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Note

Time-Reversal Invariance and Linear Multistep Methods for Integrating Dynamical Systems

It is shown that, if a linear multistep method for integrating a dynamical system is convergent and is invariant under time-reversal transformation, the multistep formula must be symmetric and the roots of its characteristic polynomial must all lie on the unit circle.

In the numerical integration of a dynamical system it is a useful check on the accuracy to confirm various invariance principles. For a system with a conservative force the energy conservation is widely used. When a system is time reversal (T.R.) invariant, comparison of physical quantities in the direct path with those in the reverse one is useful. Also, in the case of a solution of a Hamiltonian system regarded as a mapping in the phase space, invariances of the 2D area element, the whole volume (Liouville's theorem), and the Poincaré integral will be useful.

Recently we applied the T.R. principle to a study of many-body self-gravitating systems with spherical symmetry, and showed that a violent relaxation is indeed time reversible under suitable conditions [1]. There the fourth-order Runge–Kutta formula was used. However, this formula itself is not invariant under T.R. when regarded as a transformation over one step, and it is more desirable, if not absolutely necessary, to use a multistep formula which is invariant under T.R. when regarded as a transformation over multisteps. It is the purpose of this note to find conditions which the multistep formula must satisfy for T. R. invariance. Various invariances in the phase space will be discussed in a separate paper.

We consider a dynamical system whose coordinates and velocities are $x^1, x^2, \dots, x^f$ and $v^1, v^2, \dots, v^f$, respectively. The equations of motion are assumed to be written in the form

$$\frac{dx^1}{dt} = v^i, \frac{dv^i}{dt} = f^i(x^j), \qquad i = 1, \dots, f.$$

These equations are clearly invariant under T.R.

We denote values of x^i and v^i at a discrete time t_n by x_n^i and v_n^i. The times t_n are equidistant with the stepsize h. Let us write a general linear multistep formula to compute $\{x_{n+k}^i, v_{n+k}^i\}$ from a given set of $\{x_n^i, v_n^i\}$, $\{x_{n+1}^i, v_{n+1}^i\}, \dots, \{x_{n+k-1}^i, v_{n+k-1}^i\}$ in the form

$$\begin{aligned} \rho(E)\, x_n^i &= h\sigma(E)\, v_n^i, \\ \rho(E)\, v_n^i &= h\sigma(E) f_n^i, \end{aligned} \qquad i = 1, \dots, f, \tag{1}$$

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where E is an operator increasing the subscript n by 1, $\rho(\zeta)=\sum_{s=0}^{k}\alpha_s\zeta^s$, $(\alpha_k\neq 0)$, $\sigma(\zeta)=\sum_{s=0}^{k}\beta_s\zeta^s$, $(|\alpha_0|+|\beta_0|\neq 0)$, and $f_n^i=f^i(x_n^j)$. The convergent condition for formula (1) is that it is both consistent and zero-stable (see Henrici [2, Chap. 5] and Lambert [3]). The consistency means

$$\rho(1)=0, \tag{2}$$

$$\rho'(1)=\sigma(1). \tag{3}$$

The zero-stability requires that the roots of the polynomial $\rho(\zeta)$ all lie within or on the unit circle, those on the unit circle being simple. In particular,

$$\rho'(1)\neq 0. \tag{4}$$

Now we shall find the conditions for T.R. invariance. If Eq. (1) is regarded as a transformation from a given set of $\{x_n^i, v_n^i\},\ldots,\{x_{n+k-1}^i, v_{n+k-1}^i\}$ to $\{x_{n+k}^i, v_{n+k}^i\}$, then the invariance requires that the inverse transformation from a set of $\{x_{n+k}^i, -v_{n+k}^i\},\ldots,$ $\{x_{n+1}^i, -v_{n+1}^i\}$ to $\{x_n^i, -v_n^i\}$ have the same form as Eq. (1), and can be obtained directly from Eq. (1). This is realized if $\alpha_0\neq 0$ and

$$\alpha_k\alpha_s=\alpha_0\alpha_{k-s}, \qquad s=1,\ldots,k, \tag{5}$$

$$\alpha_k\beta_s=-\alpha_0\beta_{k-s}, \qquad s=0,1,\ldots,k, \tag{6}$$

or, in terms of polynomials,

$$\alpha_k\rho(\zeta^{-1})=\alpha_0\zeta^{-k}\rho(\zeta), \tag{7}$$

$$\alpha_k\sigma(\zeta^{-1})=-\alpha_0\zeta^{-k}\sigma(\zeta). \tag{8}$$

Note that here we considered the k sets of transformed variables to be independent, because we require that the method must not depend on any speciality of the system. From Eq. (5) for $s=k$, we have $\alpha_k=\pm\alpha_0$. But the case $\alpha_k=\alpha_0$ is excluded as is shown in the following theorem.

THEOREM. *If the method* (1) *is convergent and invariant under time reversal, then*

$$\alpha_s=-\alpha_{k-s}, \qquad s=0,1,\ldots,[k/2], \tag{5$'$}$$

$$\beta_s=\beta_{k-s}, \qquad s=0,1,\ldots,[k/2], \tag{6$'$}$$

or, in terms of polynomials,

$$\rho(\zeta^{-1})=-\zeta^{-k}\rho(\zeta), \tag{7$'$}$$

$$\sigma(\zeta^{-1})=\zeta^{-k}\sigma(\zeta). \tag{8$'$}$$

Therefore, all roots of $\rho(\zeta)$ *lie on the unit circle.*

Proof. Differentiating Eq. (7) and putting $\zeta = 1$, we get $(\alpha_0 + \alpha_k)\rho'(1) = 0$. Equation (4) gives $\alpha_0 + \alpha_k = 0$. The other Eqs. (5′)–(8′) follow immediately. If there is a root ζ_1 within the unit circle, Eq. (7′) implies ζ_1^{-1} is another root outside the unit circle. This contradicts the zero-stability condition. This point can be understood intuitively, as pointed out by R. H. Miller. If there is a root ζ_1 with $|\zeta_1| < 1$ in Eq. $\rho(\zeta) = 0$, the error in the solution computed by Eq. (1) contains a term ζ_1^n, where n is the number of steps. This term approaches zero with $n \to \infty$. In the reverse path the characteristic polynomial is given by $\zeta^k \rho(\zeta^{-1})$. Hence the error in the numerical solution contains a term ζ_1^{-1}, which diverges to ∞ as $n \to \infty$. This is not allowed for the T.R. invariant system.

In the case of an even k, Henrici [2, p. 285], called the conditions (5′) and (6′) symmetric and showed that the "order" of the formula of Eq. (1) is $k + 2$, which is the highest for a given k (see p. 231).

COROLLARY. *The only method which satisfies the above assumptions in the Theorem and which is strongly stable in the sense described by Lambert* [3, p. 41], *is the trapezoidal rule.*

Proof. This strong stability means that all roots of $\rho(\zeta)$ except $\zeta = 1$ lie in the unit circle. Then it is clear $k = 1$, and Eqs. (2), (3), and (6′) restrict the case to be the trapezoidal rule.

In order to get a time-reversal-invariant, strongly-stable and highly-accurate integration method, we must examine other methods more sophisticated than the linear multistep method.

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REFERENCES

1. KO AIZU, *Prog. Theor. Phys.* **70**, No. 1 (1983), 106–118.
2. P. HENRICI, "Discrete Variable Methods in Ordinary Differential Equations," Wiley, New York, 1962.
3. J. D. LAMBERT, *in* "Modern Numerical Methods for Ordinary Differential Equations" (G. Hall and J. M. Watt, Eds.), Chap. 2, Oxford Univ. Press (Clarendon), Oxford, 1976.

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