Self-Equivalent Flows Associated with the Generalized Eigenvalue Problem

D. S. Watkins*

Department of Pure and Applied Mathematics Washington State University Pullman, Washington 99164-2930

and

L. Elsner Fakultät für Mathematik Universität Bielefeld Postfach 86 40 D-4800 Bielefeld 1, Federal Republic of Germany

Submitted by Richard A. Brualdi

ABSTRACT

We present a family of flows which includes continuous analogues of the unshifted and shifted LZ and QZ algorithms for the generalized eigenvalue problem. In order to do this we use elementary Lie theory to create a general family of algorithms, of which the LZ and QZ algorithms are special cases. For each such algorithm we construct a family of associated flows, some of which are interpolants of the algorithm. We do not restrict our attention to Hessenberg-triangular forms; we consider arbitrary pairs of nonsingular matrices.

1. INTRODUCTION

In recent years there has been considerable interest in continuous analogues of the *QR* algorithm and other algorithms for calculating eigenvalues of matrices. See for example the works of Symes [18], Deift et al. [9], Nanda

^{*}Electronic mail: watkins awsumath.bitnet.

[14, 15], Chu [6], Watkins [20], and Watkins and Elsner [21], all of which have appeared since 1982. See also the earlier work of Rutishauser [16, 17] from the 1950s, which has been overlooked until recently. Given a matrix \hat{A} whose eigenvalues are desired, the QR algorithm produces a sequence A_0, A_1, A_2, \ldots such that each member of the sequence is similar to \hat{A} , and the matrices tend to upper triangular or block-triangular form. A continuous analogue of the QR algorithm produces a smooth, matrix-valued function or flow B(t), such that, for all t, B(t) is similar to \hat{A} , and $B(m) = A_m$ for $m = 0, 1, 2, \ldots$ That is, the flow interpolates the QR algorithm. More generally we may have B(t) similar to $\hat{B} = g(\hat{A})$ and $B(m) = g(A_m)$ for some specified function g. Such a flow must satisfy

$$B(t) = F(t)^{-1}\hat{B}F(t) \tag{1}$$

for some nonsingular matrix function F(t). In [21] we studied functions of the type (1), which we called *self-similar flows*.

When studying eigenvalues it is natural to employ similarity transformations, since they preserve eigenvalues. For certain other problems, such as the generalized eigenvalue problem and the singular-value problem, it is more natural to consider equivalences. Recall that two matrices $A, \tilde{A} \in \mathbb{C}^{n \times m}$ are equivalent if there exist nonsingular matrices $F \in \mathbb{C}^{n \times n}$ and $Z \in \mathbb{C}^{m \times n}$ such that $\tilde{A} = FAZ$. A matrix-valued function B(t) defined on some interval is called a self-equivalent flow if there exist smooth, nonsingular, matrix-valued functions $F(t) \in \mathbb{C}^{n \times n}$ and $Z(t) \in \mathbb{C}^{m \times m}$, and $\tilde{B} \in \mathbb{C}^{n \times m}$, such that $B(t) = F(t)\tilde{B}Z(t)$. In this paper we will develop self-equivalent flows associated with the generalized eigenvalue problem. We discussed flows associated with the singular-value decomposition in [22].

We will use elementary Lie theory to develop a family of algorithms for solving the generalized eigenvalue problem

$$\hat{A}x = \lambda \, \hat{B}x. \tag{2}$$

The family includes the LZ algorithm of Kaufman [12] and the QZ algorithm of Moler and Stewart [13], as well as new algorithms which we call SZ and HZ. We will refer to the algorithms collectively as FGZ algorithms. The usual formulations of the LZ and QZ algorithms are implicit and require that \hat{A} and \hat{B} be in unreduced upper Hessenberg and upper triangular forms, respectively. Our formulation is explicit and can be applied to arbitrary nonsingular \hat{A} and \hat{B} . While it is not recommended for practical use, our formulation does contribute to the understanding of the QZ and related algorithms and their relationship to self-equivalent flows. Associated with

1

1

е

f

1

1

each FGZ algorithm we introduce a family of FGZ flows, some of which interpolate the algorithm.

In [8] Chu introduced a flow which is an analogue of the QZ algorithm. That flow is a special case of the flows developed here. This paper also generalizes our earlier work [21], since the FG flows discussed there correspond to the case $\hat{B} = I$ in (2).

In Section 2 we summarize the basic Lie-theoretic results which we will use, and we also introduce the specific Lie groups and Lie algebras which give rise to our main examples of algorithms and flows. In Section 3 we introduce the FGZ algorithm for solving the generalized eigenvalue problem. For simplicity we stick to the unshifted case at first. In Section 4 we develop a family of flows which are continuous analogues of the unshifted FGZ algorithm, and we show that one member of this family interpolates the FGZ algorithm. In Section 5 we look at shifted and generalized FGZ algorithms, and in Section 6 we develop their continuous analogues. We show how to construct numerous flows which interpolate a given generalized FGZ algorithm. In Section 7 we demonstrate that there is some overlap between the flows presented here and the flows associated with the SVD which we introduced in [22].

2. NOTATION AND BASIC NOTIONS OF LIE THEORY

Let F denote either the real or the complex numbers, $F^{n\times n}$ the set of *n*-by-*n* matrices over F, and $\mathrm{GL}_n(F)$ the group of *n*-by-*n* nonsingular matrices with entries in F.

 $\operatorname{GL}_n(\mathsf{F})$ is a Lie group [5, 11, 19], as are all of its closed subgroups. Given a closed subgroup $\mathscr H$ of $\operatorname{GL}_n(\mathsf F)$, we will let $\Lambda(\mathscr H)$ denote the Lie algebra of $\mathscr H$ [5, 11, 19, 21]. If one views $\mathscr H$ as a real manifold, then $\Lambda(\mathscr H)$ can be viewed as the tangent space to $\mathscr H$ at the point I. The Lie algebra of $\operatorname{GL}_n(\mathsf F)$ is $\mathsf F^{n\times n}$ with the Lie product [X,Y]=XY-YX, and $\Lambda(\mathscr H)$ is a subalgebra of $\mathsf F^{n\times n}$.

Initial-value problems of the form

$$\dot{H} = HX$$
, $H(0) = H_0 \in \mathcal{H}$

or

$$\dot{H} = XH$$
, $H(0) = H_0 \in \mathcal{H}$,

where X = X(t), will play an important role in the paper. Suppose the

initial-value problem has a unique solution in some interval $[0, \tilde{t}]$. Then $H(t) \in \mathcal{H}$ for all $t \in [0, \tilde{t}]$ if and only if $X(t) \in \Lambda(\mathcal{H})$ for all $t \in [0, \tilde{t}]$. A proof is given in [21] (Theorem 5.1).

Throughout the paper \mathcal{F} and \mathcal{G} will denote two closed subgroups of $\mathrm{GL}_n(\mathsf{F})$ such that

$$\mathscr{F} \cap \mathscr{G} = \{I\} \tag{3}$$

and

$$\Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G}) = \mathbb{F}^{n \times n}. \tag{4}$$

From the condition (4) it follows [21, Theorem 5.2] that there is a neighborhood $\mathscr V$ of I in $\mathrm{GL}_n(F)$ such that every $A \in \mathscr V$ can be expressed as a product

$$A = FG \tag{5}$$

where $F \in \mathcal{F}$ and $G \in \mathcal{G}$. By (3) F and G are unique. The expression (5) is called an FG decomposition of A.

EXAMPLE 2.1L. Let \mathscr{F} be the group of unit lower triangular matrices and \mathscr{G} the group of nonsingular upper triangular matrices. Then $\Lambda(\mathscr{F})$ is the Lie algebra of strictly lower triangular matrices, and $\Lambda(\mathscr{G})$ is the Lie algebra of upper triangular matrices. Clearly $\mathbf{F}^{n\times n}=\Lambda(\mathscr{F})\oplus\Lambda(\mathscr{G})$. Therefore there exists a neighborhood \mathscr{V} of I such that every $A\in\mathscr{V}$ can be expressed as a product A=FG, where F is unit lower triangular and G is upper triangular. Of course this is a weak version of a well-known fact: every matrix whose leading principal submatrices are nonsingular (that is, almost every matrix) has a unique LU decomposition [10].

Example 2.1Q. Let \mathscr{F} be the unitary group and \mathscr{G} the group of upper triangular matrices with positive, real entries on the main diagonal. Then $\Lambda(\mathscr{F})$ is the Lie algebra of skew-Hermitian matrices, and $\Lambda(\mathscr{G})$ consists of the upper triangular matrices having real main-diagonal entries. It is easy to show that $\mathbb{C}^{n\times n}=\Lambda(\mathscr{F})\oplus\Lambda(\mathscr{G})$. Therefore there exists a neighborhood \mathscr{V} of I such that every $A\in\mathscr{V}$ can be expressed as A=FG, where F is unitary and G is upper triangular with positive main-diagonal entries. Again we have a weak version of a well-known fact: every square matrix has a QR decomposition [10]. In the real case \mathscr{F} can be taken to be either the orthogonal group or its subgroup, the rotation group, and \mathscr{G} can be taken to be the group of

nonsingular real upper triangular matrices with positive main-diagonal entries. Then $\mathbb{R}^{n\times n} = \Lambda(\mathcal{F}) \oplus \Lambda(\mathcal{G})$.

EXAMPLE 2.1S. Let \mathscr{F} be the real symplectic group in $GL_{2n}(\mathbb{R})$. This is the set of $S \in GL_{2n}(\mathbb{R})$ such that $S^TJS = J$, where $J \in \mathbb{R}^{2n \times 2n}$ is given by

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}.$$

The associated Lie algebra $\Lambda(\mathcal{F})$ is the set of $X \in \mathbb{R}^{2n \times 2n}$ such that $(JX)^T = JX$. Matrices satisfying this equation are called *Hamiltonian*. Let \mathcal{G} be the subgroup of $GL_{2n}(\mathbb{R})$ consisting of matrices of the form

$$G = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix},$$

where each block is upper triangular, G_{21} and G_{12} are strictly upper triangular, G_{11} and G_{22} are nonsingular, and diag $\{G_{11}\}=$ diag $\{G_{22}\}$. This group is discussed in greater detail in [21, Example 5.5]. Its Lie algebra is the set of matrices of the form

$$X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}$$

such that all blocks are upper triangular, X_{21} and X_{12} are strictly upper triangular, and diag $\{X_{11}\}=$ diag $\{X_{22}\}$. Again it is not hard to show that $\mathbb{R}^{2n\times 2n}=\Lambda(\mathscr{F})\oplus\Lambda(\mathscr{G})$. Thus there exists a neighborhood \mathscr{V} of I such that every $A\in\mathscr{V}$ can be expressed as a product A=FG, where F is symplectic and $G\in\mathscr{G}$. This is called the SR decomposition. In [2] and [4], for example, it is shown that almost every $A\in\mathrm{GL}_{2n}(\mathbb{R})$ has such a decomposition.

EXAMPLE 2.1H. Let $J \in \operatorname{GL}_n(\mathbb{C})$ be any diagonal matrix whose main-diagonal entries are in $\{1, -1\}$. Let \mathscr{F} be the group of J-unitary matrices. This is the set of $G \in \operatorname{GL}_n(\mathbb{C})$ such that $G^*JG = J$. Then $\Lambda(\mathscr{F})$ is the set of $X \in \mathbb{C}^{n \times n}$ such that $(JX)^* = -JX$. These are called J-skew-Hermitian matrices. Let \mathscr{G} be the group of upper triangular matrices with positive main-diagonal entries. Then $\Lambda(\mathscr{G})$ consists of the upper triangular matrices with real entries on the main diagonal. It is easy to show that $\mathbb{C}^{n \times n} = \Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G})$.

Therefore there is a neighborhood \mathscr{V} of I such that every $A \in \mathscr{V}$ can be expressed as a product A = FG, where F is J-unitary and $G \in \mathscr{G}$. This is known as the HR decomposition. For a more precise result see [2, p. 253] or [3], in which it is shown that A has an HR decomposition if and only if the leading principal minors of A^*JA have the same signs as the respective leading principal minors of J. Note that in contrast to the conditions in the preceding examples, it is not the case that this condition holds for almost all matrices, but it does hold in a neighborhood of I. In the case J = I, this example reduces to Example 2.1Q.

3. FGZ ALGORITHMS FOR THE GENERALIZED EIGENVALUE PROBLEM

Given \hat{A} , $\hat{B} \in GL_n(\mathbb{F})$ we will introduce a family of algorithms to solve the generalized eigenvalue problem

$$\hat{A}x = \lambda \, \hat{B}x.$$

For simplicity we will present the unshifted algorithms first. The shifted algorithms will be introduced in Section 6.

Given \mathscr{F} and \mathscr{G} , closed subgroups of $\mathrm{GL}_n(\mathbb{F})$ satisfying (3) and (4), the corresponding FGZ algorithm produces two sequences of matrices (A_i) and B_i) as follows: The starting matrices are $A_0 = \hat{A}$ and $B_0 = \hat{B}$. Given A_{i-1} and B_{i-1} , perform FG decompositions of $A_{i-1}B_{i-1}^{-1}$ and $B_{i-1}^{-1}A_{i-1}$:

$$A_{i-1}B_{i-1}^{-1} = \bar{F}_i\bar{G}_i, \qquad B_{i-1}^{-1}A_{i-1} = \bar{Z}_i\bar{R}_i, \tag{6}$$

where $\overline{F}_i, \overline{Z}_i \in \mathscr{F}$ and $\overline{G}_i, \overline{R}_i \in \mathscr{G}$. Then define A_i and B_i by

$$A_{i} = \overline{F}_{i}^{-1} A_{i-1} \overline{Z}_{i}, \qquad B_{i} = \overline{F}_{i}^{-1} B_{i-1} \overline{Z}_{i}.$$
 (7)

It is easy to show that A_i and B_i are also given by

$$A_i = \overline{G}_i A_{i-1} \overline{R}_i^{-1}, \qquad B_i = \overline{G}_i B_{i-1} \overline{R}_i^{-1}. \tag{8}$$

Since also

$$A_{i}B_{i}^{-1} = \overline{F}_{i}^{-1} (A_{i-1}B_{i-1}^{-1}) \overline{F}_{i} = \overline{G}_{i}\overline{F}_{i},$$

$$B_{i}^{-1}A_{i} = \overline{Z}_{i}^{-1} (B_{i-1}^{-1}A_{i-1}) \overline{Z}_{i} = \overline{R}_{i}\overline{Z}_{i},$$

we see that one step of the FGZ algorithm accomplishes one step of the FG algorithm [21] for both $A_{i-1}B_{i-1}^{-1}$ and $B_{i-1}^{-1}A_{i-1}$. Since not every matrix has an FG decomposition, it can happen that the algorithm breaks down.

For i = 0, 1, 2, ... define $F_i, Z_i \in \mathcal{F}$ and $F_i, R_i \in \mathcal{G}$ by

$$F_i = \overline{F}_1 \overline{F}_2 \cdots \overline{F}_i, \qquad Z_i = \overline{Z}_1 \overline{Z}_2 \cdots \overline{Z}_i,$$

$$G_i = \overline{G}_i \cdots \overline{G}_2 \overline{G}_1, \qquad R_i = \overline{R}_i \cdots \overline{R}_2 \overline{R}_1.$$

Then

$$A_{i} = F_{i}^{-1} \hat{A} Z_{i} = G_{i} \hat{A} R_{i}^{-1}, \tag{9}$$

$$B_{i} = F_{i}^{-1} \hat{B} Z_{i} = G_{i} \hat{B} R_{i}^{-1}, \tag{10}$$

$$A_i B_i^{-1} = F_i^{-1} (\hat{A} \hat{B}^{-1}) F_i = G_i (\hat{A} \hat{B}^{-1}) G_i^{-1}, \tag{11}$$

$$B_i^{-1}A_i = Z_i^{-1}(\hat{B}^{-1}\hat{A})Z_i = R_i(\hat{B}^{-1}\hat{A})R_i^{-1}.$$
 (12)

By an easy induction argument we get

$$\left(\hat{A}\hat{B}^{-1}\right)^{i} = F_{i}G_{i},\tag{13}$$

$$\left(\hat{B}^{-1}\hat{A}\right)^{i} = Z_{i}R_{i}. \tag{14}$$

These are the unique FG decompositions of $(\hat{A}\hat{B}^{-1})^i$ and $(\hat{B}^{-1}\hat{A})^i$, respectively.

If the algorithm does not break down, then, for certain choices of \mathcal{F} , \mathcal{G} , \hat{A} , and \hat{B} , the sequences $A_i B_i^{-1}$ and $B_i^{-1} A_i$ will converge to triangular form, revealing the generalized eigenvalues on the main diagonal. It is difficult to state exact conditions under which convergence will take place, and we will not attempt to do so here. We have chosen to describe the FGZ iteration in a very general context, but we do not claim that every choice of \mathcal{F} and \mathcal{G} yields a useful algorithm.

EXAMPLE 3.1. This example shows that convergence of $A_iB_i^{-1}$ and $B_i^{-1}A_i$ to triangular form does not imply the same for A_i and B_i . Let U be any nonsingular matrix, and let $\hat{A} = \hat{B} = U$. Then, for all i, $A_iB_i^{-1} = I$, $B_i^{-1}A_i = I$, $A_i = U$, and $B_i = U$.

4. SELF-EQUIVALENT FLOWS ASSOCIATED WITH THE GENERALIZED EIGENVALUE PROBLEM

Let F(t) and Z(t) be smooth functions such that F(0) = I, Z(0) = I, $F(t) \in \operatorname{GL}_n(\mathbb{F})$, and $Z(t) \in \operatorname{GL}_n(\mathbb{F})$ for all t. It is easy to show that the smooth function $C(t) = F(t)^{-1} \hat{C} Z(t)$ satisfies the initial-value problem

$$\dot{C} = CY - XC, \qquad C(0) = \hat{C}, \tag{15}$$

where $Y = Z^{-1}\dot{Z}$ and $X = F^{-1}\dot{F}$. Conversely, if (15) has a unique solution, then the solution is $C(t) = F(t)^{-1}\hat{C}Z(t)$, where F and Z satisfy

$$\dot{F} = FX, \qquad F(0) = I, \tag{16}$$

$$\dot{Z} = ZY, \qquad Z(0) = I, \tag{17}$$

respectively. A proof is given in [22], but this is an easy exercise. Similar results are given in [7, 8].

We will also find it useful to express self-similar flows in the form $C(t) = G(t)\hat{C}R(t)^{-1}$. Then C(t) satisfies the initial-value problem

$$\dot{C} = XC - CY, \qquad C(0) = \hat{C}, \tag{18}$$

where $X = \dot{G}G^{-1}$ and $Y = \dot{R}R^{-1}$. Conversely, if (18) has a unique solution, then the solution is $C(t) = G(t)\hat{C}R(t)^{-1}$, where G and R satisfy

$$\dot{G} = XG, \qquad G(0) = I, \tag{19}$$

$$\dot{R} = YR, \qquad R(0) = I. \tag{20}$$

Since $\mathbb{F}^{n\times n} = \Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G})$, every $M \in \mathbb{F}^{n\times n}$ can be expressed uniquely as a sum

$$M = \rho(M) + \sigma(M),$$

where $\rho(M) \in \Lambda(\mathcal{F})$ and $\sigma(M) \in \Lambda(\mathcal{G})$. Given \hat{C} , $\hat{D} \in GL_n(\mathbb{F})$ and a locally

analytic function f defined on an open set containing the common spectrum of $\hat{C}\hat{D}^{-1}$ and $\hat{D}^{-1}\hat{C}$, consider the system of differential equations

$$\dot{C} = C\rho(f(D^{-1}C)) - \rho(f(CD^{-1}))C, \qquad C(0) = \hat{C},
\dot{D} = D\rho(f(D^{-1}C)) - \rho(f(CD^{-1}))D, \qquad D(0) = \hat{D}.$$
(21)

Each of these differential equations has the form (15). The system (21) satisfies a Lipschitz condition on compact sets, so it has a unique solution on some nonempty interval $[0, \tilde{t})$. Therefore the solution is

$$C(t) = F(t)^{-1}\hat{C}Z(t),$$

$$D(t) = F(t)^{-1}\hat{D}Z(t),$$
(22)

where F and Z are solutions of

$$\dot{\mathbf{F}} = \mathbf{F}\rho(f(\mathbf{C}D^{-1})), \qquad F(0) = I,$$

$$\dot{\mathbf{Z}} = \mathbf{Z}\rho\big(f(D^{-1}C)\big), \qquad \mathbf{Z}(0) = I.$$

Since $\rho(f(D^{-1}C)) \in \Lambda(\mathcal{F})$ and $\rho(f(CD^{-1})) \in \Lambda(\mathcal{F})$, we have $F(t) \in \mathcal{F}$ and $Z(t) \in \mathcal{F}$ for all $t \in [0, \tilde{t})$ [21]. In the case when \mathcal{F} and \mathcal{G} are as in Example 2.1Q, C is upper Hessenberg, D is upper triangular, and f(x) = x, (21) reduces to the flow of Chu [8]. Using the fact that

$$f(CD^{-1})C = Cf(D^{-1}C)$$

and

$$f(CD^{-1})D = Df(D^{-1}C),$$

we see easily that the system (21) can also be expressed as

$$\dot{C} = \sigma(f(CD^{-1}))C - C\sigma(f(D^{-1}C)), C(0) = \hat{C},
\dot{D} = \sigma(f(CD^{-1}))D - D\sigma(f(D^{-1}C)), D(0) = \hat{D}.$$
(23)

It follows that

$$C(t) = G(t)\hat{C}R(t)^{-1}$$

$$D(t) = G(t)\hat{D}R(t)^{-1},$$
(24)

where

$$\dot{G} = \sigma(f(CD^{-1}))G, \qquad G(0) = I,$$

$$\dot{R} = \sigma(f(D^{-1}C))R, \qquad R(0) = I.$$

Since $\sigma(f(CD^{-1})) \in \Lambda(\mathcal{G})$ and $\sigma(f(D^{-1}C)) \in \Lambda(\mathcal{G})$, we have $G(t) \in \mathcal{G}$ and $R(t) \in \mathcal{G}$. From (22) and (24) we see that

$$C(t)D(t)^{-1} = F(t)^{-1}\hat{C}\hat{D}^{-1}F(t) = G(t)\hat{C}\hat{D}^{-1}G(t)^{-1},$$
 (25)

$$D(t)^{-1}C(t) = Z(t)^{-1}\hat{D}^{-1}\hat{C}Z(t) = R(t)\hat{D}^{-1}\hat{C}R(t)^{-1}.$$
 (26)

Furthermore, CD^{-1} and $D^{-1}C$ satisfy the differential equations

$$\frac{d}{dt}(CD^{-1}) = [CD^{-1}, \rho(f(CD^{-1}))] = [\sigma(f(CD^{-1})), CD^{-1}],$$

$$\frac{d}{dt}(D^{-1}C) = [D^{-1}C, \rho(f(D^{-1}C))] = [\sigma(f(D^{-1}C)), D^{-1}C],$$
(27)

so CD^{-1} and $D^{-1}C$ are self-similar flows of the type discussed in [21]. It follows that

$$\exp(tf(\hat{C}\hat{D}^{-1})) = F(t)G(t), \tag{28}$$

$$\exp(tf(\hat{D}^{-1}\hat{C})) = Z(t)R(t)$$
(29)

for all $t \in [0, \tilde{t})$. These are the unique FG decompositions of $\exp(tf(\hat{C}\hat{D}^{-1}))$ and $\exp(tf(\hat{D}^{-1}\hat{C}))$, respectively. Because of these equations it is possible, in certain cases, to extend the flow past singularities, as discussed in [21]. We will postpone the discussion of this topic until Section 6.

Connections between FGZ Algorithms and Flows

In the following theorems we assume that both the FGZ algorithm and the FGZ flow are defined at some integer times t = i = 0, 1, ..., m.

Theorem 4.1. The FGZ algorithm (6, 7) with initial matrices \hat{A} , \hat{B} and the FGZ flow (21) are related as follows:

(a) If $\hat{A}\hat{B}^{-1} = \exp(f(\hat{C}\hat{D}^{-1}))$, then $A_iB_i^{-1} = \exp(f(C(i)D(i)^{-1}))$ for i = 0, 1, ..., m.

(b) If $\hat{B}^{-1}\hat{A} = \exp(f(\hat{D}^{-1}\hat{C}))$, then $B_i^{-1}A_i = \exp(f(D(i)^{-1}C(i)))$ for i = 0, 1, ..., m.

Proof. Suppose $\hat{A}\hat{B}^{-1} = \exp(f(\hat{C}\hat{D}^{-1}))$. Then, comparing (13) with (28) at t = i = 0, 1, 2, ..., m, we have

$$F_i G_i = F(i)G(i). \tag{30}$$

By the uniqueness of the FG decompositions,

$$F_i = F(i), \qquad G_i = G(i)$$
 (31)

for i = 0, 1, ..., m. Therefore, by (11) and (25),

$$A_{i}B_{i}^{-1} = F_{i}^{-1}\hat{A}\hat{B}^{-1}F_{i}$$

$$= F(i)^{-1}\exp(f(\hat{C}\hat{D}^{-1}))F(i)$$

$$= \exp(f(F(i)^{-1}\hat{C}\hat{D}^{-1}F(i)))$$

$$= \exp(f(C(i)D(i)^{-1})).$$

This is the first assertion of the theorem. (We could equally well have used G_i instead of F_i^{-1} .) To get the second assertion we compare (14) with (29) at t = i = 0, 1, ..., m to obtain

$$Z_i R_i = Z(i) R(i). \tag{32}$$

These are also FG decompositions, so

$$Z_i = Z(i), \qquad R_i = R(i) \tag{33}$$

for i = 0, 1, ..., m. Now applying (12) and (26) we get that

$$B_i^{-1}A_i = \exp(f(D(i)^{-1}C(i))),$$

$$i=0,1,\ldots,m$$
.

In the special case $f(x) = \log x$ we get a much nicer result. By $\log x$ we mean any branch of the natural logarithm for which $\log(\hat{A}\hat{B}^{-1})$ and $\log(\hat{B}^{-1}\hat{A})$ are meaningful.

THEOREM 4.2. The FGZ algorithm (6, 7) with initial matrices \hat{A} , \hat{B} and the FGZ flow (21) with $f(x) = \log x$ and initial matrices $\hat{C} = \hat{A}$ and $\hat{D} = \hat{B}$ are related by

$$A_i = C(i), \quad B_i = D(i), \quad i = 0, 1, ..., m.$$

That is, the flow interpolates the FGZ algorithm.

Proof. Under the hypotheses of the theorem, the equations $\hat{A}\hat{B}^{-1} = \exp(f(\hat{C}\hat{D}^{-1}))$ and $\hat{B}^{-1}\hat{A} = \exp(f(\hat{D}^{-1}\hat{C}))$ are trivially true, so Equations (31) and (33) from the proof of Theorem 4.1 hold. Therefore

$$A_i = F_i^{-1} \hat{A} Z_i = F(i)^{-1} \hat{C} Z(i) = C(i),$$

$$B_i = F_i^{-1} \hat{B} Z_i = F(i)^{-1} \hat{D} Z(i) = D(i).$$

We could equally well have used G_i and R_i^{-1} instead of F_i^{-1} and Z_i .

5. SHIFTED AND GENERALIZED FGZ ALGORITHMS

The variants of the FGZ algorithm which are used in practice all employ shifts. A simple shifted FGZ algorithm would shift $A_{i-1}B_{i-1}^{-1}$ and $B_{i-1}^{-1}A_{i-1}$ before performing the FG decompositions. Thus instead of (6) we would

have

$$\begin{aligned} A_{i-1}B_{i-1}^{-1} - \sigma_i I &= \overline{F}_i \overline{G}_i, \\ B_{i-1}^{-1}A_{i-1} - \sigma_i I &= \overline{Z}_i \overline{R}_i, \end{aligned} \tag{34}$$

where $\sigma_1, \sigma_2, \sigma_3, \ldots$ are shifts which do not lie in the common spectrum of $\hat{A}\hat{B}^{-1}$ and $\hat{B}^{-1}\hat{A}$. The double shift FGZ algorithm replaces (6) by

$$(A_{i-1}B_{i-1}^{-1} - \sigma_{i}I)(A_{i-1}B_{i-1}^{-1} - \tau_{i}I) = \overline{F}_{i}\overline{G}_{i},$$

$$(B_{i-1}^{-1}A_{i-1} - \sigma_{i}I)(B_{i-1}^{-1}A_{i-1} - \tau_{i}I) = \overline{Z}_{i}\overline{R}_{i}.$$
(35)

In both cases A_i and B_i are defined by (7), as before. Both of these algorithms are special cases of the generalized FGZ algorithm: Let p_1, p_2, p_3, \ldots be a sequence of functions defined on the common spectrum of $\hat{A}\hat{B}^{-1}$ and $\hat{B}^{-1}\hat{A}$ such that none of the points of the spectrum is mapped to zero by any of the p_i . Let $A_0 = \hat{A}$ and $B_0 = \hat{B}$. Given A_{i-1} and B_{i-1} , define A_i and B_i as follows. First let $\bar{F}_i, \bar{Z}_i \in \mathscr{F}$ and $\bar{G}_i, \bar{R}_i \in \mathscr{G}$ be given by the FG decompositions

$$p_i(A_{i-1}B_{i-1}^{-1}) = \overline{F}_i\overline{G}_i, \qquad p_i(B_{i-1}^{-1}A_{i-1}) = \overline{Z}_i\overline{R}_i.$$
 (36)

Then define

$$A_{i} = \overline{F}_{i}^{-1} A_{i-1} \overline{Z}_{i}, \qquad B_{i} = \overline{F}_{i}^{-1} B_{i-1} \overline{Z}_{i}.$$
 (37)

Using the identities $A_{i-1}p_i(B_{i-1}^{-1}A_{i-1}) = p_i(A_{i-1}B_{i-1}^{-1})A_{i-1}$ and $B_{i-1}p_i(B_{i-1}^{-1}A_{i-1}) = p_i(A_{i-1}B_{i-1}^{-1})B_{i-1}$, one shows easily that A_i and B_i are also given by

$$A_{i} = \overline{G}_{i} A_{i-1} \overline{R}_{i}^{-1}, \qquad B_{i} = \overline{G}_{i} B_{i-1} \overline{R}_{i}^{-1}. \tag{38}$$

If we take $p_i(x) = x - \sigma_i$, (36) reduces to (34), whereas if $p_i(x) = (x - \sigma_i)(x - \tau_i)$, (36) reduces to the double shift algorithm (35).

Equations (9) through (12), which hold for the unshifted FGZ algorithm, continue to be valid for the generalized FGZ algorithm. Equations (13, 14)

are replaced by the generalizations

$$\prod_{j=1}^{i} p_{j}(\hat{A}\hat{B}^{-1}) = F_{i}G_{i}, \qquad (39)$$

$$\prod_{j=1}^{i} p_{j}(\hat{B}^{-1}\hat{A}) = Z_{i}R_{i}. \tag{40}$$

EXAMPLE 5.1L. Let \mathcal{F} be the group of unit lower triangular matrices, and \mathcal{G} the group of nonsingular upper triangular matrices. Defining p_i as in (35), we get an algorithm equivalent to Kaufman's LZ algorithm [12] without pivoting. Of course the actual implementation of [12] is an implicit formulation which is very different from what is indicated by (35) and (37).

EXAMPLE 5.1Q. Let \mathscr{F} be the unitary group and \mathscr{G} the group of upper triangular matrices with positive entries on the main diagonal. Defining p_i as in (35), we get an algorithm equivalent to the QZ algorithm of Moler and Stewart [13]. Once again the actual implementation of [13] is implicit.

Example 5.1S. Let $\mathscr{F} \in GL_{2n}(\mathbb{R})$ be the real symplectic group defined in Example 2.1S, and let \mathscr{G} also be as defined in Example 2.1S. The resulting algorithm is called the SZ algorithm. Like the LZ and QZ algorithms, it can be implemented implicitly. We plan to discuss questions of implementation in general in a subsequent paper.

Example 5.1H. If we take \mathcal{F} and \mathcal{G} as in Example 2.1H, we get an algorithm which we will call the HZ algorithm.

6. FLOWS ASSOCIATED WITH GENERALIZED FGZ ALGORITHMS

Given a generalized FGZ algorithm, we would like to find self-equivalent flows which interpolate the algorithm. To this end we consider flows satisfying nonautonomous initial value problems of the form

$$\dot{C} = C\rho(f(t, D^{-1}C)) - \rho(f(t, CD^{-1}))C, \qquad C(0) = \hat{C},
\dot{D} = D\rho(f(t, D^{-1}C)) - \rho(f(t, CD^{-1}))D, \qquad D(0) = \hat{D},$$
(41)

where f(t, x) is piecewise continuous in t and locally analytic in x. Solutions of (41) satisfy the following theorem, which generalizes Theorems 6.1 and 9.1 of [21].

THEOREM 6.1. Let $\hat{C} \in \mathbf{F}^{n \times n}$, $\hat{D} \in \operatorname{GL}_n(\mathbf{F})$, and let f(t,x) be any function which is piecewise continuous in t and, for each t, locally analytic in x on an open set containing the common spectra of $\hat{C}\hat{D}^{-1}$ and $\hat{D}^{-1}\hat{C}$. Then the initial-value problem (41) has a unique solution on some nonempty interval $[0, \tilde{t})$. The solution satisfies

$$C(t) = F(t)^{-1}\hat{C}Z(t) = G(t)\hat{C}R(t)^{-1}$$

$$D(t) = F(t)^{-1}\hat{D}Z(t) = G(t)\hat{D}R(t)^{-1},$$
(42)

where F, G, Z, and R are solutions of

$$\dot{F} = F\rho(f(t, CD^{-1})), \qquad F(0) = I, \tag{43}$$

$$\dot{G} = \sigma(f(t, CD^{-1}))G, \qquad G(0) = I, \tag{44}$$

$$\dot{Z} = Z\rho(f(t, D^{-1}C)), \qquad Z(0) = I,$$
(45)

$$\dot{R} = \sigma(f(t, D^{-1}C))R, \qquad R(0) = I.$$
 (46)

F(t), $Z(t) \in \mathcal{F}$ and G(t), $R(t) \in \mathcal{G}$ for all $t \in [0, \tilde{t})$. They are related by the equations

$$\exp\{M(t)\} = F(t)G(t), \tag{47}$$

$$\exp\{N(t)\} = Z(t)R(t), \tag{48}$$

where

$$M(t) = \int_0^t f(s, \hat{C}\hat{D}^{-1}) ds$$
 and $N(t) = \int_0^t f(s, \hat{D}^{-1}\hat{C}) ds$.

Equations (47) and (48) represent FG decompositions of $\exp\{M(t)\}$ and $\exp\{N(t)\}$, respectively.

Proof. There exists a neighborhood $\mathscr V$ of I such that every $A \in \mathscr V$ has an FG decomposition. Choose $\tilde t > 0$ such that $\exp\{M(t)\} \in \mathscr V$ and

 $\exp\{N(t)\}\in\mathscr{V}$ for all $t\in[0,\tilde{t})$, and let $F(t),Z(t)\in\mathscr{F}$ and $G(t),R(t)\in\mathscr{G}$ be defined uniquely on $[0,\tilde{t})$ by (47) and (48). Clearly F(0)=G(0)=Z(0)=R(0)=I. Define C(t) and D(t) by $C(t)=F(t)^{-1}\hat{C}Z(t)$ and $D(t)=F(t)^{-1}\hat{D}Z(t)$. Then $C(0)=\hat{C}$ and $D(0)=\hat{D}$. The next step is to differentiate (47) and (48). Notice that

$$\frac{d}{dt}\exp\{M(t)\}=f(t,\hat{C}\hat{D}^{-1})\exp\{M(t)\}.$$

This would be obvious if M(t) were a scalar-valued function. It is false in general for matrix functions because of noncommutativity, but it is valid in this case because all matrices involved are functions of $\hat{C}\hat{D}^{-1}$. Differentiating (47), we have

$$f(t,\hat{C}\hat{D}^{-1})\exp\{M(t)\} = \dot{F}(t)G(t) + F(t)\dot{G}(t).$$

Multiplying on the left by $F(t)^{-1}$ and on the right by $G(t)^{-1}$, and noting that $C(t)D(t)^{-1} = F(t)^{-1}\hat{C}\hat{D}^{-1}F(t)$, we find that

$$f(t,C(t)D(t)^{-1}) = F(t)^{-1}\dot{F}(t) + \dot{G}(t)G(t)^{-1}.$$
 (49)

Since $F(t)^{-1}\dot{F}(t) \in \Lambda(\mathscr{F})$ and $\dot{G}(t)G(t)^{-1} \in \Lambda(\mathscr{G})$, we see that (49) gives the unique decomposition of $f(t,C(t)D(t)^{-1})$ into components in $\Lambda(\mathscr{F})$ and $\Lambda(\mathscr{G})$:

$$F^{-1}\dot{F} = \rho(f(t, CD^{-1}))$$
 and $\dot{G}G^{-1} = \sigma(f(t, CD^{-1}))$.

Rearranging these equations, we find that F and G are the unique solutions of (43) and (44), respectively. We now differentiate (48) and perform an analogous sequence of manipulations to find that Z and R are the unique solutions of (45) and (46), respectively. Since (43) and (45) have the form (16,17), C(t) must satisfy a differential equation of the form (15). This is just the first equation of (41). Similarly D(t) must satisfy the second equation of (41). Since the right-hand side of (41) satisfies a Lipschitz condition on compact sets, the solution is unique. Our definition of C(t) and D(t) establishes half of (42). The other half follows from the fact that (41) can also be written as

$$\dot{C} = \sigma(f(t, CD^{-1}))C - C\sigma(f(t, D^{-1}C)), \qquad C(0) = \hat{C},$$

$$\dot{D} = \sigma(f(t, CD^{-1}))D - D\sigma(f(t, D^{-1}C)), \quad D(0) = \hat{D}.$$

Each of these equations has the form (18), so $C(t) = G(t)\hat{C}R(t)^{-1}$ and $D(t) = G(t)\hat{D}R(t)^{-1}$. This completes the proof.

Our proof was based on the differentiation formula

$$\frac{d}{dt}\exp\{P(t)\}=\dot{P}(t)\exp\{P(t)\}.$$

One can just as well use the formula

$$\frac{d}{dt}\exp\{P(t)\}=\exp\{P(t)\}\dot{P}(t).$$

In this case one defines C and D by $C(t) = G(t)\hat{C}R(t)^{-1}$ and D(t) = $G(t)\hat{D}R(t)^{-1}$ and works in the opposite direction.

Taking F and S as in Examples 2.1L, 2.1Q, 2.1S, and 2.1H, we get families of flows which we will call LZ, QZ, SZ, and HZ flows, respectively.

Singularities in the Flows

Just as in [21], one can show that the flow (41) has singularities at exactly those t for which one of the FG decompositions (47, 48) fails to exist. Thus QZ flows never have singularities. All of the other types of flows which we have considered can have singularities. A flow can be continued after a singularity provided that the decompositions (47) and (48) exist after the singularity. This is always the case for LZ and SZ flows with autonomous differential equations (21), because the points at which the decompositions fail to exist are isolated in time [21]. For general LZ and SZ flows (41) we cannot say categorically that the singularities are isolated, because M(t) and N(t) are not necessarily analytic. It is nevertheless generically true that the singularities are isolated. In order to extend the HZ flows one must extend the definition of the HR decomposition as in [1-3, 21]. The definition of the generalized HZ flows can then be extended in a natural way. There is no need to carry out that extension here, since the important ideas are already given in [21].

The Connection Between Generalized FGZ Algorithms and Flows

Theorem 6.2. Let φ be a locally analytic function defined on an open set containing the common spectrum of $\hat{C}\hat{D}^{-1}$ and $\hat{D}^{-1}\hat{C}$, and let all other terms be as defined earlier in this section. Suppose

$$\int_{j-1}^{j} f(s,x) ds = \log p_{j}(\varphi(x)), \qquad j = 1, 2, 3, \dots$$
 (50)

(a) If $\hat{A}\hat{B}^{-1} = \varphi(\hat{C}\hat{D}^{-1})$, then the generalized FGZ algorithm based on p_1, p_2, p_3, \ldots , with initial pair \hat{A} , \hat{B} , and the generalized FGZ flow based on f, with initial pair \hat{C} , \hat{D} , are related by

$$A_i B_i^{-1} = \varphi(C(i)D(i)^{-1}), \quad i = 0, 1, 2,$$

(b) If $\hat{B}^{-1}\hat{A} = \varphi(\hat{D}^{-1}\hat{C})$, then the generalized FGZ algorithm based on p_1, p_2, p_3, \ldots , with initial pair \hat{A} , \hat{B} , and the generalized FGZ flow based on f, with initial pair \hat{C} , \hat{D} , are related by

$$B_i^{-1}A_i = \varphi(D(i)^{-1}C(i)), \quad i = 0, 1, 2,$$

Proof. Suppose $\hat{A}\hat{B}^{-1} = \varphi(\hat{C}\hat{D}^{-1})$. Substituting $\hat{C}\hat{D}^{-1}$ for x in (50), summing j from 1 to i, and taking exponents, we find that for i = 1, 2, 3, ...,

$$\exp\left\{\int_0^i f(s,\hat{C}\hat{D}^{-1}) ds\right\} = \prod_{j=1}^i p_j(\hat{A}\hat{B}^{-1}).$$

Then by (39) and (47) with t = i, we have $F(i)G(i) = F_iG_i$ for i = 0, 1, 2, ...By the uniqueness of the FG decomposition, $F(i) = F_i$ and $G(i) = G_i$, i = 0, 1, 2, ... Therefore

$$A_{i}B_{i}^{-1} = F_{i}^{-1}\hat{A}\hat{B}^{-1}F_{i} = F(i)^{-1}\varphi(\hat{C}\hat{D}^{-1})F(i) = \varphi(C(i)D(i)^{-1})$$

for i = 0, 1, 2, ... This proves the first assertion. The proof of the second assertion is similar.

If we take $\varphi(x) = x$, we get a flow which interpolates the FGZ algorithm:

THEOREM 6.3. Suppose f and p_1, p_2, p_3, \ldots are related by

$$\int_{j-1}^{j} f(s, x) ds = \log p_{j}(x), \qquad j = 1, 2, 3, \dots$$
 (51)

Then the generalized FGZ algorithm based on p_1, p_2, p_3, \ldots , with initial pair \hat{A} , \hat{B} , and the generalized FGZ flow based on f, with initial pair \hat{C} , $\hat{D} = \hat{A}$, \hat{B} , are related by

$$A_i = C(i), \quad B_i = D(i), \quad i = 0, 1, 2, \dots$$

Proof. Substituting $\hat{A}\hat{B}^{-1}$ (= $\hat{C}\hat{D}^{-1}$) into (51), summing j from 1 to i, and taking exponents, we find that

$$\exp\left\{\int_0^i f(s,\hat{C}\hat{D}^{-1}) ds\right\} = \prod_{j=1}^i p_j(\hat{A}\hat{B}^{-1}).$$

Similarly

$$\exp\left\{\int_0^i f(s, \hat{D}^{-1}\hat{C}) ds\right\} = \prod_{j=1}^i p_j(\hat{B}^{-1}\hat{A}).$$

Comparing (39) and (40) with (47) and (48), respectively, and invoking the uniqueness of FG decompositions, we find that $F(i) = F_i$, $G(i) = G_i$, $Z(i) = Z_i$, and $R(i) = R_i$, for $i = 0, 1, 2, \ldots$ Thus

$$A_i = F_i^{-1} \hat{A} Z_i = F(i)^{-1} \hat{C} Z(i) = C(i),$$

$$B_i = F_i^{-1} \hat{B} Z_i = F(i)^{-1} \hat{D} Z(i) = D(i)$$

for i = 0, 1, 2, ...

REMARK. We could have drawn the same conclusion using G and R^{-1} instead of F^{-1} and Z.

Provided that $p_1, p_2, p_3,...$ are chosen so that $\log p_i(\hat{C}\hat{D}^{-1})$ and $\log p_i(\hat{D}^{-1}\hat{C})$ are always meaningful, there are many ways to choose f(t,x) so that the equations (51) are satisfied. Some examples are given in [21] (Examples 9.4–9.7). There is no need to repeat them here.

7. RELATIONSHIP TO FLOWS ASSOCIATED WITH THE SVD

There is some overlap between the flows discussed in this paper and the flows associated with the singular-value decomposition which we discussed in [22]. Consider the flow (41) in the case when FG is QR. In this case $\rho(M)$ is skew-Hermitian for all M. Using this fact and the identity $(d/dt)(D^{-1}) = -D^{-1}\dot{D}D^{-1}$, we find that the differential equation for D can be transformed to

$$\frac{d}{dt}(D^{*-1}) = D^{*-1}\rho(f(t,D^{-1}C)) - \rho(f(t,CD^{-1}))D^{*-1}.$$

Thus D^{*-1} and C satisfy the same differential equation. It follows that if $\hat{D}^{*-1} = \hat{C}$, then $D(t)^{*-1} = C(t)$ for all t. Thus (41) reduces to the single matrix differential equation

$$\dot{C} = C\rho(f(t, C^*C)) - \rho(f(t, CC^*))C, \qquad C(0) = \hat{C},$$

which is exactly the form of the flows considered in [22], except that in [22] we allowed singular and even nonsquare C.

REFERENCES

- 1 M. A. Brebner and J. Grad, Eigenvalues of $Ax = \lambda Bx$ for real symmetric matrices A and B computed by reduction to a pseudosymmetric form and the HR process, Linear Algebra Appl. 43:99-118 (1982).
- W. Bunse and A. Bunse-Gerstner, Numerische Lineare Algebra, B. G. Teubner, Stuttgart, 1985.
- 3 A. Bunse-Gerstner, An analysis of the HR algorithm for computing the eigenvalues of a matrix, Linear Algebra Appl. 35:155-178 (1981).
- 4 A. Bunse-Gerstner, Matrix factorizations for symplectic QR-like methods, Linear Algebra Appl. 83:49-77 (1986).
- 5 P. M. Cohn, Lie Groups, Cambridge U.P., 1957.
- 6 M. Chu, The generalized Toda flow, the *QR* algorithm, and the centre manifold theory, *SIAM J. Algebraic Methods* 5:187-201 (1984).
- 7 M. Chu, A differential equation approach to the singular value decomposition of bidiagonal matrices, *Linear Algebra Appl.* 80:71-80 (1986).
- 8 M. Chu, A continuous approximation to the generalized Schur decomposition, Linear Algebra Appl. 78:119-132 (1986).
- 9 P. Deift, T. Nanda, and C. Tomei, Differential equations for the symmetric eigenvalue problem, SIAM J. Numer. Anal. 20:1-22 (1983).

- 10 G. Golub and C. Van Loan, Matrix Computations, Johns Hopkins U.P., Baltimore, 1983.
- S. Helgason, Differential Geometry, Lie Groups and Symmetric Spaces, Aca-11 demic, New York, 1978.
- 12 L. Kaufman, The LZ algorithm to solve the generalized eigenvalue problem, SIAM J. Numer. Anal. 11:997-1024 (1974).
- C. B. Moler and G. W. Stewart, An algorithm for generalized matrix eigenvalue problems, SIAM J. Numer. Anal. 10:241-256 (1973).
- 14 T. Nanda, Isospectral Flows on Band Matrices, Doctoral Dissertation, Courant Inst., New York, 1982.
- 15 T. Nanda, Differential equations and the QR algorithm, SIAM J. Numer. Anal. 22:310-321 (1985).
- 16 H. Rutishauser, Ein Infinitesimales Analogon zum Quotienten-Differenzen-Algorithmus, Arch. Math. 5:132-137 (1954).
- H. Rutishauser, Solution of eigenvalue problems with the LR-transformation, Nat. Bur. Standards Appl. Math. Ser. 49:47-81 (1958).
- 18 W. W. Symes, The QR algorithm and scattering for the finite nonperiodic Toda lattice, Phys. D 4D:275-280 (1982).
- 19 F. W. Warner, Foundations of Differentiable Manifolds and Lie Groups, Springer, New York, 1983.
- 20 D. S. Watkins, Isospectral flows, SIAM Rev. 26:379-391 (1984).
- D. S. Watkins and L. Elsner, Self-similar flows, Linear Algebra Appl.,
- 22 D. S. Watkins and L. Elsner, Self-equivalent flows associated with the singularvalue decomposition, SIAM J. Matrix Anal. Appl. 10 (1989), to appear.

Received 18 February 1988; final manuscript accepted 9 September 1988