Conservative Methods for Ordinary Differential Equations on Quadratic Groups

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In the last few years numerical analysts have shown a growing interest in the numerical solution of matrix systems of ODEs whose solutions preserve, during the evolution, certain qualitative features of the initial matrices, such as orthogonality, symplecticness, isospectrality. In general, if the theoretical solution evolves on a matrix Lie group $\mathcal{G}$, then *ad-hoc* numerical procedures could be applied in order to obtain a numerical solution on the same matrix Lie group. In the case of isospectral problems we have to solve the Lax system

$$L' = [B(L), L], \qquad L(0) = L_0, \tag{1}$$

where L_0 is a constant symmetric matrix, $B(\cdot)$ maps symmetric matrices into skew-symmetric matrices, and $[B(L), L]$ is the commutator of $B(L)$ and L. Two different procedures, based on the approach proposed in [2] (the MGLRK methods), are suggested. Such an approach is a computational form for the Flaschka formulation of (1). Our numerical procedures consist in solving (1) by a Runge Kutta method, then, a single step of a Gauss Legendre Runge Kutta (GLRK) method may be applied to the Flaschka formulation of (1) (see [9], [8]). In the first procedure we compute the approximation of the Lax system by a continuous explicit RK method, instead, the second procedure computes the approximation of the Lax system by a GLRK method (the same method used for the Flaschka system). For matrix differential systems evolving on a quadratic group the mathematical form is the following:

$$Y'(t) = F(t, Y(t))Y(t), \qquad Y(0) = Y_0 \in \mathcal{G}, \qquad t \geq 0, \tag{2}$$

where $F(t, Y) \in \mathtt{g}$ for every $(t, Y) \in \mathbb{R}^+ \times \mathcal{G}$, and $\mathtt{g}$ denotes the Lie algebra of the group $\mathcal{G}$. It is well-known that the theoretical solution $Y(t)$ of (2) lies in $\mathcal{G}$ for all $t > 0$. *Quadratic Groups* include matrix groups of importance for physicists, such as the symplectic group, the Lorentz group but also the orthogonal group.

Definition (see [7]). *Let H be a nonsingular, symmetric or skew-symmetric $n \times n$ matrix. The quadratic group $\mathcal{H}_n(\mathbb{R})$ related to H, is given by the set of all matrices $Y \in \mathbb{R}^{n\times n}$ such that $Y^T H Y = H$. The Lie algebra $\mathtt{h}$ of $\mathcal{H}_n(\mathbb{R})$ is the set $\mathtt{h} = \{A \in \mathbb{R}^{n\times n} | A^T H + HA = 0\}$.*

If H is the identity matrix I_n of size n, we obtain the orthogonal group $O_n(\mathbb{R})$ with Lie algebra given by the set of skew-symmetric matrices $\mathtt{o} = \{A \in \mathbb{R}^{n\times n} | \ A^T + A = 0\}$. If H is the $2n \times 2n$ canonical symplectic matrix J we get the symplectic group $SP_{2n}(\mathbb{R})$ with Lie algebra given by the set of *Hamiltonian* matrices $\mathtt{sp} = \{A \in \mathbb{R}^{2n\times 2n} | \ A^T J + JA = 0\}$. The Lorentz group $SO_{p,m}(\mathbb{R})$ is the quadratic group of the diagonal matrix $D = \mathrm{diag}(I_p, -I_m)$, where its Lie algebra $\mathtt{l}$ is given by the set of matrices $A \in \mathbb{R}^{n\times n}$, with $n = p + m$, of the following form:

$$A = \begin{pmatrix} A_1 & A_2 \\ A_2^T & A_3 \end{pmatrix} \tag{3}$$

where A_1 and A_3 are skew-symmetric matrices in $\mathbb{R}^{p\times p}$ and $\mathbb{R}^{m\times m}$ respectively while $A_2 \in \mathbb{R}^{p\times m}$. If $p = 3$ and $m = 1$ we obtain the classical Lorentz group studied in the special theory of relativity.
To solve differential system on quadratic groups we have proposed methods based on the Cayley transform (see [4]). We denote by $\mathcal{R}(z)$ the Cayley map $\mathcal{R}(z) = (1+z)(1-z)^{-1}$, for $z \in \mathbb{C} - \{1\}$. Let $\mathcal{H}_n(\mathbb{R})$ be the quadratic group of H and let $Y(t)$ be the solution of 2 If -1 is not an eigenvalue of $Y(t)$ for any $t \in [0, T]$, then $Y(t)$ may be written as

$$Y(t) = \mathcal{R}[A(t)], \qquad t \in [0, T], \tag{4}$$

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where $A(t)$ belongs to $C^1([0,T] \to \mathbb{R}^{n\times n})$ and satisfies the differential system

$$\begin{aligned} A' &= \tfrac{1}{2}(I-A)F(t,\mathcal{R}(A))(I+A), \qquad t\in[0,T], \\ A(0) &= A_0 = \mathcal{R}^{-1}(Y_0). \end{aligned} \tag{5}$$

If $1 \notin \sigma[A(t)]$, then $A(t)$ belongs to the Lie algebra $\mathtt{h}$ for any $t \in [0,T]$.
We recall that any numerical method applied to (5) provides a numerical solution in the Lie algebra $\mathtt{h}$. Thus the Cayley methods are derived by a computational approximation of (5). If we apply explicit RK methods to solve (5) we obtain a class of semi-explicit methods to solve the differential system (2) in the Lie group. This approach has also been used to solve isospectral flows (see [5]).
To solve differential systems in the manifold of rectangular orthogonal matrices $\mathcal{O}_{n,q}(\mathbb{R}) = \{Y \in \mathbb{R}^{n\times q} | Y^TY = I_q\}$ with $q<n$ and where $F : \mathcal{O}_{n,q}(\mathbb{R}) \to \mathbb{R}^{n\times n}$ satisfies the weak skew-symmetric condition:

$$\forall Y \in \mathcal{O}_{n,p}(\mathbb{R}) : \quad Y^T[F^T(Y)+F(Y)]Y = 0. \tag{6}$$

can be used the same approach but we have to distinguish two cases. If $F(Y)$ is a skew-symmetric matrix for all Y in $\mathcal{O}_{n,q}(\mathbb{R})$ at each $t \geq 0$ we consider an orthogonal extension $V(t)$ of $Y(t)$ by means of $W(t) \in \mathbb{R}^{n\times(n-q)}$, such that $V(t) = (Y(t), W(t)) \in O_n(\mathbb{R})$. Thus we solve the square orthogonal system $V' = F(Y)V$, $V_0 = (Y_0, W_0) \in O_n(\mathbb{R})$ and $Y(t)$ may be given in the form $Y(t) = \mathcal{R}[A(t)]Y(t_k)$. If $F(Y)$ is not a skew-symmetric matrix but only weakly skew-symmetric, we can show that the rectangular differential system is equivalent to the new differential system where the matrix function is skew-symmetric (see [10]):

$$\begin{aligned} &Y'(t) = G(Y(t))Y(t), \qquad t\in[0,T] \\ &Y(0) = Y_0 \in \mathcal{O}_{n,q}(\mathbb{R}), \end{aligned} \tag{7}$$

where G is the following skew-symmetric matrix function

$$\forall Y \in \mathcal{O}_{n,q}(\mathbb{R}) : \qquad G(Y) = F(Y)YY^T - YY^TF^T(Y). \tag{8}$$

The Cayley approach have been used to develop a Fortran90 subroutine to integrate orthogonal differential systems and in particular to solve square and rectangular systems, to find the Lyapunov exponents of dynamical systems and to solve isospectral problems (see [6]).

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