ORTHOSYMPLECTIC INTEGRATION OF LINEAR HAMILTONIAN SYSTEMS

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Abstract. The authors describe a continuous, orthogonal and symplectic factorization procedure for integrating unstable linear Hamiltonian systems. The method relies on the development of an orthogonal, symplectic change of variables to block triangular Hamiltonian form. Integration is thus carried out within the class of linear Hamiltonian systems. Use of an appropriate timestepping strategy ensures that the symplectic pairing of eigenvalues is automatically preserved. For long-term integrations, as are needed in the calculation of Lyapunov exponents, the favorable qualitative properties of such a symplectic framework can be expected to yield improved estimates. The method is illustrated and compared with other techniques in numerical experiments on the Hénon-Heiles and spatially discretized Sine-Gordon equations.

1. Introduction

Accurate computation of the fundamental matrix solution is essential for the numerical treatment of boundary value problems [1] and for the determination of the Lyapunov exponents of a nonlinear system along a sampling trajectory [10], [11], [14], [22]. When the linearized system is unstable, the naive approach of integrating the identity matrix forward in time fails due to the eventual dominance of components in the unstable directions. The task is better accomplished by applying an appropriate change of variables to reduce the problem to one which can be easily solved by quadrature. It is well known (see [12]) that for general bounded continuous linear system a time dependent orthogonal transformation can be found to bring the problem to upper triangular form. Orthogonal transformations are desirable because they are well conditioned, easy to invert, and preserve the trace of the linear system. The use of numerical techniques that preserve orthogonality has been investigated (see [9]) for general linear systems, but not in the context of Hamiltonian systems.

In this paper, we show how continuous orthogonal-symplectic (*orthosymplectic*) transformations can be used to bring linear Hamiltonian systems to a block triangular Hamiltonian form. By using an appropriate discretization scheme, the well-known double-pairing of the spectrum of the solution matrix [20] is then automatically preserved and both stable and unstable directions are resolved during the

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integration. Using this approach, computed Lyapunov exponents occur in exact plus/minus pairs, i.e. in pairs of exponents that sum to zero. Recent results on symplectic methods (for a survey, see e.g. [7]) have indicated that preserving the symplectic structure leads to improved numerical behavior in long-term simulations. For example, the approximate flow map of a symplectic discretization method corresponds closely to the exact flow of a nearby Hamiltonian system (see [16] for a constructive formulation of this result for several classes of symplectic schemes); a consequence is that one generally observes better preservation of the Hamiltonian in symplectic computations over very long time intervals than one expects from nonsymplectic schemes. In [25], a symplectic numerical scheme was used to integrate displacement vectors in tandem with the trajectory; this produced improved numerical calculations of the *principal* Lyapunov exponent of the Hénon-Heiles problem over standard methods. For one degree of freedom Hamiltonian problems, Habib and Ryne [17] developed an analytical method for determining both Lyapunov exponents. This scheme, based upon an analysis of the eigenvalues of the Oseledec matrix [19], does not readily extend to a practical numerical method for general N degree of freedom systems.

This article is organized as follows. In §2, we show that the orthogonal factorizations of [9] can be derived from a constrained formulation, and we indicate how this formulation can be extended to develop orthosymplectic integrators. In §3, we derive a system of differential equations for the orthosymplectic transformation Q. We show how these equations can be reduced in dimension by using the patent symplectic structure and in such a way that the orthogonality persists as an integral invariant structure. In §4, we consider numerical methods for computing the transformation for linearization in tandem with a numerical trajectory. Finally, in §5, we compute the Lyapunov exponents of the Hénon-Heiles problem and a discrete version of the Sine-Gordon equation in the vicinity of a particular unstable orbit considered in [21]. We compare second order methods that preserve the orthosymplectic structure with a method that preserves only orthogonality and show that the symplectic approaches yield improved numerical estimates of the exponents.

2. Constrained Formulation

For $A(t) \in \mathbf{R}^{N\times N}$ a real, continuous, bounded matrix function consider the linear differential equation

$$\left\{ \begin{array}{rcl} \dot{Y}(t) & = & A(t)Y(t) \\ Y(t_0) & = & Y_0. \end{array} \right. \tag{1}$$

We consider the problem of determining the projection of the real matrix solution $Y(t) \in \mathbf{R}^{N\times N}$ onto the orthogonals. One approach is to solve the original system and then project onto the constraint $Y^tY = I$, e.g. by computing the QR decomposition of $Y(t)$. Alternatively, we can introduce the continuous factorization $Y(t) = Q(t)R(t)$, into an orthogonal matrix $Q(t)$ and upper triangular matrix

$R(t)$; following the approach of [9], this leads to a system of equations of the form

$$\dot{Q} = AQ - QB$$

where $B = \dot{R}R^{-1}$ is upper triangular. The $\frac{N(N+1)}{2}$ elements of B are then determined from the imposition of $\frac{N(N+1)}{2}$ constraints of the form $Q^tQ = I$. Ignoring the significance of R, we can view our problem as a constrained system of differential equations (a differential-algebraic system):

$$\begin{aligned} \dot{Q} &= AQ - QB \\ Q^tQ &= I \end{aligned}$$

where B consists of multipliers which enforce the constraint. This problem, which has index two in the standard terminology, can be solved by any suitable numerical integrator (see [4]). The method of [9] can be viewed as reducing this differential-algebraic system by differentiation of the constraint and elimination of the multiplier B, leaving a system of differential equations of the form $\dot{Q} = S(Q)Q$, with $S(Q)$ skew-symmetric, which automatically maintains the orthogonality as an integral invariant structure. A suitable quadratic integral-preserving scheme such as Gauss-Legendre RK discretization can then be employed to solve the unconstrained system. This method resulted in improvements in numerical behavior over standard coordinate projections in the experiments of [9, 10].

Now consider a linear Hamiltonian problem of the form

$$\left\{ \begin{aligned} \dot{Y}(t) &= JA(t)Y(t) \\ Y(t_0) &= Y_0, \end{aligned} \right. \tag{2}$$

where $A = A(t)$ is a continuous, bounded, symmetric matrix function,

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

and Y_0 is symplectic.

We could apply the orthogonal integration technique as before, but this approach would destroy the known symplectic structure of the matrix Y. Instead, in the next section we will see that both the orthogonality and the symplectic structure of Q can be preserved by means of an oblique projection onto the constraints of the form:

$$\begin{aligned} \dot{Q} &= JAQ - QJB \\ Q^tQ &= I \end{aligned}$$

where B is symmetric and of the block form

$$B = \begin{bmatrix} 0 & B_{12} \\ B_{12}^t & B_{22} \end{bmatrix}$$

with B_{12} lower triangular and B_{22} symmetric. There are thus only $\frac{N}{2}(\frac{N}{2}+1)$ free multipliers whereas there remain $N(N+1)/2$ constraints, so the equations are formally overdetermined, however it turns out that they do have an exact solution $B = B(Q)$ which is constructed explicitly in the next section.

Once B is known we are left with unconstrained equations

$$\dot{Q} = JAQ - QJB(Q)$$

This system can be rewritten (using the constraint) so as to retain the orthogonality as a first integral of the differential equations. On the other hand, for the symplectic property $Q^tJQ - J = 0$, we have (assuming that Q is orthogonal):

$$\begin{aligned} \frac{d}{dt}(Q^tJQ - J) &= Q^tJ\dot{Q} + \dot{Q}^tJQ \\ &= Q^tJ(JAQ - QJB) + (JAQ - QJB)^tJQ \\ &= -Q^tAQ - Q^tJQJB + Q^tAJ^tJQ - B^tJ^tQ^tJQ \\ &= -(Q^tJQ)JB + BJ(Q^tJQ) \end{aligned}$$

If Q^tJQ were replaced by J in the right hand side, the right hand side would vanish. This means that the equation $Q^tJQ - J = 0$ is a so-called *weak invariant* (see [13, 18]). Such invariants are not preserved by standard integration schemes. Hence if we integrate the system directly over a lengthy time interval by a method such as one of the Gauss-Legendre schemes, we would expect the symplectic structure to be destroyed over time. The key to preventing this is to introduce a partial, global parameterization of the group of orthosymplectic matrices. This can be done by substituting the orthosymplectic form

$$Q = \begin{bmatrix} Q_1 & Q_2 \\ -Q_2 & Q_1 \end{bmatrix} \tag{3}$$

with the parametrizing matrices subject to constraining relations of the form $Q_1^tQ_1 + Q_2^tQ_2 = I$ and $Q_1^tQ_2 = Q_2^tQ_1$ (see [6, 5, 8]). (This is very similar to the introduction of Euler parameters in treating rigid body motion.) All that is left is then the solution of the resulting equations of motion for Q_1 and Q_2.

3. Development of the Continuous Orthosymplectic Factorization

We will now show how to compute a continuous factorization of Y in (2) of the form

$$Y(t) = Q(t)X(t) \tag{4}$$

where Q, of form (3) is both orthogonal and symplectic, and X is a 2×2 block upper triangular matrix of the form

$$X = \begin{bmatrix} X_{11} & X_{12} \\ 0 & X_{22} \end{bmatrix} \tag{5}$$

with X_{11} upper triangular, and X_{22} lower triangular. Note that for Q of the block form (3), the conditions for Q to be symplectic and the conditions for Q to be orthogonal are the same:

$$Q_1^t Q_1 + Q_2^t Q_2 = I \quad \text{and} \quad Q_1^t Q_2 - Q_2^t Q_1 = 0.$$

With the ansatz (4), and substituting into (2), we find

$$\dot{Q}X + Q\dot{X} = JAQX.$$

Since X is symplectic it satisfies $\dot{X} = JBX$ for some symmetric matrix function B. Consequently, after multiplying on the right by X^{-1}, we obtain

$$\dot{Q} = JAQ - Q\dot{X}X^{-1} = JAQ - QJB. \tag{6}$$

After multiplying this last equation by Q^t we obtain

$$Q^t\dot{Q} = Q^t JAQ - Q^t QJB. \tag{7}$$

At this point, we have a choice: (i) we can attempt to solve for JB ignoring the orthogonality of Q, in which case we would recover that orthogonality as a first integral of (6), or (ii) we can utilize the orthogonality explicitly in the derivation of JB. We take the latter approach since it allows us to easily obtain a closed form solution for JB, however, it turns the orthogonality into a weak invariant. (Below we will show how the integral $Q^tQ = I$ can be recovered.) With the assumption of the orthogonality, and assuming also the symplecticness of Q so that $Q^tJ = JQ^t$, we find

$$JB = JQ^tAQ - Q^t\dot{Q}.$$

Since Q is orthogonal, $Q^tQ = I$, so $Q^t\dot{Q}$ is skew symmetric. Note that X^{-1}, $\dot{X}$ and JB all have the same zero structure as X. Hence the matrix

$$JQ^tAQ - Q^t\dot{Q}$$

also has this structure. If we block the matrices into four equal sized submatrices and use subscripted indices i, j to refer to the (i, j) block, then we have

$$(Q^t\dot{Q})_{21} = (JQ^tAQ)_{21} = -(Q^tAQ)_{11}.$$

The skew-symmetry of $Q^t\dot{Q}$ and the symmetry of A implies that

$$(Q^t\dot{Q})_{12} = (Q^tAQ)_{11}^t = (Q^tAQ)_{11}^t.$$

Also, using superscripts to index components within the block, we find

$$S_{11}^{ij} := (Q^t\dot{Q})_{11}^{ij} = (Q^t\dot{Q})_{22}^{ij} = \begin{cases} (Q^tAQ)_{12}^{ji}, & i > j, \\ 0, & i = j, \\ -(Q^tAQ)_{12}^{ij}, & i < j. \end{cases} \tag{8}$$

Having expressed $Q^t\dot{Q}$ in terms of the elements of Q^tAQ, we can give similar formulas for JB:

$$\begin{aligned} (JB)_{11}^{ij} &= (Q^tAQ)_{12}^{ji} - (Q^t\dot{Q})_{11}^{ij} \\ &= (Q^tAQ)_{12}^{ji} - S_{11} \\ &= \begin{cases} 2(Q^tAQ)_{12}^{ij}, & i<j, \\ (Q^tAQ)_{12}^{ij}, & i=j, \\ 0, & i>j. \end{cases} \end{aligned}$$

and

$$(JB)_{22}^{ij} = -(JB)_{11}^{ji}, \quad (JB)_{21} = 0, \quad \text{and} \quad (JB)_{12} = (Q^tAQ)_{22} - (Q^tAQ)_{11}.$$

Differential equations for Q are obtained as

$$\dot{Q} = \begin{bmatrix} \dot{Q}_1 & \dot{Q}_2 \\ -\dot{Q}_2 & \dot{Q}_1 \end{bmatrix} = \begin{bmatrix} Q_1S_{11} - Q_2(Q^tAQ)_{11} & Q_1(Q^tAQ)_{11} + Q_2S_{11} \\ -Q_1(Q^tAQ)_{11} - Q_2S_{11} & Q_1S_{11} - Q_2(Q^tAQ)_{11} \end{bmatrix} =: E. \tag{9}$$

3.1. Reduction to equations of motion for Q_1 and Q_2. For computation, we would like to compute Q_1 and Q_2 directly. That is, we would like to reduce equation (6) to a system of equations for Q_1 and Q_2.

Unfortunately, the straightforward approach of simply picking two components of (6) fails since one then finds that the orthogonality constraints are only weak invariants. However, it is possible to alter the differential equations in such a way as to insure that the orthogonality constraints are strong invariants of the differential equations. First note that (9) can be written as

$$\dot{Q} = QD$$

where for E in (9)

$$D = Q^tE \quad = \quad \begin{bmatrix} S_{11} & (Q^tAQ)_{11} \\ -(Q^tAQ)_{11} & S_{11} \end{bmatrix}$$

where S_{11} is as in (8).

Now,

$$\dot{Q}^t = D^tQ^t$$

or, in terms of the first column of blocks of Q,

$$\frac{d}{dt}\begin{bmatrix} Q_1^t \\ Q_2^t \end{bmatrix} = D^t \begin{bmatrix} Q_1^t \\ Q_2^t \end{bmatrix} \tag{10}$$

These reformulated equations are equivalent to the original equations along the orthogonality constraints. Moreover, since D is skew symmetric, $Q_1^tQ_1 + Q_2^tQ_2 = I$ is an integral invariant of the flow; it is also easy to check that the other condition for orthogonality, $Q_1^tQ_2 - Q_2^tQ_1 = 0$ is also an integral invariant of the flow of this system.

In the case of a *separable* Hamiltonian system the coefficient matrix JA takes the special form

$$JA = \begin{bmatrix} 0 & I \\ -K(t) & 0 \end{bmatrix}. \tag{11}$$

with K a symmetric matrix. In this case the differential equations for Q_1^t and Q_2^t are of the form

$$\begin{pmatrix} \dot{Q}_1^t \\ \dot{Q}_2^t \end{pmatrix} = \begin{bmatrix} -S_{11} & -(Q_2^tQ_2 + Q_1^tKQ_1) \\ (Q_2^tQ_2 + Q_1^tKQ_1) & -S_{11} \end{bmatrix} \begin{pmatrix} Q_1^t \\ Q_2^t \end{pmatrix}. \tag{12}$$

4. Numerical Methods

The primary application of the continuous orthosymplectic factorization lies in the computation of the variational equations for a nonlinear problem along some (numerically computed) trajectory. This involves solving the given nonlinear problem and either the linear variational equation or the equation for the orthosymplectic transformation in tandem. In this section we describe the numerical techniques that will be employed to solve the original Hamiltonian system, the linear variational equation, the equation for the decoupling transformation Q, and to determine the Lyapunov exponents. We first describe three general algorithms that will be compared, and then describe the specific implementations that will be employed.

4.1. Algorithms. The QR based techniques for determining fundamental matrix solutions of linear systems and hence the Lyapunov exponents of a linear system form two general classes, the continuous QR methods and the discrete QR methods. The continuous QR method involves first determining the change of variables Q and then determining the fundamental matrix solution of the transformed linear system. We will concentrate our efforts on the computation of Q and the determination of the diagonal entries of the transformed system, i.e. the Lyapunov exponents. The discrete QR method involves integrating for the fundamental matrix solution and then reorthogonalizing to avoid the difficulty with exponentially increasing and/or decreasing components.

Regardless of whether a discrete or continuous QR method is to be employed, the Hamiltonian system

$$\dot{x} = J\nabla H(x) \tag{13}$$

must be solved numerically.

For the symplectic continuous QR method (SCQR) me must also solve for Q_1 and Q_2 using equation (10) or in the special case of a separable Hamiltonian using equation (12). To determine Lyapunov exponents one forms the time averages of the diagonal elements of JB. Thus, the i^{th} Lyapunov exponent is given as

$$\lambda_i = \limsup_{t\to\infty} \frac{1}{t} \int_0^t (JB)^{ii}(s)ds. \tag{14}$$

One easily sees from this construction and the structure of the transformed coefficient matrix JB that the Lyapunov exponents and in the fact the finite time Lyapunov exponents occur in $\pm$ pairs (see also [2] and [20]).

We consider the use of the so called *symplectic discrete QR method* (SDQR) using the symplectic QR decomposition (see [5], [6]) as well as the standard discrete QR method (DQR) using the modified Gram-Schmidt method (see [15]). To use either of these, we must also solve the equation

$$\dot{Y} = J\nabla^2 H(x(t))Y \equiv JA(t)Y. \tag{15}$$

Given a step size h, let Y_n denote the local fundamental matrix solution on the interval $[nh, (n+1)h]$ with $Y(nh) = I$. For the DQR method let Q_0 denote a random $2N \times 2N$ orthogonal matrix, then the method is obtained as

$$Q_{n+1}R_{n+1} = Y_n Q_n \tag{16}$$

for $n = 0, 1, 2, ...$ where $Q_{n+1}R_{n+1}$ is the QR decomposition of Y_nQ_n. For the SDQR method we choose Q_0 to be a random orthosymplectic matrix and in (16) replace the standard QR decomposition of Y_nQ_n with the symplectic QR decomposition. For both of the discrete methods the Lyapunov exponents are determined as

$$\lambda_i = \lim_{k\to\infty} \frac{1}{kh} \sum_{j=0}^{k} \log((R_j)^{ii}). \tag{17}$$

4.2. Implementation Details. In our numerical experiments, we treat examples with the separable Hamiltonian form

$$H(q,p) = \frac{1}{2}p^t p + V(q),$$

so that (13) has the form

$$\dot{q} = p, \tag{18}$$

$$\dot{p} = -\nabla V(q). \tag{19}$$

We solve this separable system using the leapfrog scheme

$$\begin{aligned} q_{n+1} &= q_n + hp_{n+\frac{1}{2}}, \\ p_{n+\frac{1}{2}} &= p_n - \frac{h}{2}\nabla V(q_n), \\ p_{n+1} &= p_{n+\frac{1}{2}} - \frac{h}{2}\nabla V(q_{n+1}). \end{aligned}$$

For the continuous method SCQR we solve (12) for Q_1^t and Q_2^t using the implicit midpoint scheme (the second order Gauss Runge-Kutta scheme) and the orthogonality preserving fixed point iteration of [9]. Note that both orthogonality and the symplectic structure of Q will be preserved by the fixed point iteration since the orthogonality is preserved and the conditions for preserving orthogonality are the same as the conditions for preserving the symplectic structure. We approximate the integral in (14) using the composite trapezoidal rule. Since knowledge of K is required at the half steps (to apply the implicit midpoint rule for Q_1^t and Q_2^t) and at the full steps (to form the Lyapunov exponents), we use the leap frog method to approximate the solution of the original Hamiltonian system on a twice fine mesh.

For the discrete methods SDQR and DQR we solve for the fundamental matrix solution in (15) by applying the leap frog scheme to each column. We then apply either the modified Gram-Schmidt method (see [15]) for DQR or the symplectic QR decomposition (see [5] and [6]) for SDQR. We note that for the symplectic QR decomposition it is necessary to post–process the solution in order to obtain a block upper triangular matrix with positive diagonal elements. We do so by multiplying Q_{n+1} on the right and R_{n+1} of the left by a symplectic diagonal matrix of with ± 1 along the diagonal. If desired, the approximate Lyapunov exponents are obtained by forming a partial sum in (17).

5. Numerical Experiments

In this section we employ the algorithms described previously to find Lyapunov exponents of Hamiltonian systems. We consider the Hénon-Heiles system and a spatial discretization of the Sine-Gordon equation. We compare the orthosymplectic or symplectic continuous QR method (SCQR) with the standard discrete QR method (DQR) and the symplectic discrete QR method (SDQR). All the computations were performed on a Silicon Graphics Indigo[2] workstation in double precision (i.e. machine epsilon $\epsilon_M \approx 2.2E-16$). Throughout this section we order the Lyapunov exponents $\{\lambda_i\}_{i=1}^{2N}$ so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{2N-1} \geq \lambda_{2N}$.

5.1. Hénon-Heiles Hamiltonian System.

We first consider the computation of Lyapunov exponents for the Hénon-Heiles problem with Hamiltonian

$$\begin{aligned} H(q_1, q_2, p_1, p_2) &= \frac{1}{2}(p_1^2 + p_2^2) + \phi(q_1, q_2) \\ &= \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3 \end{aligned}$$

Our experiment was based on similar calculations in [3] of Lyapunov exponents for points inside and outside the chaotic regime. The differential equations are

$$\begin{aligned} \dot{q}_1 &= p_1 \\ \dot{q}_2 &= p_2 \\ \dot{p}_1 &= -q_1(1+2q_2) \\ \dot{p}_2 &= -q_2 - q_1^2 + q_2^2 \end{aligned}$$

with Hessian

$$K(q) = \begin{bmatrix} 1+2q_2 & 2q_1 \\ 2q_1 & 1-2q_2 \end{bmatrix}.$$

Experiments were performed with each of the initial conditions in Table 1 that were obtained by fixing q_2, p_2, setting $q_1 = 0$, and choosing p_1 to make the value of the Hamiltonian 0.125 to 6 significant digits.

Table 1. (Initial Conditions for Hénon-Heiles)

IC	q_2	p_2	p_1
1	0.2	0.02	0.463609
2	0.33	0.14	0.381389
3	0.015	0.25	0.432755
4	0.20	0.14	0.442417
5	-0.15	0.02	0.474183
6	0.25	0.30	0.328506

Table 2. (Hénon-Heiles, $T = 10,000$, $h = 10^{-3}$)

IC	Method	λ_1	λ_2	$\lvert\sum_{i=1}^{2N}\lambda_i\rvert$	$\sup_i \lvert\lambda_i + \lambda_{2N+1-i}\rvert$
1	SCQR	$7.14E-04$	$5.23E-04$	0	0
1	SDQR	$6.13E-04$	$6.14E-04$	$1.12E-16$	$5.61E-17$
1	DQR	$6.13E-04$	$6.14E-04$	$1.67E-17$	$7.42E-05$
2	SCQR	$5.57E-04$	$3.10E-04$	0	0
2	SDQR	$5.32E-04$	$4.99E-04$	$6.97E-16$	$4.91E-16$
2	DQR	$5.32E-04$	$4.99E-04$	$1.76E-16$	$2.59E-04$
3	SCQR	$3.32E-04$	$9.69E-05$	0	0
3	SDQR	$4.91E-04$	$9.78E-05$	$2.31E-16$	$2.93E-16$
3	DQR	$4.91E-04$	$9.78E-05$	$4.04E-17$	$1.46E-04$
4	SCQR	$4.18E-02$	$5.53E-04$	0	0
4	SDQR	$4.18E-02$	$8.98E-05$	$7.55E-16$	$4.84E-16$
4	DQR	$4.18E-02$	$8.98E-05$	$1.87E-16$	$5.50E-05$
5	SCQR	$6.03E-02$	$6.25E-04$	0	0
5	SDQR	$6.03E-02$	$5.77E-04$	$5.01E-16$	$4.20E-16$
5	DQR	$6.03E-02$	$5.77E-04$	$1.68E-15$	$3.55E-05$
6	SCQR	$3.32E-02$	$4.95E-04$	0	0
6	SDQR	$3.32E-02$	$7.03E-04$	$4.40E-16$	$4.09E-16$
6	DQR	$3.32E-02$	$7.03E-04$	$2.71E-16$	$6.23E-05$

The results of our numerical experiments are contained in Table 2. Notice that the standard discrete QR method correctly approximates the sum of the finite time approximate Lyapunov exponents, but not the fact that the exponents occur in plus/minus pairs. This is further confirmation of the observation made in [10] that the standard discrete QR method may not effectively approximate negative exponents. Observe that for IC1-3, the symplectic continuous QR method appears to resolve differences between the first two exponents. For IC4-6 the three methods give nearly identical results for the largest exponent. For all of the initial conditions considered the discrete QR methods give identical results for the first two exponents. This is due in part to the fact that both of these methods involve decomposing the same approximate fundamental matrix solution (which has both exponentially increasing and exponentially decreasing components).

5.2. Sine-Gordon Equation. We consider the Sine-Gordon equation with periodic boundary conditions:

$$u_{tt} = u_{xx} + \sin u, \qquad u = u(x,t), \qquad u(0,t) = u(L,t), \qquad u_x(0,t) = u_x(L,t)$$

If we let $q = u$ and $p = u_t$, then the Hamiltonian is $H = \int_0^L (\frac{1}{2}p^2 + \frac{1}{2}q_x^2 - \cos q)dx$. Notation here is directly from [21]. Upon discretizing in space we obtain the Hamiltonian (see [21], [23], [24])

$$\hat{H} = \sum_{j=0}^{N} (\frac{1}{2}P_j^2 + \frac{1}{2\Delta x^2}(Q_{j+1} - Q_j)^2 - \cos Q_j)$$

and the equations of motion

$$\begin{aligned} \dot{Q}_j &= P_j \\ \dot{P}_j &= \frac{1}{\Delta x^2}(Q_{j-1} - 2Q_j + Q_{j+1}) - \sin Q_j \end{aligned}$$

(respecting the periodic BC's: $Q_{-1} \equiv Q_N$, $Q_{N+1} \equiv Q_0$).

This is in the separable Hamiltonian form. The Hessian matrix is

$$K(Q) = \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots \\ \vdots & & & & & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 1 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix} - \begin{bmatrix} \cos(Q_1) & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \cos(Q_N) \end{bmatrix}$$

We consider the initial condition

$$u(x,0) = \pi + 0.1 \cos \mu x, \qquad u_t(x,0) = 0$$

with $\mu = 2\pi/L$ and $L = 2\sqrt{2}\pi$. These parameter values appear to allow only a single unstable mode (see [21]).

Tables 3 and 4 contain the results of our numerical experiments. In Table 3 the time step is fixed and the spatial grid is varied, while in Table 4 the time step varies and the spatial grid is fixed. Note in Table 3 that the discrete QR method, DQR, is unable to resolve the plus/minus pairing of the exponents. We see in Table 4 that the two discrete QR methods agree for the positive exponents, but not for the negative exponents. The symplectic methods give similar results, so the choice between the two is not clear. In general the symplectic continuous method is more expensive, but we anticipate that it may give better results for larger stepsizes than the symplectic discrete method since the differential equation for Q represents a reduction of the full dynamical system to one in the space of orthogonal matrices and thus eliminates a source of potential exponential instability.

Table 3. (Sine-Gordon, $T = 1,000$, $h = 10^{-2}$)

N	Method	λ_1	λ_2	λ_3	$\sup_i \lvert\lambda_i + \lambda_{2N+1-i}\rvert$
16	SCQR	$1.72E-01$	$1.11E-01$	$3.34E-02$	0
16	SDQR	$1.72E-01$	$1.06E-01$	$3.89E-02$	$6.80E-16$
16	DQR	$1.72E-01$	$1.06E-01$	$3.89E-02$	$4.25E-03$
32	SCQR	$6.51E-02$	$2.04E-02$	$6.94E-03$	0
32	SDQR	$6.57E-02$	$2.24E-02$	$6.12E-03$	$1.10E-15$
32	DQR	$6.57E-02$	$2.24E-02$	$6.12E-03$	$1.61E-03$

Table 4. (Sine-Gordon, $T = 1,000$, $N = 16$)

h	Method	λ_1	λ_2	λ_{16}	λ_{17}	λ_{31}	λ_{32}
5E-02	SCQR	$1.38E-01$	$7.63E-02$	$6.03E-04$	$-6.03E-04$	$-7.63E-02$	$-1.38E-01$
5E-02	SDQR	$1.40E-01$	$7.32E-02$	$8.43E-04$	$-8.43E-04$	$-7.32E-02$	$-1.40E-01$
5E-02	DQR	$1.40E-01$	$7.32E-02$	$8.43E-04$	$-8.37E-04$	$-7.44E-02$	$-1.40E-01$
5E-03	SCQR	$1.07E-01$	$6.79E-02$	$1.44E-04$	$-1.44E-04$	$-6.79E-02$	$-1.07E-01$
5E-03	SDQR	$1.07E-01$	$6.80E-02$	$1.36E-04$	$-1.36E-04$	$-6.80E-02$	$-1.07E-01$
5E-03	DQR	$1.07E-01$	$6.80E-02$	$1.37E-04$	$-7.21E-04$	$-6.93E-02$	$-1.07E-01$
5E-04	SCQR	$1.36E-01$	$6.38E-02$	$4.99E-04$	$-4.99E-04$	$-6.38E-02$	$-1.36E-01$
5E-04	SDQR	$1.36E-01$	$6.33E-02$	$4.98E-04$	$-4.98E-04$	$-6.33E-02$	$-1.36E-01$
5E-04	DQR	$1.36E-01$	$6.33E-02$	$4.98E-04$	$-5.64E-04$	$-6.46E-02$	$-1.36E-01$

6. Conclusion

For Hamiltonian problems both the continuous symplectic or discrete symplectic QR methods appear to be superior to the standard discrete QR method. The symplectic methods are useful for determining fundamental matrix solutions and Lyapunov exponents. Both the standard QR and symplectic QR methods preserve the sum of the Lyapunov exponents (which is zero for Hamiltonian systems), but the symplectic QR methods also preserve the fact the Lyapunov exponents occur in plus/minus pairs for Hamiltonian systems. The differences in the standard QR and symplectic QR methods is plainly evident from the numerical experiments. For discrete Hamiltonian dynamical systems the discrete symplectic QR

method should be preferred over the standard discrete QR method. For continuous Hamiltonian systems either the continuous or discrete symplectic QR method should be employed. The continuous symplectic QR method may possess advantages over the discrete symplectic QR method in some applications since the fundamental matrix solution does not need to be computed (a process which tends to restrict the stepsize for the discrete methods).

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