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Note

Canonical Transformation Invariance and Linear Multistep Formula for Integration of Hamiltonian Systems

It is shown that, if a linear multistep formula applied to numerical integration of hamiltonian systems is also to be a canonical transformation, it must essentially be a two-term formula. © 1985 Academic Press, Inc.

In numerical integration of dynamical systems it is useful to confirm various invariance properties. Although it is not always necessary that an integration formula itself has invariance properties, it will be interesting to find conditions that the formula must satisfy in order to have these properties. In a recent note [1] we found conditions under which a linear multistep formula is invariant under time reversal transformation. In this note we shall examine under what conditions a linear multistep formula, when applied to integration of hamiltonian systems, is to be a canonical transformation.

A hamiltonian system is described by canonical coordinates $q^1,..., q^f$ and conjugate momenta $p^1,..., p^f$. It is convenient to regard these variables as a vector $y = \{y^\mu\} = \{q^i, p^i\}$ in the $2f$-dimensional phase space. With a hamiltonian function $H(y) = H(q, p)$ the equations of motion are written in the form

$$dy/dt = f(y), \tag{1}$$

$$f(y) = \{f^\mu(y)\} = \{\partial H/\partial p^i, \ -\partial H/\partial q^i\}. \tag{2}$$

Let a solution of these equations be $y(t) = y(t; y_0, t_0)$, where y_0 is an initial value of y at a time t_0. This solution can be regarded as a transformation from y_0 to $y(t)$. It is called a canonical transformation if it satisfies the following condition: Let two infinitesimal variations of y_0 be δy_0 and $\delta' y_0$, and their time developments be δy and $\delta' y$, respectively. Then a normalized skew-symmetric bilinear form made with δy and $\delta' y$

$$[\delta y \, \delta' y] = \sum_{i=1}^{f} (\delta q^i \, \delta' p^i - \delta p^i \, \delta' q^i) = (\delta y)^{\mathrm{T}} J (\delta' y) \tag{3}$$

must be constant in time. Here the superscript T means the transposition and J is a $2f \times 2f$ matrix $J = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$.

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The equations for δy and $\delta' y$ are derived from Eq. (1) as

$$d(\delta y)/dt = F\,\delta y \qquad \text{and} \qquad d(\delta' y)/dt = F\,\delta' y,$$

where F is a $2f \times 2f$ matrix:

$$(F^\mu_\nu) = (\partial f^\mu/\partial y^\nu) = \begin{pmatrix} \partial^2 H/\partial p^i\,\partial q^j & \partial^2 H/\partial p^i\,\partial p^j \\ -\partial^2 H/\partial q^i\,\partial q^j & -\partial^2 H/\partial q^i\,\partial p^j \end{pmatrix}. \tag{4}$$

Here the superscripts i and j indicate rows and columns, respectively, of four $f \times f$ matrices. Then it can easily be shown that the expression (3) is constant in time, since

$$F^{\mathrm{T}} J + JF = 0. \tag{5}$$

Now we shall show that if a linear one-step formula applied to a hamiltonian system is regarded as a transformation, the formula is a canonical transformation. Let the formula to compute y_{n+1} from y_n be written in the form

$$y_{n+1} - y_n = h\{\beta f_{n+1} + (1-\beta) f_n\}, \tag{6}$$

where h is a step size, y_n the value of y at $t = t_0 + nh$, and y_{n+1} has a similar meaning, $f_n = f(y_n)$ and $f_{n+1} = f(y_{n+1})$, and β is a constant with $0 \leqslant \beta \leqslant 1$. For infinitesimal variations we have

$$\delta y_{n+1} - \delta y_n = h\{\beta F_{n+1}\,\delta y_{n+1} + (1-\beta)\,F_n\,\delta y_n\},$$

where F_n is a matrix F given by Eq. (4) with $y = y_n$. From this equation we find δy_{n+1} to the first order of h

$$\delta y_{n+1} = [1 + h\{\beta F_{n+1} + (1-\beta)\,F_n\}]\,\delta y_n.$$

Hence,

$$\begin{aligned} [\delta y_{n+1}\,\delta' y_{n+1}] &= (\delta y_n)^{\mathrm{T}} [J + h\{\beta(F^{\mathrm{T}}_{n+1} J + JF_{n+1}) \\ &\quad + (1-\beta)(F^{\mathrm{T}}_n J + JF_n)\}]\,\delta' y_n \\ &= [\delta y_n\,\delta' y_n]. \end{aligned}$$

In the last step Eq. (5) is used. We note that this proof is a discrete version of the proof for constancy in time of the expression (3).

Next we consider the case of a general linear multistep formula to compute y_{n+k} from $y_n, \ldots, y_{n+k-1}$. The formula is written in the form

$$\rho(E)\,y_n = \sigma(E) f_n, \tag{7}$$

where E is an operator increasing the subscript n by one, $\rho(\zeta) = \sum_{s=0}^k \alpha_s \zeta^s$ ($\alpha_k = 1$), and $\sigma(\zeta) = \sum_{s=0}^k \beta_s \zeta^s$ ($|\alpha_0| + |\beta_0| \neq 0$). The convergence condition for formula (7) is that it is both consistent and zero-stable (see Henrici [2, Chap. 5] and Lambert [3]). The consistency means

$$\rho(1)=0, \tag{8}$$

$$\rho'(1)=\sigma(1). \tag{9}$$

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

$$\rho'(\zeta_1)\neq 0 \qquad \text{for} \quad |\zeta_1|=1. \tag{10}$$

Now we shall find under what conditions this linear multistep formula is to be a canonical transformation. From Eq. (7) we get a multistep formula for infinitesimal variations δy

$$\rho(E)\,\delta y_n = h\sigma(E)\,F_n\,\delta y_n.$$

From this equation we get δy_{n+k} to the first order of h

$$\delta y_{n+k}=\sum{}'\,\{-\alpha_s+h(-\alpha_s\beta_k F_{n+k}+\beta_s F_{n+s})\}\,\delta y_{n+s},$$

where $\sum'$ means summation over s from 0 to $k-1$. We assume that transformations from δy_n to δy_{n+1},..., from δy_{n+k-2} to δy_{n+k-1} are all canonical transformations. Then all normalized skew-symmetric bilinear forms for δy_n,..., δy_{n+k-1} are equal to each other, and are put equal to I:

$$[\delta y_n\,\delta' y_n]=\cdots=[\delta y_{n+k-1}\,\delta'_{n+k-1}]=I. \tag{11}$$

Now we calculate $[\delta y_{n+k}\,\delta' y_{n+k}]$ and put it equal to I. After some algebra we obtain

$$\begin{aligned} I=\left(\sum{}'\,\alpha_s^2\right)I+&\sum_{s\neq s'}{}'\sum{}'\alpha_s\alpha_{s'}(\delta y_{n+s})^{\mathrm{T}}J\delta' y_{n+s'}\\ &-h\sum_{s\neq s'}{}'\sum{}'(\delta y_{n+s})^{\mathrm{T}}(\alpha_{s'}\beta_s M_{n+s}-\alpha_s\beta_{s'}M_{n+s'})\,\delta' y_{n+s'}, \end{aligned} \tag{12}$$

where the $2f\times 2f$ matrix M_{n+s} is given by

$$M_{n+s}=F^{\mathrm{T}}_{n+s}J=\begin{pmatrix}\partial^2H/\partial q^i\,\partial q^j & \partial^2H/\partial q^i\,\partial p^j\\ \partial^2H/\partial p^i\,\partial q^j & \partial^2H/\partial p^i\,\partial p^j\end{pmatrix}_{y=y_{n+s}}$$

Here the superscripts i and j have the same meaning as in Eq. (4). Equation (12) must hold to every order of h. Also it must hold for any dynamical system. In particular, for a free particle system the matrix M reduces to $M'=\left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)$, where we assume the mass of each particle is one. Then, we have

$$I=\left(\sum{}' \alpha_s^2\right) I+\sum_{s\neq s'}{}'\sum{}' \alpha_s\alpha_{s'}(\delta y_{n+s})^{\mathrm{T}} J\delta' y_{n+s'},$$

$$\sum_{s\neq s'}{}'\sum{}' (\alpha_{s'}\beta_s-\alpha_s\beta_{s'})(\delta y_{n+s})^{\mathrm{T}} M'\,\delta' y_{n+s'}=0.$$

These equations must hold for any values of δy_{n+s} and $\delta' y_{n+s'}$ which satisfy Eq. (11). Using Lagrange's method of undetermined multipliers, we obtain

$$\sum{}' \alpha_s^2=1, \tag{13}$$

$$\alpha_s\alpha_{s'}=0 \qquad \text{for} \quad 0\leqslant s<s'<k, \tag{14}$$

$$\alpha_{s'}\beta_s=\alpha_s\beta_{s'} \qquad \text{for} \quad 0\leqslant s<s'<k. \tag{15}$$

As Eq. (8) means $1+\sum' \alpha_s=0$, there is at least one $\alpha_l\neq 0$ for $s=l$. As Eq. (14) implies $\alpha_s=0$ for $s\neq l$, $\alpha_l=-1$ is the only α_s which is not zero. These α_s's satisfy Eq. (13). Equation (15) implies $\beta_s=0$ except $s=l$. Thus the polynomial $\rho(\zeta)$ has only two, and the polynomial $\sigma(\zeta)$ has at most two terms different from zero:

$$\rho(\zeta)=\zeta^k-\zeta^l, \tag{16}$$

$$\sigma(\zeta)=\beta_k\zeta^k+\beta_l\zeta^l, \tag{17}$$

and Eq. (9) gives

$$\beta_k+\beta_l=k-l.$$

Also Eq. (16) satisfies Eq. (10). Hence we get the following theorem.

THEOREM. *If a linear multistep formula Eq.* (7) *is convergent and is further a canonical transformation, it must be a two-term formula as Eq.* (16) *and Eq.* (17).

Finally, we shall make three remarks:

First, as for higher-order invariant forms such as the $2f$-dimensional volume element in the phase space, we note that invariance of these forms can be derived from that of the normalized skew-symmetric bilinear form Eq. (3) (see, for example, Weyl [4, Chap. 6]).

Second, if the formula Eq. (7) is convergent, is a canonical transformation, and is further invariant under time reversal transformation, it must be a one-step formula as given by Eq. (6) (Aizu [1]).

Third, in practical computations a two-term formula may not give highly accurate results. If a non-invariant formula in current use gives good results to invariant quantities, we must examine why such a non-invariant formula gives good results.

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References

1. K. Aizu, *J. Comput. Phys.* **55** (1984), 154–156.
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), London/New York, 1976.
4. H. Weyl, "Classical Groups," Princeton Univ. Press, Princeton, N.J., 1946.

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