Journal of Computational and Applied Mathematics 308 (2016) 263–275

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

On solving an isospectral flow

Amandeep Kaur

Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, England, United Kingdom

ARTICLE INFO

Article history:
Received 26 May 2015
Received in revised form 12 May 2016

Keywords:
Isospectral flow
Eigenvalues
Magnus expansion
Lie algebra
Binary trees

ABSTRACT

In this paper we expand the solution of the matrix ordinary differential system, originally due to Bloch and Iserles, of the form $X' = [N, X^2]$, $t \geq 0$, $X(0) = X_0 \in \mathrm{Sym}(n)$, $N \in \mathfrak{so}(n)$, where $\mathrm{Sym}(n)$ denotes the space of real $n \times n$ symmetric matrices and $\mathfrak{so}(n)$ denotes the Lie algebra of real $n \times n$ skew-symmetric matrices. The flow is solved using explicit Magnus expansion, which respects the isospectrality of the system. We represent the terms of expansion as binary rooted trees and deduce an explicit formalism to construct the trees recursively.

1. Introduction

Isospectral flows are matrix systems of ordinary differential equations of the form

$$X' = [B(X), X], \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n), \tag{1}$$

where $B(X) : \mathrm{Sym}(n) \to \mathfrak{so}(n)$. Their main structural feature is that they preserve the eigenvalues of the solution matrix. Isospectral flows occur in many important applications. First and the best known example is the Toda lattice, a one-dimensional lattice of particles whose motion is described by a nearest-neighbour interaction of an exponential type. It can be used to model a wide range of particle systems, ranging from the hard-sphere limit to the atomic case [1,2]. Another important example is the QR flow. The QR method for finding the eigenvalues of a matrix can be executed as an isospectral flow at unit intervals. QR flow is the generalization of non-periodic Toda flow. Such flows were first investigated by Symes [3] and subsequently in [4–9] and elsewhere.

Other well known examples include *eigenvalue problems* and *inverse eigenvalue problems for symmetric Toeplitz matrices* [10].

Note that if we let $B(X) = [N, X]$, in (1) where $N \in \mathrm{Sym}(n)$ then it leads to the *double-bracket flows*. Double bracket flows are isospectral flows given by the equations

$$X' = [[N, X], X], \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n) \tag{2}$$

where $N \in \mathrm{Sym}(n)$. They were introduced by Brockett [11] and Chu and Driessel [12]. Double bracket flows were discretized and then solved by Iserles by the method of Magnus series [13] and were generalized for more parameters [14]. Also, methods based on Magnus expansion are proposed for the numerical integration of the double-bracket flow and a bound on the convergence domain is provided by F. Casas [15].

In this paper we are concerned with the discretization of the matrix differential equation

$$X' = [N, X^2], \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n), \quad N \in \mathfrak{so}(n). \tag{3}$$

E-mail address: A.kaur@damtp.cam.ac.uk.

http://dx.doi.org/10.1016/j.cam.2016.05.033

The system (3) is known as the Bloch–Iserles (BI) equations. It is isospectral (preserves the eigenvalues of $X(t)$), is endowed with a Poisson structure and is integrable as proved by Bloch and Iserles [16]. We discretize this system using a similar approach, for instance in [13] and [15]. However, solving BI is much more complicated since it contains X^2 in the expression.

The above system is of interest for a number of reasons. Firstly, we can easily verify that it can be written in the form

$$X' = [N, X]X + X[N, X], \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n). \tag{4}$$

For $N \in \mathfrak{so}(n)$ and $X \in \mathrm{Sym}(n)$, we have $[N, X] \in \mathrm{Sym}(n)$, therefore it is a special case of a *congruent flow*

$$X' = A(X)X + XA^T(X), \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n), \tag{5}$$

where $A : \mathrm{Sym}(n) \to M(n)$, where $M(n)$ is the set of real $n \times n$ matrices, is sufficiently smooth. It is easy to verify that $X(t) = V(t)X_0V^T(t)$, where $V' = A(VX_0V^T)V$, $V(0) = I$. That means the solution is an outcome of the *general linear group* $\mathrm{GL}(n)$ acting on $\mathrm{Sym}(n)$ by congruence. That proves that the *signature* of $X(t)$ is constant [17]. Another interesting aspect of the given set of equations is that they are dual to the *generalized rigid body equations*

$$M' = [\Omega, M], \quad t \geq 0, \qquad M(0) \in \mathfrak{so}(n),$$

where $M = \Omega J + J\Omega$, $J \in \mathrm{Sym}(n)$ therefore $\Omega \in \mathfrak{so}(n)$ [18].

Also, it is clear that (3) can be rewritten in the form

$$X' = [XN + NX, X], \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n), \quad N \in \mathfrak{so}(n).$$

Since $XN + NX \in \mathfrak{so}(n)$ for $X \in \mathrm{Sym}(n)$, $N \in \mathfrak{so}(n)$, it follows that the system (3) is indeed isospectral.

It is obvious that we can discretize isospectral flows by traditional numerical methods (e.g. Runge–Kutta and multistep), but, once $n \geq 3$, these methods cannot respect the isospectrality of the system, i.e. the numerical solution changes the eigenvalues [19]. Isospectrality is essential for applications ranging from classical mechanics, like Toda flows and N-body systems, to linear algebra, like QR flows and inverse eigenvalue problems, so we need to solve (3) by a method that respects it [20,19,21].

In this paper we solve the given isospectral flow using the method of Magnus series. We show that the solution of (3) can be represented in the form $X(t) = e^{\Omega(t)}X_0e^{-\Omega(t)}$, where instead of computing X at the first place, we obtain the Taylor expansion of Ω. Note that this ensures automatically that the numerical solution, being similar to X_0, is isospectral. We will see that the Taylor expansion of Ω can be formed algorithmically from X_0 and N and linear combinations of their commutators and anti-commutators. The goal of this paper is to determine the rules for finding the terms of Ω to an arbitrary accuracy. For the solution, first we convert the isospectral flow to a Lie-group flow and then translate it into a Lie-algebraic equation. This method preserves the isospectrality and gives the desired structure of the solution with large time steps. In Section 2 we solve the given system of differential equations using the Magnus expansion to obtain the Taylor expansion of Ω. Finally, in Section 3 the terms are represented by binary rooted trees and an algorithm is formed to construct the next tree by recursion and to calculate the coefficient of each tree. This lays the foundations to a more general setting, namely the explicit representation of the solution of (3) when $B(X)$ can be represented in a finite "alphabet". The representation as binary trees is very important because otherwise, as the number of terms in each iteration grows exponentially, the complexity of manual computation becomes prohibitive. By indexing the terms in the expansion with a subset of binary trees, it is convenient to derive explicit recurrence relations. Also, it is remarkable that the skew-symmetry and Jacobi identity obeyed by the commutator help us to reduce the number of terms by cancelling or writing certain terms as the linear combination of other terms.

2. An expansion of the solution

As stated above, the Bloch–Iserles system can be rewritten in the form

$$X' = [B(X), X], \quad t \geq 0, \qquad X(0) = X_0 \in \mathrm{Sym}(n)$$

with $B(X) = NX + XN$, where $B(X) : \mathrm{Sym}(n) \to \mathfrak{so}(n)$. This system is seen to be isospectral and it is standard to verify that

$$X(t) = Q(t)X_0Q^T(t), \quad t \geq 0, \tag{6}$$

where $Q(t) \in \mathrm{SO}(n)$ is the solution of

$$Q'(t) = (Q(t)X_0Q^T(t)N + NQ(t)X_0Q^T(t))Q(t), \qquad Q(0) = I. \tag{7}$$

In a similar way as Magnus [22] did for linear equations, our idea is to represent the solution of (7) in the form

$$Q(t) = e^{\Omega(t)},$$

where

$$\Omega' = \sum_{0}^{\infty} \frac{\mathrm{B}_r}{r!} \mathrm{ad}_{\Omega}^r (e^{\Omega}X_0e^{-\Omega}N + Ne^{\Omega}X_0e^{-\Omega}), \qquad \Omega(0) = 0. \tag{8}$$