i = 1, 2, 3)$ by multiplicative extrapolation method because the sum of the three composition coefficients c_1, c_2, c_3 is 1, and the coefficient c_2 is negative.

Yoshida[2] get the same result for symplectic explicit operators used to solve separable Hamiltonian systems. The result we get here is based on Yoshida's work and can be applied to non-Hamiltonian systems and non-symplectic integrators.

An example: The trapezoid method is self-adjoint and of order 2, then

$$\begin{cases} y_1 = y_0 + \dfrac{1}{2(2 - 2^{\frac{1}{3}})}\tau(f(y_0) + f(y_1)) \\ y_2 = y_1 + \dfrac{-2^{\frac{1}{3}}}{2(2 - 2^{\frac{1}{3}})}\tau(f(y_1) + f(y_2)) \\ y_3 = y_2 + \dfrac{1}{2(2 - 2^{\frac{1}{3}})}\tau(f(y_2) + f(y_3)) \end{cases} \tag{14}$$

is a scheme of order 4.

At last we point out that the Gauss-Legendre methods are self-adjoint, and they are also multi-stage, one-step methods, so the multiplicative extrapolation in this paper can also be applied to them as to trapezoid method in the above example.

References

[1] Feng Kang, The calculus of formal power series for diffeomorphisms and vector fields, Preprint, Acad. Sin. Comp. Ctr. 1991.

[2] Haruo Yoshida, Construction of higher order symplectic integrators, *Physics Letters A*, 150 (5-7), (1990), 262-269.

[3] E.Hairer S.P.Norsett and G.wanner, Solving Ordinary Differential Equations, non-stiff problems I, Springer-Verlag 1987, Chapter 2(§.7.8,12,13)

[4] Stanly Steinberg, Lie series and nonlinear ordinary differential equations. *Journal of Mathematical Analysis and Applications*, **101** : 1 (1984), 39-63.

[5] V.I.Arnold, Mathematical Methods of Classical Mechanics.Spinger- Verlag, 1978, 208-212.

[6] Alex J.Dragt and John M.Finn, Lie series and invariant functions for analytic symplectic ways. *Journal of Mathematical Physics*, **17** : 12 (1976), 2215.

[7] Feng Kang and Qin Meng-Zhao, Hamiltonian algorithms for hamiltonian systems and a comparative numerical study, *Computer Physics Communications*, 65 (1991), 173-187.

[8] F.Neri, Lie algebras and canonical integration, Department of Physics , University of Maryland, College Park, MD.20742.