VOLUME PRESERVING RK METHODS FOR LINEAR SYSTEMS*

QIN MENGZHAO (秦孟兆) LI HONGWEI (李洪伟)

(*LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, the Academy of Mathematics and Systems Sciences, the Chinese Academy of Sciences, Beijing* 100080, *China*)

Abstract

In this article, we analyze and study under what conditions a source-free system has volume-preserving RK schemes. For linear systems, we give a comparatively thorough discussion about RK methods to be phase volume preserving integrators. We also analyze the relationship between volume-preserving integrators and symplectic integrators.

Key words. Runge-Kutta method, volume preserving method, symplectic method

1. Introduction

In recent years, there has been a great interest in constructing numerical integration schemes for ODEs in such a way that some qualitative geometrical properties of the solution of the ODEs are exactly preserved. Ruth[1] and Feng Kang[2,3] has proposed symplectic algorithms for Hamiltonian systems, and since then structures-preserving methods for dynamical systems have been systematically developed[4−7]. The symplectic algorithms for Hamiltonian systems, the volume-preserving integrators for source-free systems and the contact algorithms for contact systems are all structure-preserving methods. These methods are often referred to as geometric algorithms as they have obvious geometrical meaning.

A linear source-free system of ordinary differential equations generally takes the form

$$\dot{y} = My \tag{1}$$

where M is an $n \times n$ square matrix with trace (M)=0. If det $(M) \equiv 0$, the system can degrade to a lower stage case, so we assume det $(M) \neq 0$. And now we assume that M is a constant matrix. An RK method, says (A, b, c), applied to system (1) takes the form

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij}MY_j, \qquad y_{n+1} = y_n + h\sum_{j=1}^{s} b_jMY_j, \tag{2}$$

where $A = (a_{ij})_{s\times s}$, $b = (b_1, b_2, \cdots, b_s)^T$.

Lemma 1. Let $sl(n)$ denote the set of all $n \times n$ real matrices trace equal to zero and $SL(n)$ the set of all $n \times n$ real matrices determinant equal to one. Then for any real analytic function $\phi(z)$ defined in a neighborhood of z=0 in c satisfying the conditions: 1)

Received January 25, 1999. Revised April 28, 1999.

* This work is supported by State Key Project "Large scale scientific and engineering computing".

$\phi(0) = 1$ and 2) $\phi'(0) = 1$, we have that $\phi\big(sl(n)\big) \subset SL(n)$ for some $n \geq 3$ if and only if $\phi(z) = \exp(z)$.

The proof of this lemma can be found in [6]. This lemma says that there are no consistent analytic approximations to the exponential function sending at the same time $sl(n)$ into $SL(n)$ other than the exponential itself. It shows that it is impossible to construct volume-preserving algorithms analytically depending on some source-free vector fields. Thus all the conventional methods including the well-known RK methods, *linear multistep methods* are non-volume-preserving. In that article, the authors have explored new ways to construct volume-preserving algorithms. By means of the essentially Hamiltonian decompositions of source-free vector fields and the symplectic difference schemes for 2-dimensional Hamiltonian systems they showed a general way to construct volume-preserving difference schemes for source-free systems. But in this paper, we just talk about RK method, and according to Lemma 1, we can't find a general volume-preserving RK method. So our hope is to distinguish M into different classes and find out whether there are volume-preserving RK methods in any class.

Now we need the following notations

$$\begin{aligned} &\overline{A} = A \otimes E_n, \qquad \overline{M} = \operatorname{diag}(M, M, \cdots, M) = E_s \bigotimes M, \qquad \bar{b} = b^T \otimes E_n, \\ &Y = (Y_1, Y_2, \cdots, Y_s)^T \qquad \overline{y}_n = (y_n, y_n, \cdots, y_n)^T, \qquad \bar{e} = e \otimes e_n, \end{aligned} \tag{3}$$

where E_n is an n-stage identical matrix, $e = (1, 1, \cdots, 1)^T$ is a n-dimensioned vector. For RK methods to be volume preserving, we have an equivalent condition: $\det \frac{\partial(y_{n+1})}{\partial(y_n)} \equiv 1$. So we need to calculate the matrix $\frac{\partial(y_{n+1})}{\partial(y_n)}$. In matrix notations, RK method (2) reads

$$y_{n+1} = y_n + hM\bar{b}Y, \qquad Y = (I - h\overline{M}\,\overline{A})^{-1}\overline{y_n}. \tag{4}$$

So,

$$y_{n+1} = [E_n + hM\bar{b}(I - h\overline{M}\overline{A})^{-1}\bar{e}]\, y_n \Longrightarrow \frac{\partial(y_{n+1})}{\partial(y_n)} = E_n + hM\bar{b}(I - h\overline{M}\,\overline{A})^{-1}\bar{e}. \tag{5}$$

Lemma 2. Let A and D be non-degenerate $m \times m$ and $n \times n$ matrices respectively, B an $m \times n$ and C an $n \times m$ matrix. Then

$$\det(A)\,\det(D + CA^{-1}B) = \det(D)\det(A + BD^{-1}C). \tag{6}$$

The proof can be found in any textbook on linear algebra.

By the lemma2, it's easy to get from (5)

$$\det\Big(\frac{\partial(y_{n+1})}{\partial(y_n)}\Big) = \frac{\det(I - h\overline{M}\,\overline{A} - \bar{e}M\bar{b})}{\det(I - h\overline{M}\,\overline{A})}.$$

Additionally, we define the notations

$$A^- = (a_{ij}^-), \qquad a_{ij}^- = a_{ij} - b_j, \qquad N = A \otimes M, \qquad N^- = A^- \otimes M. \tag{7}$$

In these notations (5) reads

$$\det\Big(\frac{\partial(y_{n+1})}{\partial(y_n)}\Big) = \frac{\det(I - hN^-)}{\det(I - hN)}. \tag{8}$$

Now letting (8) be identical to one, we arrive at the criterion for RK method (2) to be volume-preserving schemes:

$$\det(\lambda I - \mathrm{N}^-) = \det(\lambda \mathrm{I} - \mathrm{N}), \qquad \forall \lambda \in \mathrm{R}. \tag{9}$$

Theorem 2. If the dimension of M is odd, then all the RK methods based on high order quadrature formulas such as Gauss, Radau, Labatto are not volume preserving.

Proof. Notice $N = A \otimes M$, $N^- = A^- \otimes M$. If the method is volume preserving, then

$$\begin{aligned}\det(N) = \det(N^-) &\Longleftrightarrow \det(A \otimes M) = \det(A^- \otimes M)\\ &\Longleftrightarrow (\det A)^n(\det(M))^s = (\det(A^-))^n(\det M)^s\\ &\Longleftrightarrow (\det A)^n = (\det(A^-))^n\\ &\Longleftrightarrow \det(A) = \det(A^-).\end{aligned} \tag{10}$$

Now, we need the W-transformation proposed by Hairer and Wanner[8]. They introduced a generalized square matrix W defined by

$$W = \big(p_0(c), p_1(c), \cdots, p_{s-1}(c)\big), \tag{11}$$

where the normalized shifted Legendre polynomials are defined by

$$p_k(x) = \sqrt{2k+1}\sum_{i=0}^{k}(-1)^{k+i}C_k^iC_{k+l}^ix^i, \qquad k = 0, 1, \cdots. \tag{12}$$

For Gauss method, letting $X = W^{-1}AW$, then

$$X = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & -\xi_2 & & \\ & \xi_2 & \ddots & \ddots & \\ & & \ddots & \ddots & -\xi_{s-1} \\ & & & \xi_{s-1} & 0 \end{pmatrix}, \tag{13}$$

where $\xi_k = \frac{1}{2\sqrt{4k^2-1}}$, $k = 0, 1, \cdots, s-1$.

However, letting $X^- = W^{-1}A^-W$, then

$$X^- = \begin{pmatrix} -\frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & -\xi_2 & & \\ & \xi_2 & \ddots & \ddots & \\ & & \ddots & \ddots & -\xi_{s-1} \\ & & & \xi_{s-1} & 0 \end{pmatrix}. \tag{14}$$

It's easy to verify that $\det(X) \neq \det(X^-) \Longrightarrow \det(A) \neq \det(A^-)$. So, Gauss method is not volume preserving.

By using the following table, the remaining part of the proof is similar.

Method	$X_{s,s-1}$	$X_{s-1,s}$	$X_{s,s}$
Lobatt ⅢA	$\xi_{s-1}u$	0	0
Lobatt ⅢB	0	$-\xi_{s-1}u$	0
lobatt ⅢC	$\xi_{s-1}u$	$-\xi_{s-1}u$	$u^2/2(2s-1)$
Lobatt ⅢS	$\xi_{s-1}u\sigma$	$-\xi_{s-1}u\sigma$	0
Radau IA	ξ_{s-1}	$-\xi_{s-1}$	$1/(4s-2)$
Radau ⅡA	ξ_{s-1}	$-\xi_{s-1}$	$1/(4s-2)$
Radau IB	ξ_{s-1}	$-\xi_{s-1}$	0
Radau Ⅱ B	ξ_{s-1}	$-\xi_{s-1}$	0

where $u, \sigma \in R$, $u\sigma \neq 0$.

Theorem 3. If the dimension of M is even,then the RK methods based on high order quadrature formulas such as Lobatt Ⅲ A, Lobatt Ⅲ B, Lobatt Ⅲ S, Radau I B and Radau Ⅱ B are volume preserving if and only if

$$\lambda(M) = (\lambda_1, \lambda_2, \cdots, \lambda_{\frac{n}{2}}, -\lambda_1, -\lambda_2, -\cdots, -\lambda_{\frac{n}{2}}). \tag{15}$$

Proof. Assume A and B are $n \times n$ and $m \times m$ matrices respectively, and their eigenvalues are respectively $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ and $\{\mu_1, \mu_2, \cdots, \mu_m\}$. Then according to the property of Kronecker product, we have $\lambda(A \otimes B) = \{\lambda_i \mu_j,\ i = 1, \cdots, n,\ j = 1, \cdots, m\}$. For RK methods to be volume-preserve schemes, according to (9), N and N^- must have same eigenvalues, that's to say, $A \otimes M$ and $A^- \otimes M$ must have the same eigenvalues. By using the property of Kronecker product above, the proof is not difficult. For example, for Gauss method, $\lambda(A) = \lambda(X)$, $\lambda(A^-) = \lambda(X^-)$, and on the other hand, it's obvious that $\lambda(X) = -\lambda(X^-)$; so according to the properties of Kronecker product, we can easily verify that $A \otimes M$ and $A^- \otimes M$ have the same eigenvalues.

Notation 1. If (1) is a Hamiltonian system, that's to say, $M = J^{-1}S$, where $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, $S' = S$ is an $n \times n$ invertible matrix, then $\lambda(M) = (\lambda_1, \lambda_2, \cdots, \lambda_{\frac{n}{2}}, -\lambda_1, -\lambda_2, -\cdots, -\lambda_{\frac{n}{2}})$. So the RK methods based on high order quadrature formulas such as Gauss, Lobatt Ⅲ A, Lobatt Ⅲ B, Lobatt Ⅲ S, Radau I B, Radau Ⅱ B are volume preserving. The theorem says that for the methods to preserve volume, the system, in some sense, must be similar to a Hamiltonian system. And if the matrix M is similar to an infinitesimally symplectic matrix, i.e., there is an invertible matrix P, subjected to $P^{-1}MP = JS$, $S^T = S$, then we can transform the system to a Hamiltonian system by a coordinate transformation. In this situation, the volume preserving RK methods and the symplectic RK methods almost have no differences, that is to say, if P is a symplectic matrix then volume-preserving RK methods are equivalent to symplectic RK methods; and in the other case, they can be transformed to each other by a linear transformation.

Notation 2. It should be pointed put that in the discussion of the conditions under which an RK method will be volume-preserving we assume that the system can't reduce to a lower stage case. That is to say, $\det(M) \neq 0$. But in practice some systems are naturally reducible. For example,

$$\dot{x} = cy - bz, \qquad \dot{y} = az - cx, \qquad \dot{z} = bx - ay, \qquad a, b, c \in \mathrm{R}.$$

For this system, the centered Euler method is volume-preserving. In fact, Labott Ⅲ A, Labott Ⅲ B, Labott Ⅲ S, Radau I B, Radau Ⅱ B are also volume-preserving. If we examine the process in Section Ⅱ, it's easy to get the following theorem.

Theorem 2*. If the dimension of M is odd, then the RK methods based on high order quadrature formulas such as Lobatt Ⅲ A, Lobatt Ⅲ B, Lobatt Ⅲ S, Radau I B and Radau Ⅱ B are volume preserving if and only if

$$\lambda(M) = (\lambda_1, \lambda_2, \cdots, \lambda_{\frac{n}{2}}, 0, -\lambda_1, -\lambda_2, -\cdots, -\lambda_{\frac{n}{2}}).$$

We also find that in Theorem 3, $\det(M) \neq 0$ is not necessary.

As for nonlinear systems, we can't give some satisfactory results. A nonlinear system

$$\dot{y} = f(y), \qquad t \in \mathrm{R}, \ \ \mathrm{y} \in \mathrm{R}^n$$

is said to be source free if $\operatorname{div}(f) = \sum_{i=1}^{n} \frac{\partial f_i}{\partial y_i}(y) = 0$. Such systems preserve the phase volume on the phase space R^n. For these systems, we only point out that the Euler central scheme is volume preserving if and only if the Jacobian $\frac{\partial f_i}{\partial y_i} = M$ is, in some sense, similar to an infinitesimally symplectic matrix. That is to say, the eigenvalues of M can be specified as $\lambda(M) = (\lambda_1, \lambda_2, \cdots, \lambda_{\frac{n}{2}}, -\lambda_1, -\lambda_2, \cdots, -\lambda_{\frac{n}{2}})$, or $\lambda(M) = e(\lambda_1, \lambda_2, \cdots, \lambda_{\frac{n}{2}}, 0, -\lambda_1, -\lambda_2, \cdots, -\lambda_{\frac{n}{2}})$[4].

References

1 R.D. Ruth. A Canonical Integration Technique. *IEEE Trans. On Nucl. Sci.*, NS-30, 1983, 2669–2671

2 Feng Kang. On Difference Scheme and Symplectic Geometry. Proceeding of the 1984 Beijing, Symposium on Differential Geometry and Differential Equations-Computation of Partial Differential Equations, ed. Feng Kang. Science press, Beijing, 1985, 42–58

3 Feng Kang, Qin Mengzhao. The Symplectic Methods for the Computation of Hamiltonian Equations. Lecture Notes in Mathematics 1297. Springer-Verlag, Berlin, 1987, 1–37

4 Qin MengZhao, Zhu WJ Volume Preserving Schemes and Numerical Experiments. *Computers Math. Applic.*, 1993, 26(4): 33–42

5 Yuri B. Suris. Partitioned Runge-Kutta Methods as Phase Volume Preserving Integrators. *Physics Letters* (Series A), 1996, 220, 63–69

6 Feng Kang, Z.J. Shang. Volume-preserving Algorithms For Source-free Dynamical Systems. *Numerisch Math.*, 1995, 71: 451–463

7 R.I. McLachlan, G.R.W. Quispel, G.S. Turner. Numerical Integrations that Preserve Symmetrics and Reversing Symmetrres. *SIAM J. Numer. Anal.*, 1998, 35 (2): 586–599

8 E. Hairer, S.P. Nϕrett, G. Wanner. Solving Ordinary Differential Equations I: Nonstiff Problems. Springer, Berlin, 1992

9 Feng Kang. Symplectic, Contact and Volume-preserving Algorithms. Proc. 1-st China-Japan Conf. on Numer. Math., Beijing, 1992, World Scientific, Singapore, 1993

10 Sun Geng. Construction of High Order Symplectic PRK Methods. *Journal of Computational Mathematics*, 1995, 13(1): 40–50