Self-Similar Flows

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ABSTRACT

Large classes of self-similar (isospectral) flows can be viewed as continuous analogues of certain matrix eigenvalue algorithms. In particular there exist families of flows associated with the QR, LR, and Cholesky eigenvalue algorithms. This paper uses Lie theory to develop a general theory of self-similar flows which includes the QR, LR, and Cholesky flows as special cases. Also included are new families of flows associated with the SR and HR eigenvalue algorithms. The basic theory produces analogues of unshifted, single-step eigenvalue algorithms, but it is also shown how the theory can be extended to include flows which are continuous analogues of shifted and multiple-step eigenvalue algorithms.

1. INTRODUCTION

W. W. Symes [29] discovered that the finite, nonperiodic Toda flow [14, 22] is a continuous analogue of the well-known QR algorithm [15, 31, 33]. Generalizations of the Toda flow were made in [10, 12, 23, 24]. All of these generalizations are related to the QR algorithm, so we refer to them as QR flows. In [32] a family of LR *flows*, flows related to the LR eigenvalue

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algorithm, was introduced. In this paper we use elementary Lie theory to develop a general theory of self-similar flows, in which the QR and LR flows appear as special cases. Other interesting special cases are flows associated with the SR algorithm [5, 8], and the HR algorithm [4–6]. We refer to the eigenvalue algorithms collectively as FG algorithms. We will establish the existence of FG flows associated with a very general class of FG algorithms.

Very recently we discovered that the theory of self-similar flows is older than we had thought. The basic LR flow was developed by Rutishauser in the fifties. The paper [27], one of the earliest works on the LR algorithm, contains a section in which the flow is derived as a limiting case of the LR algorithm. All of the important equations associated with the flow are given, but the interpolation property of the flow is not mentioned. Even earlier Rutishauser [26] derived a continuous analogue of the quotient-difference algorithm, the predecessor of the LR algorithm. See also [17]. These developments seem to have been overlooked up to now.

The flows which we are studying are known as isospectral flows because the evolution of each such flow is described by a square matrix $B(t)$ whose spectrum is invariant in time. This isospectral property follows from the fact that $B(t) = F(t)^{-1}B(0)F(t)$ for some nonsingular $F(t)$. Thus, for all t, $B(t)$ is similar to the initial matrix $B(0)$. In general this self-similarity property is stronger than the isospectral property, so we have decided to adopt the new name *self-similar flows*.

In Section 2 we characterize the differential equations which give rise to selfsimilar flows, and in Section 3 we discuss the general properties of FG algorithms. In Section 4 we establish the connection between self-similar flows and FG algorithms but do not establish the existence of flows associated with FG algorithms. Section 5 summarizes the required material on Lie groups and Lie algebras and introduces the examples associated with the special cases QR, LR, SR, and HR. Section 6 draws on the Lie theory to establish the existence of self-similar flows associated with FG algorithms. Section 7 handles the problem of continuing an FG flow after a singularity. The HR flows, like the HR algorithm, present special difficulties in this regard. These problems are addressed in Section 8.

In Section 9 we make a further generalization which includes flows associated with shifted, double-step, and other multiple-step FG algorithms. Section 10 generalizes in a different direction to include the Cholesky flows of [32]. Finally, in Section 11 we present some simple theorems which show which special structures such as bandedness and symmetry properties, when present in the initial condition, are preserved by the various classes of FG flows.

This paper is by no means the first to use Lie theory in the study of the Toda flow and its generalizations. Other works are [1, 2, 19, 25, 28]. All of the flows considered in these papers are QR flows. The reason for this is that the generalizations have been inspired by the classical theory of semisimple Lie algebras [16]. In this theory the important group decompositions all have a compact factor. In specific examples this compact factor is just a subgroup of the unitary group. In order to obtain flows associated with the LR, SR, and HR algorithms, one must consider group decompositions which do not have a compact factor.

A recent paper by Chu and Norris [11] studies classes of flows which are more general in the sense that they are generated by subspace decompositions which are not necessarily Lie algebra decompositions.

All matrices appearing in this paper are square matrices with real or complex entries.

2. THE DIFFERENTIAL EQUATION OF A SELF-SIMILAR FLOW

Each of the self-similar flows studied in [32] and elsewhere arises from a matrix differential equation of the form

$$\dot{B} = BC - CB = [B, C].$$

Indeed one can prove the following theorem (cf. Lax [20], Flaschka [14]), which shows that just about any differential equation of this form gives rise to a self-similar flow.

THEOREM 2.1.

(a) *Consider the initial-value problem*

$$\dot{B} = [B, C] \qquad B(0) = \hat{B} \in \mathbf{C}^{n\times n}, \tag{1}$$

where $C = C(t, B)$ *is Lipschitz continuous in a neighborhood of* $(0, \hat{B})$. *Then* (1) *has a unique solution* $B(t)$ *in some nonempty interval* $[0, \hat{t})$. *The solution satisfies*

$$B(t) = F(t)^{-1}\hat{B}F(t), \tag{2}$$

where $F(t)$ *is the solution of the initial-value problem*

$$\dot{F}(t) = F(t)C(t, B(t)), \qquad F(0) = I. \tag{3}$$

(b) *Conversely, suppose B satisfies* (2), *where F is some differentiable matrix function satisfying $F(0) = I$. Then $B(t)$ satisfies an initial-value problem of the form* (1), *where C is given by $C(t) = F(t)^{-1}\dot{F}(t)$.*

Proof. (a): The fact that (1) has a unique local solution is classical. The linear initial-value problem (3) also has a unique solution F on $[0, \hat{t})$. $F(t)$ is nonsingular throughout $[0, \hat{t})$; its inverse is the unique solution of the initial-value problem $\dot{H} = -CH$, $H(0) = I$. To see that B satisfies (2), let $\tilde{B}(t) = F(t)^{-1}\hat{B}F(t)$. Differentiate $\tilde{B}$ to show that $\tilde{B}$ satisfies (1). By the uniqueness of the solution, $\tilde{B} = B$. (b): Conversely, suppose B satisfies (2), and define C by $C = F^{-1}\dot{F}$. Just differentiate B to verify that it satisfies (1). ∎

Obviously a self-similar flow can also be expressed in the form $B(t) = G(t)\hat{B}G(t)^{-1}$. In analogy with Theorem 2.1 we have

THEOREM 2.1′.

(a) *Consider the initial-value problem*

$$\dot{B} = [E, B], \qquad B(0) = \hat{B} \in \mathbf{C}^{n\times n}, \tag{4}$$

where $E = E(t, B)$ is Lipschitz continuous in a neighborhood of $(0, \hat{B})$. Then (4) *has a unique solution $B(t)$ in some nonempty interval $[0, \hat{t})$. The solution satisfies*

$$B(t) = G(t)\hat{B}G(t)^{-1}, \tag{5}$$

where $G(t)$ is the solution of the initial-value problem

$$\dot{G}(t) = E(t, B(t))G(t), \qquad G(0) = I. \tag{6}$$

(b) *Conversely, suppose B satisfies* (5), *where G is some differentiable matrix function satisfying $G(0) = I$. Then $B(t)$ satisfies an initial-value problem of the form* (4), *where E is given by $E(t) = \dot{G}(t)G(t)^{-1}$.*

The proof is analogous to that of Theorem 2.1. Of course Theorems 2.1 and 2.1′ say the same thing. If we take $E = -C$, then (4) is identical to (1), F^{-1} is the solution of (6), and consequently $F^{-1} = G$. Thus (5) and (2) are also identical. The reason for writing the theorem in two different ways is that it is sometimes convenient to take $E \neq -C$. For example, compare the differential equations (1) and (4) when C and E are chosen so that $C + E = B$.

It is easy to check that they are identical. The reason this works is that B commutes with itself. In fact, (1) and (4) are identical if and only if $C+E$ commutes with B. Consider, therefore, the more general situation in which $C(t,B)+E(t,B)=f(t,B)$, where for each $\tilde{t}$, $f(\tilde{t},x):\mathbf{C}\to\mathbf{C}$ is a function defined on the spectrum of $\hat{B}$. Then since $f(t,B)$ commutes with B, (1) and (4) are identical. It follows that the self-similar solution $B(t)$ can be expressed in two different ways: $B(t)=F(t)^{-1}\hat{B}F(t)=G(t)\hat{B}G(t)^{-1}$, where $G(t)\neq F(t)^{-1}$.

3. ALGORITHMS OF QR TYPE (FG ALGORITHMS)

The finite, nonperiodic Toda flow and most of the generalizations which have appeared in the literature are continuous analogues of the QR algorithm for calculating the eigenvalues of a matrix. The LR (or LU) flows introduced in [32] are related in the same way to the LR eigenvalue algorithm. These algorithms have the following general properties: Associated with each algorithm is a pair of sets $\mathscr{F}$ and $\mathscr{G}$, each of which is a closed subgroup of the general linear group $\mathrm{GL}_n(\mathbf{F})$ ($\mathbf{F}=\mathbf{R}$ or $\mathbf{C}$), such that $\mathscr{F}\cap\mathscr{G}=\{I\}$. The latter property guarantees that each $A\in\mathrm{GL}_n(\mathbf{F})$ has at most one factorization of the form $A=FG$, where $F\in\mathscr{F}$ and $G\in\mathscr{G}$. Such a factorization will be called an FG *decomposition*. Starting from a given matrix $\hat{A}\in\mathrm{GL}_n(\mathbf{F})$, the algorithm produces a sequence of matrices $\hat{A}=A_0, A_1, A_2,\dots$ as follows: A_i is factored into a product $A_i=\overline{F}_{i+1}\overline{G}_{i+1}$, where $\overline{F}_{i+1}\in\mathscr{F}$ and $\overline{G}_{i+1}\in\mathscr{G}$. Then the factors are multiplied together in the reverse order to yield A_{i+1}. Thus

$$A_i=\overline{F}_{i+1}\overline{G}_{i+1},\qquad \overline{G}_{i+1}\overline{F}_{i+1}=A_{i+1}. \tag{7}$$

We will refer to this general scheme as an FG *algorithm*. It is not guaranteed that every A_i has an FG decomposition. If some A_i fails to have an FG decomposition, the algorithm breaks down.

In the QR algorithm $\mathscr{F}$ is taken to be the subgroup of unitary matrices, and $\mathscr{G}$ is the subgroup of upper triangular matrices with positive entries on the main diagonal. Since every $A\in\mathrm{GL}_n(\mathbf{C})$ can be expressed as a product of matrices of this form, the QR algorithm never fails to produce an infinite sequence. In the LR algorithm $\mathscr{F}$ is taken to be the subgroup of unit lower triangular matrices, and $\mathscr{G}$ is the subgroup of nonsingular upper triangular matrices. Since not every nonsingular matrix has an LR decomposition, this algorithm sometimes breaks down. Other FG algorithms are the SR and HR algorithms, which will be introduced in Section 5.

There are two fundamental relationships which are satisfied by every *FG* algorithm. The first is self-similarity: every A_i is similar to the starting matrix A. From (7) we see immediately that

$$A_{i+1} = \bar{F}_{i+1}^{-1} A_i \bar{F}_{i+1} = \bar{G}_{i+1} A_i \bar{G}_{i+1}^{-1}, \qquad i = 0, 1, 2, \ldots .$$

Letting

$$F_m = \bar{F}_1 \bar{F}_2 \cdots \bar{F}_m \in \mathscr{F}, \qquad G_m = \bar{G}_m \bar{G}_{m-1} \cdots \bar{G}_1 \in \mathscr{G},$$

we have

$$A_m = F_m^{-1} \hat{A} F_m = G_m \hat{A} G_m^{-1}, \qquad m = 0, 1, 2, \ldots . \tag{8}$$

Thus (A_m) is a discrete analogue of a self-similar flow. In particular the spectrum is preserved. The second fundamental relationship is

$$\hat{A}^m = F_m G_m, \qquad m = 0, 1, 2, \ldots . \tag{9}$$

This is easily proved by induction on m. Since $F_m \in \mathscr{F}$ and $G_m \in \mathscr{G}$, (9) gives the unique *FG* decomposition of $\hat{A}^m$. If $\mathscr{F}$, $\mathscr{G}$, and $\hat{A}$ satisfy certain conditions, it can be proved that the sequence (A_m) converges to triangular form or some other simple form from which the eigenvalues of $\hat{A}$ can be obtained. The key equation in the convergence proof is (9).

4. THE CONNECTION BETWEEN SELF-SIMILAR FLOWS AND *FG* ALGORITHMS

Let $\mathscr{F}$ and $\mathscr{G}$ be two closed subgroups of $GL_n(\mathbb{F})$ such that $\mathscr{F} \cap \mathscr{G} = \{I\}$. (One more hypothesis will be added in Section 6.) There is an *FG* algorithm associated with this pair of subgroups. Let us see how we might associate self-similar flows with this *FG* algorithm.

Every self-similar flow satisfies

$$B(t) = F(t)^{-1} \hat{B} F(t) \tag{10}$$

for some differentiable F with $F(0) = I$. Let us suppose we have in hand a flow which satisfies a number of specific properties. To begin with, suppose $F(t) \in \mathcal{F}$ for all t. Suppose further that the flow has a second description

$$B(t) = G(t)\hat{B}G(t)^{-1}, \tag{11}$$

where $G(0) = I$ and $G(t) \in \mathcal{G}$ for all t. Associated with the functions $F(t)$ and $G(t)$, respectively, are functions $C(t) = F(t)^{-1}\dot{F}(t)$ and $E(t) = \dot{G}(t)G(t)^{-1}$. The fact that (10) and (11) describe the same flow implies that $C(t) + E(t)$ commutes with $B(t)$ for all t. Let us make the final assumption that there exists a function f defined on the spectrum of $\hat{B}$ such that

$$C(t) + E(t) = f(B(t)) \qquad \forall t \geqslant 0. \tag{12}$$

This is consistent with the commutativity requirement.

How is this flow related to the FG algorithm? Equations (10) and (11) are analogues of (8). We also need an equation which corresponds to (9). An analogue of (9) would have the form

$$\hat{A}^t = F(t)G(t). \tag{13}$$

To obtain necessary conditions for this equation, differentiate both sides:

$$\begin{aligned}(\ln \hat{A})\hat{A}^t &= \dot{F}G + F\dot{G} \\ &= FCG + FEG \\ &= Ff(B)G \\ &= F\left[F^{-1}f(\hat{B})F\right]G \\ &= f(\hat{B})FG \\ &= f(\hat{B})\hat{A}^t.\end{aligned} \tag{14}$$

Since $\hat{A}^t$ is nonsingular, we conclude that $\ln \hat{A} = f(\hat{B})$; that is, $\hat{A} = e^{f(\hat{B})}$. This establishes the relationship which $\hat{A}$ and $\hat{B}$ must satisfy. Furthermore, a second look at the chain of equations (14) reveals that $F(t)G(t)$ is a solution of the initial-value problem

$$\dot{K} = f(\hat{B})K, \qquad K(0) = I.$$

This problem has the unique solution $K = e^{f(\hat{B})t}$. Thus

$$e^{f(\hat{B})t} = F(t)G(t). \tag{15}$$

This is the analogue of (9). Of course this is the same as (13) if $\hat{A} = e^{f(\hat{B})}$.

The connection between the flow and the FG algorithm is this: If the initial matrices $\hat{A}$ and $\hat{B}$ are related by $\hat{A} = e^{f(\hat{B})}$, then

$$A_m = e^{f(B(m))}, \qquad m = 0, 1, 2, \dots . \tag{16}$$

If it happens that $f(x) = \ln x$, then

$$A_m = B(m), \qquad m = 0, 1, 2, \dots .$$

That is, the values of the self-similar flow at integer times coincide with the iterates of the FG algorithm. To prove (16) compare (15) at $t = m$ with its analogue (9). Since $\hat{A} = e^{f(\hat{B})}$, and the FG decomposition is unique,

$$F(m) = F_m, \quad G(m) = G_m, \qquad m = 0, 1, 2, \dots .$$

From (10), $e^{f(B(t))} = F(t)^{-1} e^{f(\hat{B})} F(t) = F(t)^{-1} \hat{A} F(t)$. Thus, at integer times,

$$e^{f(B(m))} = F_m^{-1} \hat{A} F_m. \tag{17}$$

Comparing (17) with (8), we obtain (16).

In order to obtain this connection we made a number of assumptions about the flow: $F(t) \in \mathscr{F}$, $G(t) \in \mathscr{G}$, and $C(t) + E(t) = f(B(t))$. How can we construct a flow which satisfies these conditions? As we shall see, the key results come from Lie theory. The requirement that $F(t) \in \mathscr{F}$ for all t implies that the related function $C(t)$ must lie in $\Lambda(\mathscr{F})$ for all t, where $\Lambda(\mathscr{F})$ denotes the Lie algebra associated with $\mathscr{F}$. Similarly, the condition $G(t) \in \mathscr{G}$ for all t implies that $E(t) \in \Lambda(\mathscr{G})$ for all t. Thus Equation (12) amounts to a Lie-algebra decomposition. In order to satisfy (12) we must be able to express $f(B(t))$ (which could be any matrix) as a sum of two matrices, one from $\Lambda(\mathscr{F})$, the other from $\Lambda(\mathscr{G})$. We shall see that if such a Lie algebra decomposition exists, then the FG decomposition (15) also exists for t in some interval $0 \leqslant t < \hat{t}$. The existence of the FG flow follows.

5. SUMMARY OF LIE-THEORETIC RESULTS

We summarize briefly the results on Lie groups and Lie algebras which we will need. This section also introduces the principal examples which will be used to illustrate the theory. Some good references to Lie theory are [3, 9, 13, 16, 18, 30]. A *Lie group* is an analytic manifold which has a group structure whose multiplication and inversion operations are continuous with respect to the topology of the manifold. The general linear group $GL_n(\mathbf{C})$ is a Lie group, and so are its closed subgroups. As matrix practitioners we prefer to work with matrices. Thus we view $GL_n(\mathbf{C})$ as a group of matrices, and we restrict our attention to $GL_n(\mathbf{C})$ and its closed subgroups. Some important examples of Lie groups of matrices are the nonsingular upper (lower) triangular matrices, the unit upper (lower) triangular matrices (1's on the main diagonal), the unitary matrices, and the real orthogonal matrices.

A Lie algebra is a real vector space on which a nonassociative multiplication operation satisfying certain properties is defined. We need not list those properties here. Two examples of Lie algebras are the real vector spaces $\mathbf{R}^{n\times n}$ and $\mathbf{C}^{n\times n}$ with the commutator product

$$[X,Y]=XY-YX.$$

A Lie *subalgebra* of $\mathbf{C}^{n\times n}$ is any subspace (under real scalar multiplication) which is closed under the commutator product. $\mathbf{R}^{n\times n}$ is a subalgebra of $\mathbf{C}^{n\times n}$. All of the Lie algebras which we shall consider are subalgebras of $\mathbf{C}^{n\times n}$. Some examples are the upper (lower) triangular matrices, the strictly upper (lower) triangular matrices, the skew-Hermitian matrices, and the real skew-symmetric matrices.

Let $\mathbf{F}=\mathbf{R}$ or $\mathbf{C}$. Associated with each Lie group $\mathscr{G}\subseteq GL_n(\mathbf{F})$ is a Lie algebra $\Lambda(\mathscr{G})$. The simplest interpretation of $\Lambda(\mathscr{G})$ is that it is the tangent space of $\mathscr{G}$ at the identity element I. This viewpoint is too simplistic for certain aspects of the theory, but it will suffice for our needs. A matrix $X\in\mathbf{F}^{n\times n}$ is a member of $\Lambda(\mathscr{G})$ if and only if there exists a differentiable function $G(t)$ defined on a neighborhood of $t=0$ such that $G(t)\in\mathscr{G}$ for all t, $G(0)=I$, and $\dot{G}(0)=X$. It follows easily from the differentiation rules $(d/dt)(G_1G_2)=\dot{G}_1G_2+G_1\dot{G}_2$ and $(d/dt)G(\alpha t)=\alpha\dot{G}(\alpha t)$ that $\Lambda(\mathscr{G})$ is a vector space over the real numbers. Its dimension equals the dimension of (the real manifold) $\mathscr{G}$. It is also easy to show that $\Lambda(\mathscr{G})$ is closed under the commutator product; that is, it is a Lie algebra. For this we need to introduce two preliminary results:

(1) If $G\in\mathscr{G}$ and $X\in\Lambda(\mathscr{G})$, then $GXG^{-1}\in\Lambda(\mathscr{G})$.

(2) If X is a differentiable function and $X(t)\in\Lambda(\mathscr{G})$ for all t, then $\dot{X}(t)\in\Lambda(\mathscr{G})$ for all t.

These are both easy to prove. Now let $X, Y \in \Lambda(\mathcal{G})$. Then there exists a function $G(t) \in \mathcal{G}$ such that $G(0) = I$ and $\dot{G}(0) = X$. From the two results just stated, $(d/dt)[G(t)YG(t)^{-1}]_{t=0}$ is a member of $\Lambda(\mathcal{G})$. Direct calculation shows that this derivative is just $[X, Y]$. Thus $[X, Y] \in \Lambda(\mathcal{G})$.

For each of the groups which we will consider, it is easy to determine the associated Lie algebra. A short list follows:

Group	Algebra
Nonsingular upper (lower) triangular	Upper (lower) triangular
Unit upper (lower) triangular	Strictly upper (lower) triangular
Unitary	Skew-Hermitian
Real orthogonal	Real skew-symmetric
Rotation	Real skew-symmetric
Symplectic	Hamiltonian

Since the tangent space at I is completely determined by the characteristics of $\mathcal{G}$ in any neighborhood of I, it can happen that two distinct subgroups of $GL_n(\mathbf{C})$ have the same Lie algebra. For example, the Lie algebra of both the orthogonal group and the rotation group is the skew-symmetric Lie algebra. Let $\kappa(\mathcal{G})$ denote the connected component of $\mathcal{G}$ which contains I. Then, since I has a connected neighborhood, $\Lambda(\kappa(\mathcal{G})) = \Lambda(\mathcal{G})$. More generally $\Lambda(\mathcal{G}_1) = \Lambda(\mathcal{G}_2)$ if and only if $\kappa(\mathcal{G}_1) = \kappa(\mathcal{G}_2)$. In particular, two connected subgroups of $GL_n(\mathbf{C})$ have the same Lie algebra if and only if they are equal.

The exponential function plays an important role in Lie theory, as it serves as a link between a Lie group and its associated Lie algebra. Indeed, for any matrix $C \in \mathbf{C}^{n\times n}$ and any Lie subgroup $\mathcal{F}$ of $GL_n(\mathbf{C})$, $C \in \Lambda(\mathcal{F})$ if and only if $e^C \in \mathcal{F}$. Another way to say this is that if $F(t)$ is the unique solution of the initial-value problem $\dot{F} = FC$, $F(0) = I$, then $F(t) \in \mathcal{F}$ for all t if and only if $C \in \Lambda(\mathcal{F})$. It turns out that this remains valid when C is allowed to vary as a function of t. This is one of the two key results for our development.

THEOREM 5.1. *Let $C(t)$ be a continuous function from $[t_0, t_1]$ into $\mathbf{C}^{n\times n}$, and let $F(t)$ be the solution of an initial-value problem*

$$\dot{F} = FC, \qquad F(t_0) \in \mathcal{F} \tag{18}$$

on $[t_0, t_1]$, where $\mathcal{F}$ is any closed subgroup of $GL_n(\mathbf{C})$. Then $F(t) \in \mathcal{F}$ for all $t \in [t_0, t_1]$ if and only if $C(t) \in \Lambda(\mathcal{F})$ for all $t \in [t_0, t_1]$.

Proof. The hypotheses of the theorem imply that $F(t)$ is nonsingular for all $t \in [t_0, t_1]$, so $C(t) = F(t)^{-1}\dot{F}(t)$. Suppose $F(t) \in \mathscr{F}$ for all $t \in [t_0, t_1]$. To see that $C(\hat{t}) \in \Lambda(\mathscr{F})$ for $\hat{t} \in [t_0, t_1]$, simply note that the function $G(t) = F(\hat{t})^{-1}F(\hat{t}+t)$ satisfies $G(t) \in \mathscr{F}, G(0) = I$, and $\dot{G}(0) = C(\hat{t})$.

Conversely, suppose $C(t) \in \Lambda(\mathscr{F})$ for all $t \in [t_0, t_1]$. Let $\hat{t} = \sup\{t \in [t_0, t_1] \mid F(t) \in \mathscr{F}\}$. We must show that $\hat{t} = t_1$, so suppose $\hat{t} < t_1$. Since $\mathscr{F}$ is closed, $F(\hat{t}) \in \mathscr{F}$. It is easy to see that the tangent space of $\mathscr{F}$ at a given point F is just the set $\{FX \mid X \in \Lambda(\mathscr{F})\}$. Thus the quantity FC defines a time-dependent, continuously varying vector field on the manifold $\mathscr{F}$, tangent to $\mathscr{F}$. It follows that the initial-value problem $\dot{F} = FC$, $F(\hat{t}) \in \mathscr{F}$, has a unique solution $F(t) \in \mathscr{F}$ for t in some neighborhood of $\hat{t}$. This solution must coincide with the solution of (18), which is also unique. Thus $F(t) \in \mathscr{F}$ for some $t > \hat{t}$, a contradiction. ∎

A companion to Theorem 5.1 is the following.

THEOREM 5.1^T. *Let $E(t)$ be a continuous function from $[t_0, t_1]$ into $\mathbf{C}^{n\times n}$, and let $G(t)$ be the solution of an initial-value problem*

$$\dot{G} = EG, \qquad G(t_0) \in \mathscr{G}$$

on $[t_0, t_1]$, where $\mathscr{G}$ is any closed subgroup of $\mathrm{GL}_n(\mathbf{C})$. *Then $G(t) \in \mathscr{G}$ for all $t \in [t_0, t_1]$ if and only if $E(t) \in \Lambda(\mathscr{G})$ for all $t \in [t_0, t_1]$.*

This can be proved by arguments analogous to those used to prove Theorem 5.1. Alternatively the theorem can be deduced from Theorem 5.1 by taking transposes. One need only note that the transpose of a Lie group of matrices is also a group, the transpose of a Lie algebra of matrices is also a Lie algebra, and $\Lambda(\mathscr{G}^T) = \Lambda(\mathscr{G})^T$.

The next theorem is the other key result. It establishes conditions under which matrices in a neighborhood of I can be guaranteed to have an FG decomposition. As before, let $\mathbf{F} = \mathbf{R}$ or $\mathbf{C}$.

THEOREM 5.2. *Let $\mathscr{F}$ and $\mathscr{G}$ be two closed subgroups of* $\mathrm{GL}_n(\mathbf{F})$ *such that $\mathscr{F} \cap \mathscr{G} = \{I\}$. (Thus $\Lambda(\mathscr{F}) \cap \Lambda(\mathscr{G}) = \{0\}$.) Suppose $\mathbf{F}^{n\times n} = \Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G})$. Then there exists an open set $\mathscr{U} \subseteq \mathrm{GL}_n(\mathbf{F})$ containing I, such that every $A \in \mathscr{U}$ can be expressed (uniquely) as a product $A = FG$, where $F \in \mathscr{F}$ and $G \in \mathscr{G}$.*

Proof. (Cf. [16, Lemma 2.4, p. 115].) Let $X_1, \ldots, X_j$ be a basis for (the real vector space) $\Lambda(\mathscr{F})$, and $X_{j+1}, \ldots, X_k$ a basis for $\Lambda(\mathscr{G})$. Then $X_1, \ldots, X_k$

is a basis for (the real vector space) $\mathbf{F}^{n\times n}$. The map

$$(c_1,\ldots,c_k)\to \exp\left(\sum_{i=1}^{j} c_i X_i\right)\exp\left(\sum_{i=j+1}^{k} c_i X_i\right)$$

is an analytic map of $\mathbf{R}^k$ into $GL_n(\mathbf{F})$. Since its Jacobian is nonzero at $(c_1,\ldots,c_k)=0$, it maps some neighborhood of zero injectively onto a neighborhood $\mathscr{U}$ of I in $GL_n(\mathbf{F})$. Thus every $A\in\mathscr{U}$ is the image of some $(c_1,\ldots,c_k)$, and therefore $A=FG$, where $F=\exp(\sum_{i=1}^{j}c_iX_i)\in\mathscr{F}$ and $G=\exp(\sum_{i=j+1}^{k}c_iX_i)\in\mathscr{G}$. ∎

EXAMPLE 5.3. 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 $\mathbf{C}^{n\times n}=\Lambda(\mathscr{F})\oplus\Lambda(\mathscr{G})$. Therefore, by Theorem 5.2, there exists a neighborhood $\mathscr{U}$ of I such that every $A\in\mathscr{U}$ 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.

EXAMPLE 5.4. 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 $\mathbf{C}^{n\times n}=\Lambda(\mathscr{F})\oplus\Lambda(\mathscr{G})$. Therefore, by Theorem 5.2, there exists a neighborhood $\mathscr{U}$ of $\mathscr{I}$ such that every $A\in\mathscr{U}$ 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. 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 $\mathbf{R}^{n\times n}=\Lambda(\mathscr{F})\oplus\Lambda(\mathscr{G})$.

EXAMPLE 5.5. Define $J\in\mathbf{R}^{2n\times 2n}$ by

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

The *real symplectic group* is the set of $S \in GL_{2n}(\mathbf{R})$ such that $S^TJS = J$. Let $\mathcal{F}$ be the real symplectic group. Then $\Lambda(\mathcal{F})$ is the set of $X \in \mathbf{R}^{2n\times 2n}$ such that $(JX)^T = JX$. Matrices satisfying this equation are called *Hamiltonian*. A matrix in $\mathbf{R}^{2n\times 2n}$ is Hamiltonian if and only if it has the form

$$\begin{bmatrix} A & N \\ K & -A^T \end{bmatrix},$$

where $K = K^T$ and $N = N^T$. Let $\tilde{\mathcal{G}}$ be the subgroup of $GL_{2n}(R)$ 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} is strictly upper triangular, and G_{11} and G_{22} are nonsingular. It is not hard to show that $\tilde{\mathcal{G}}$ is a group. In fact it is the group of upper triangular matrices in disguise: Let P be the matrix of the perfect shuffle permutation, which permutes the rows via

$$k \to \begin{cases} 2k-1 & \text{if} \quad k \leqslant n, \\ 2k-2n & \text{if} \quad k > n. \end{cases}$$

Then $P\tilde{\mathcal{G}}P^T$ is exactly the group of nonsingular upper triangular matrices in $GL_{2n}(R)$. The Lie algebra $\Lambda(\tilde{\mathcal{G}})$ 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 and X_{21} is strictly upper triangular. Of course $P\Lambda(\tilde{\mathcal{G}})P^T$ is the Lie algebra of upper triangular matrices in $\mathbf{R}^{2n\times 2n}$. Let $\mathcal{G}$ be the subgroup of $\tilde{\mathcal{G}}$ consisting of those matrices for which $\operatorname{diag}\{G_{11}\} = \operatorname{diag}\{G_{22}\}$, and G_{12} is strictly upper triangular. In the corresponding Lie algebra $\operatorname{diag}\{X_{11}\} = \operatorname{diag}\{X_{22}\}$, and X_{12} is strictly upper triangular.

These groups and algebras have complex analogues. We have restricted our attention to the real case because only this case is of interest in this paper.

Again it is not hard to show that $\mathbf{R}^{2n\times 2n} = \Lambda(\mathcal{F}) \oplus \Lambda(\mathcal{G})$. Thus there exists a neighborhood $\mathcal{U}$ of I such that every $A \in \mathcal{U}$ can be expressed as a product $A = FG$, where F is symplectic and $G \in \mathscr{G}$. This is also known. In [5] and [7], for example, it is shown that almost every $A \in \mathrm{GL}_{2n}(\mathbf{R})$ has such a decomposition. All that is required is that the leading even principal minors of PA^TJAP^T be nonzero. This is called the *SR* decomposition. There is no complex variant of this theorem [5, p. 247; 7]. The *SR* decomposition gives rise to the *SR* algorithm, which is useful for calculating the eigenvalues of Hamiltonian matrices [8]. The Hamiltonian eigenvalue problem arises in the problem of solving the algebraic Riccati equation of control theory [9].

EXAMPLE 5.6. Let $J \in \mathrm{GL}_n(\mathbf{C})$ 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 $G \in \mathrm{GL}_n(\mathbf{C})$ such that $G^*JG = J$. Then $\Lambda(\mathscr{F})$ is the set of $X \in \mathbf{C}^{n\times n}$ 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 $\mathbf{C}^{n\times n} = \Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G})$. Therefore there is a neighborhood $\mathscr{U}$ of I such that every $A \in \mathscr{U}$ can be expressed as a product $A = FG$, where F is J-unitary and G is upper triangular. This is known as the *HR* decomposition. For a more precise result see [5, p. 253] or [6], 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.

6. EXISTENCE OF FLOWS ASSOCIATED WITH *FG* ALGORITHMS

Let $\mathscr{F}$ and $\mathscr{G}$ be closed subgroups of $\mathrm{GL}_n(\mathbf{F})$ such that $\mathscr{F} \cap \mathscr{G} = I$ and $\mathbf{F}^{n\times n} = \Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G})$. Thus every $M \in \mathbf{F}^{n\times n}$ can be expressed uniquely as a sum

$$M = \rho(M) + \sigma(M), \tag{19}$$

where $\rho(M) \in \Lambda(\mathscr{F})$ and $\sigma(M) \in \Lambda(\mathscr{G})$. Equation (19) defines linear projectors $\rho: \mathbf{F}^{n\times n} \to \Lambda(\mathscr{F})$ and $\sigma: \mathbf{F}^{n\times n} \to \Lambda(\mathscr{G})$. Associated with the subspace pair $(\mathscr{F}, \mathscr{G})$ is an *FG* algorithm, as described in Section 3. The following theorem establishes the existence of associated self-similar flows.

THEOREM 6.1. *Let $\hat{B} \in \mathbf{F}^{n\times n}$, and let f be any locally analytic function defined on the spectrum of $\hat{B}$. Then, defining ρ and σ as in (19), the* *initial-value problem*

$$\dot{B} = [B, \rho(f(B))] = [\sigma(f(B)), B], \qquad B(0) = \hat{B} \tag{20}$$

has a unique solution on some nonempty interval $[0, \hat{t})$. *The solution satisfies*

$$B(t) = F(t)^{-1}\hat{B}F(t) = G(t)\hat{B}G(t)^{-1}, \qquad t \in [0, \hat{t}), \tag{21}$$

where F and G are the solutions of

$$\dot{F} = F\rho(f(B)), \qquad F(0) = I, \tag{22}$$

$$\dot{G} = \sigma(f(B))G, \qquad G(0) = I, \tag{23}$$

respectively. $F(t) \in \mathscr{F}$ *and* $G(t) \in \mathscr{G}$ *for all* $t \in [0, \hat{t})$. *They are related by the equation*

$$e^{f(\hat{B})t} = F(t)G(t), \qquad t \in [0, \hat{t}), \tag{24}$$

which gives the FG decomposition of $e^{f(\hat{B})t}$.

Proof. By Theorem 5.2 there exists a neighborhood $\mathscr{U}$ of I such that every member of $\mathscr{U}$ has an FG decomposition. For values of t near zero, $e^{f(\hat{B})t}$ lies in $\mathscr{U}$. Choose $\hat{t} > 0$ so that $e^{f(\hat{B})t} \in \mathscr{U}$ for all $t \in [0, \hat{t})$, and let $F(t) \in \mathscr{F}$ and $G(t) \in \mathscr{G}$ be uniquely defined on $[0, \hat{t})$ by (24). Clearly $F(0) = I$ and $G(0) = I$. Differentiating (24), we obtain

$$f(\hat{B})e^{f(\hat{B})t} = \dot{F}(t)G(t) + F(t)\dot{G}(t).$$

Premultiplying by $F(t)^{-1}$ and postmultiplying by $G(t)^{-1}$, we find that

$$F(t)^{-1}f(\hat{B})F(t) = F(t)^{-1}\dot{F}(t) + \dot{G}(t)G(t)^{-1}. \tag{25}$$

Define $B(t)$ for $t \in [0, \hat{t})$ by $B(t) = F(t)^{-1}\hat{B}F(t)$. Then the left-hand side of (25) is just $f(B(t))$. Let $C(t) = F(t)^{-1}\dot{F}(t)$ and $E(t) = \dot{G}(t)G(t)^{-1}$. By Theorems 5.1 and 5.1^T, respectively, $C(t) \in \Lambda(\mathscr{F})$ and $E(t) \in \Lambda(\mathscr{G})$. Thus

(25) gives the unique decomposition of $f(B(t))$ into components in $\Lambda(\mathscr{F})$ and $\Lambda(\mathscr{G})$:

$$F^{-1}\dot{F} = C = \rho(f(B)), \tag{26}$$

$$\dot{G}G^{-1} = E = \sigma(f(B)). \tag{27}$$

Applying Theorem 2.1, part (b), we see that B is a solution of the initial-value problem (20). Since the right-hand side of (20) is locally Lipschitz, this solution is unique. Rearranging (26) and (27) we find that F and G are the (unique) solutions of (22) and (23), respectively. Our definition of $B(t)$ establishes half of (21). The other half is a consequence of part (a) of Theorem 2.1′. Since (24) also holds by definition, the proof is now complete. ∎

In the proof we used the differentiation formula

$$\frac{d}{dt}e^{f(\hat{B})t} = f(\hat{B})e^{f(\hat{B})t}.$$

It is instructive to repeat the proof using the alternative formula

$$\frac{d}{dt}e^{f(\hat{B})t} = e^{f(\hat{B})t}f(\hat{B}).$$

One then defines B by $B(t) = G(t)\hat{B}G(t)^{-1}$ and applies Theorems 2.1′, part (b), and 2.1, part (a), instead of 2.1, part (b), and 2.1′, part (a).

Theorem 6.1 establishes the existence of flows satisfying all of the conditions outlined in Section 4. Thus these flows are continuous analogues of the FG algorithm, in the sense that (16) is satisfied.

EXAMPLE 6.2 (QR flows). Taking $\mathscr{F}$ to be the unitary group and $\mathscr{G}$ the group of upper triangular matrices with positive entries on the main diagonal, we obtain the QR flows.

EXAMPLE 6.3 (LR flows). Taking $\mathscr{F}$ to be the group of unit lower triangular matrices and $\mathscr{G}$ the group of nonsingular, upper triangular matrices, we obtain the LR or LU flows introduced in [32].

EXAMPLE 6.4 (*SR* flows). Taking $\mathscr{F}$ and $\mathscr{G}$ to be as in Example 5.5, we obtain the family of *SR* flows, continuous extensions of the *SR* algorithm.

EXAMPLE 6.5 (*HR* flows). Taking $\mathscr{F}$ and $\mathscr{G}$ as in Example 5.6, we obtain *HR* flows.

It is useful to restate as a theorem some of the conclusions of the proof of Theorem 6.1.

THEOREM 6.6. *Let $\mathscr{F}$, $\mathscr{G}$, $\hat{B}$, and f be as specified at the beginning of this section. Let $\mathscr{I}$ be a nonempty interval, and suppose that for all $t \in \mathscr{I}$*

$$e^{f(\hat{B})t} = F(t)G(t),$$

where $F(t) \in \mathscr{F}$ and $G(t) \in \mathscr{G}$. Let $B(t) = F(t)^{-1}\hat{B}F(t) = G(t)\hat{B}G(t)^{-1}$. Then F, G, and B satisfy the differential equations $\dot{F} = F\rho(f(B))$, $\dot{G} = \sigma(f(B))G$, and $\dot{B} = [B, \rho(f(B))] = [\sigma(f(B)), B]$, respectively, on $\mathscr{I}$.

The proof is contained in the proof of Theorem 6.1.

7. SINGULARITIES IN SELF-SIMILAR FLOWS

The existence of a solution to the initial-value problem (20) is guaranteed only on some bounded interval $[0, \hat{t})$, which could be very short. The solution fails to exist at $\hat{t}$ if and only if

$$\lim_{t \to \hat{t}-} \|B(t)\| = \infty.$$

It is clear from Theorem 6.6 that $B(t)$ cannot have such a singularity as long as $e^{f(\hat{B})t}$ has an *FG* decomposition (24). Conversely, as long as the solution exists, so does the *FG* decomposition of $e^{f(\hat{B})t}$. For suppose $B(t)$ exists and remains bounded on $[0, \hat{t}]$. Then the linear differential equations (22) and (23) each satisfy a Lipschitz condition, so they have unique solutions $F(t)$ and $G(t)$, respectively, on $[0, \hat{t}]$. By Theorems 5.1 and 5.1^T, $F(t) \in \mathscr{F}$ and $G(t) \in \mathscr{G}$ for all $t \in [0, \hat{t}]$. The equations (14) with $C = \rho(f(B))$ and $E = \sigma(f(B))$ show that the product $F(t)G(t)$ satisfies the initial-value problem $\dot{K} = f(\hat{B})K$, $K(0) = I$. Thus $e^{f(\hat{B})t} = F(t)G(t)$; that is, $e^{f(\hat{B})t}$ has an *FG* decomposition.

This answers the question of when singularities occur. Since the QR decomposition never fails to exist, the QR flows never have singularities. The other examples of flows which we have considered all can exhibit singularities.

One can also ask what happens after a singularity. The decomposition $e^{f(\hat{B})t} = F(t)G(t)$ provides a canonical way of continuing the flow, provided that this decomposition exists after the singularity. Using the $F(t)$ or the $G(t)$ so defined, we can define $B(t) = F(t)^{-1}\hat{B}F(t)$ or equivalently $B(t) = G(t)\hat{B}G(t)^{-1}$. This B satisfies the differential equation $\dot{B} = [B, \rho(f(B))] = [\sigma(f(B)), B]$.

The LR and SR flows can always be continued after a singularity, because the points (in time) at which the LR or SR decomposition fails to exist are isolated. We will prove this in the LR case, the SR case being similar. The LR decomposition fails to exist if and only if one of the leading principal minors of $e^{f(\hat{B})t}$ is zero. Let $f_i(t)$ denote the ith leading principal minor of $e^{f(\hat{B})t}$, and let $f(t) = f_1(t)f_2(t)\cdots f_n(t)$. Then $f(t)$ is an analytic function whose zeros mark the points at which $e^{f(\hat{B})t}$ fails to have an LR decomposition. Since f is analytic and nonzero, these points must be isolated.

Another way of viewing the continuation of flows is to regard $B(t)$ as a function of a complex variable. Suppose the decomposition $e^{f(\hat{B})t} = F(t)G(t)$ exists except at isolated singular points in the complex plane. The functions $F(t)$ and $G(t)$ are in fact analytic functions of the complex variable t, as is $B(t) = F(t)^{-1}\hat{B}F(t) = G(t)\hat{B}G(t)^{-1}$. Thus a singularity on the real axis can be sidestepped in a unique manner by making a short detour into the complex plane.

8. CONTINUING THE HR FLOWS

The problem of continuing the HR flows is somewhat more complicated than that of the LR and SR flows. Recall from Example 5.6 that the groups for the HR algorithm are the set of upper triangular matrices with positive main-diagonal entries and the set of J-unitary matrices—that is, the matrices satisfying $H^*JH = J$, where J is a given diagonal matrix with ± 1's on the main diagonal. Let $\mathcal{R}$ denote the former group and $\mathcal{H}$ the latter. The problem is that the set of matrices A which can be expressed as a product $A = HR$, where $H \in \mathcal{H}$ and $R \in \mathcal{R}$, is too small. This problem affects not only the HR flows, but the discrete HR algorithm as well. In the case of the discrete algorithm the problem is handled as follows: Instead of requiring that H satisfy $H^*JH = J$, it is allowed that $H^*JH = \hat{J}$, where $\hat{J}$, like J, is diagonal with ± 1's on the main diagonal. Such an H is called *$(J, \hat{J})$-unitary*. By

Sylvester's law of inertia J and $\hat{J}$ must have the same number of -1's on the main diagonal. For a given J, almost every $A \in GL_n(C)$ can be written (uniquely) as a product $A = HR$, where H is $(J, \hat{J})$-unitary for some $\hat{J}$, and $R \in \mathcal{R}$. The exact result is as follows:

THEOREM 8.1. *Given $A \in GL_n(C)$, there exist unique $(J, \hat{J})$-unitary H and $R \in \mathcal{R}$ such that $A = HR$ if and only if the ith principal minor A^*JA agrees in sign with the ith principal minor of $\hat{J}$ for $i = 1, 2, \dots, n$.*

For a proof see for example [6, Theorem 2.3] or [5, p. 253].

The only matrices which do not have an HR decomposition of any kind are those A for which one of the leading principal minors of A^*JA is zero. This is a set of Lebesgue measure zero in $C^{n \times n}$.

Modified to accommodate changes in J, the HR algorithm has the following form: Given initial $\hat{A}$ and J, let $A_0 = \hat{A}$ and $J_0 = J$. Then given A_{i-1} and J_{i-1}, the ith step produces A_i and J_i by

$$A_{i-1} = \overline{H}_i \overline{R}_i, \qquad \overline{R}_i \overline{H}_i = A_i,$$

where $\overline{H}_i$ is (J_{i-1}, J_i)-unitary and $\overline{R}_i \in \mathcal{R}$. The algorithm breaks down at step i if and only if some leading principal minor of $A_{i-1}^* J_{i-1} A_{i-1}$ is zero.

Defining $H_m = \overline{H}_1 \overline{H}_2 \cdots \overline{H}_m$ and $R_m = \overline{R}_m \cdots \overline{R}_2 \overline{R}_1$, the fundamental equations for the analysis of the HR algorithm are

$$A_m = H_m^{-1} \hat{A} H_m \tag{28}$$

$$\hat{A}^m = H_m R_m. \tag{29}$$

Notice that H_i is (J_0, J_i)-unitary.

The HR flows can be extended in the same spirit. Given $\hat{B}$, J, and f, consider the decomposition

$$e^{f(\hat{B})t} = H(t)R(t), \tag{30}$$

where $H(t)$ is $(J, J(t))$-unitary for some $J(t)$, and $R(t) \in \mathcal{R}$. This decomposition exists, provided that the leading principal minors of $A(t)^*JA(t)$ are nonzero, where $A(t) = e^{f(\hat{B})t}$. We can define $B(t)$ at all such points by

$$B(t) = H(t)^{-1} \hat{B} H(t) = R(t) \hat{B} R(t)^{-1}.$$

This flow evaluated at integer times coincides with the HR algorithm in the sense described in Section 4. That is, if $\hat{A} = e^{f(\hat{B})}$, then $A_m = e^{f(B(m))}$ for $m = 1, 2, 3, \ldots$. Indeed, (30) evaluated at integer times gives

$$\hat{A}^m = H(m)R(m).$$

Comparing this equation with (29) and recalling that the HR decomposition is unique, we conclude that $H(m) = H_m$, $R(m) = R_m$, and $J(m) = J_m$. Thus $A_m = H_m^{-1}\hat{A}H_m = H(m)^{-1}e^{f(\hat{B})}H(m) = e^{f(B(m))}$.

We note further that the flow has a singularity at each point at which $J(t)$ changes: The leading principal minors of $J(t)$ have the same sign as the leading principal minors of

$$[e^{f(\hat{B})t}]^* J [e^{f(\hat{B})t}]. \tag{31}$$

This determines $J(t)$ uniquely. In order for $J(t)$ to change, one of the leading principal minors of (31) must pass through zero; that is, the flow must have a singularity. The converse is almost true as well: If one of the leading principal minors becomes zero, this will almost always signal a change in $J(t)$. However, it can occasionally happen that the minor touches the t-axis without changing sign. In these rare cases a singularity occurs without a change in $J(t)$.

Finally we show that the function $B(t)$ also satisfies a differential equation of the form

$$\dot{B} = [B, \rho(f(B))] = [\sigma(f(B)), B], \tag{32}$$

for appropriate choices of ρ and σ, on each interval in which the flow has no singularities. Suppose $\mathscr{I}$ is an open interval in which the flow has no singularities. Throughout this interval $J(t)$ is constant, say $J(t) = \hat{J}$ for all $t \in \mathscr{I}$. Let $\mathscr{H}$ denote the group of $\hat{J}$-unitary matrices, and let ρ and σ be the unique projectors for which $M = \rho(M) + \sigma(M)$, $\rho(M) \in \Lambda(\mathscr{H})$, and $\sigma(M) \in \Lambda(\mathscr{R})$. We claim that for this choice of ρ and σ, $B(t)$ satisfies (32) on $\mathscr{I}$. Throughout $\mathscr{I}$ the HR decomposition (30) exists, where $H(t)$ is $(J, \hat{J})$-unitary. Proceeding as in the proof of Theorem 6.1 we differentiate (30) to find that

$$f(B(t)) = H(t)^{-1}\dot{H}(t) + \dot{R}(t)R(t)^{-1}.$$

Let $C(t) = H(t)^{-1}\dot{H}(t)$. At this point we would like to invoke Theorem 5.1 to conclude that $C(t) \in \Lambda(\mathscr{H})$ for all $t \in \mathscr{I}$. However Theorem 5.1 does not apply, because $H(t)$ does not belong to $\mathscr{H}$; $H(t)$ is $(J,\hat{J})$-unitary. It is nevertheless true that $C(t) \in \mathscr{L}(\mathscr{H})$. Given $\hat{t} \in \mathscr{I}$, let $H_1(t) = H(\hat{t})^{-1}H(\hat{t}+t)$. Then $H_1(t) \in \mathscr{H}$ for values of t near zero, $H_1(0) = I$, and $\dot{H}(0) = C(\hat{t})$. Therefore $C(\hat{t}) \in \Lambda(\mathscr{H})$. Now we can proceed exactly as in Theorem 6.1 to show that $B(t)$ satisfies (32) in $\mathscr{I}$. It is important to realize that the projectors ρ and σ change whenever $J(t)$ changes.

9. FLOWS ASSOCIATED WITH SHIFTED AND GENERALIZED *FG* ALGORITHMS

Generalized FG Algorithm

Let $\hat{A} \in \mathbf{F}^{n\times n}$, and let $\mathscr{F}$ and $\mathscr{G}$ be closed subgroups of $GL_n(\mathbf{F})$ such that $\mathbf{F}^{n\times n} = \Lambda(\mathscr{F}) \oplus \Lambda(\mathscr{G})$. Let $p_1, p_2, p_3, \ldots$ be a sequence of functions defined on the spectrum of $\hat{A}$, such that $p_i(\hat{A})$ is nonsingular for $i = 1,2,3,\ldots$. Let $A_0 = \hat{A}$, and for $i = 1,2,3,\ldots$ define $\overline{F}_i \in \mathscr{F}$ and $\overline{G}_i \in \mathscr{G}$ by the *FG* decomposition

$$p_i(A_{i-1}) = \overline{F}_i\overline{G}_i.$$

Then define A_i by

$$A_i = \overline{F}_i^{-1}A_{i-1}\overline{F}_i = \overline{G}_iA_{i-1}\overline{G}_i^{-1}.$$

This is the generalized *FG* algorithm. It contains the shifted *FG* algorithm as a special case: $p_i(t) = t - \sigma_i$, where $\sigma_1, \sigma_2, \sigma_3, \ldots$ is the sequence of shifts. The double-shift *FG* algorithm is gotten by taking $p_i(t) = (t-\sigma_i)(t-\tau_i)$, where (σ_i, τ_i) is the pair of shifts for the ith double step. Define

$$F_i = \overline{F}_1\overline{F}_2\cdots\overline{F}_i, \qquad G_i = \overline{G}_i\cdots\overline{G}_2\overline{G}_1.$$

The fundamental equations for the generalized *FG* algorithm are

$$A_m = F_m^{-1}\hat{A}F_m = G_m\hat{A}G_m^{-1} \tag{33}$$

and

$$p_m(\hat{A})\cdots p_2(\hat{A})p_1(\hat{A}) = F_mG_m. \tag{34}$$

The first is obvious; the second is proved by induction on m.

The goal of this section is to construct flows

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

such that $B(j) = A_j$ for $j = 0, 1, 2, \dots$ or, more generally,

$$\varphi(B(j)) = A_j, \qquad j = 0, 1, 2, \dots,$$

for some given function φ.

Generalizing the FG Flows

Let $\rho : \mathbb{F}^{n\times n} \to \Lambda(\mathcal{F})$ and $\sigma : \mathbb{F}^{n\times n} \to \Lambda(\mathcal{G})$ be the projectors defined in Section 6. Let $f(t, x)$ be a function defined on $[0,\infty)\times \mathrm{sp}(\hat{B})$, where $\mathrm{sp}(\hat{B})$ denotes the spectrum of $\hat{B}$. Suppose f is piecewise continuous in t and locally analytic in x. We will consider flows defined by differential equations of the form

$$\dot{B} = \left[B, \rho(f\{t, B(t)\})\right] = \left[\sigma(f\{t, B(t)\}), B\right], \qquad B(0) = \hat{B}. \quad (35)$$

The following generalization of Theorem 6.1 holds.

THEOREM 9.1. *The initial-value problem* (35) *has a unique solution on some nonempty interval* $[0, \hat{t})$. *The solution satisfies*

$$B(t) = F(t)^{-1}\hat{B}F(t) = G(t)\hat{B}G(t)^{-1}, \qquad (36)$$

where F and G are the solutions of

$$\dot{F} = F\rho(f\{t, B(t)\}), \qquad F(0) = I, \qquad (37)$$

$$\dot{G} = \sigma(f\{t, B(t)\})G, \qquad G(0) = I, \qquad (38)$$

respectively. $F(t) \in \mathcal{F}$ *and* $G(t) \in \mathcal{G}$ *for all* $t \in [0, \hat{t})$. *They are related by the equation*

$$\exp\left\{\int_0^t f(s, \hat{B})\,ds\right\} = F(t)G(t), \qquad (39)$$

which gives the FG decomposition of $\exp\{\int_0^t f(s, \hat{B})\,ds\}$.

Proof. The proof is the same as that of Theorem 6.1. The only significant difference is that $f(\hat{B})t$ is replaced by the integral

$$M(t) = \int_0^t f(s, \hat{B})\, ds.$$

The differentiation formulas which are needed are

$$\frac{d}{dt} e^{M(t)} = e^{M(t)} f(t, \hat{B})$$

$$= f(t, \hat{B}) e^{M(t)}.$$

They are valid because all matrices involved are functions of $\hat{B}$. Thus all commute with $\hat{B}$ and with each other. ∎

Corresponding to Theorem 6.6 we have

THEOREM 9.2. *Let $\mathcal{I}$ be any nonempty interval, and suppose that for all $t \in \mathcal{I}$*

$$\exp\left\{ \int_0^t f(s, \hat{B})\, ds \right\} = F(t)G(t),$$

where $F(t) \in \mathcal{F}$ and $G(t) \in \mathcal{G}$. Let $B(t) = F(t)^{-1}\hat{B}F(t) = G(t)\hat{B}G(t)^{-1}$. Then F, G, and B satisfy the differential equations (37), (38), *and* (35), *respectively, on $\mathcal{I}$.*

The Connection between the Generalized FG Algorithms and FG Flows

THEOREM 9.3. *Let φ be a locally analytic function defined on the spectrum of $\hat{B}$, and let all other terms be as defined earlier in this section. Suppose $\hat{A} = \varphi(\hat{B})$, and*

$$\int_{i-1}^{i} f(s, x)\, ds = \log p_i(\varphi(x)), \qquad i = 1, 2, 3, \ldots, \tag{40}$$

for all x in the spectrum of $\hat{B}$. Then the generalized FG algorithm and the FG *flow based on f are related by*

$$A_m = \varphi(B(m)), \qquad m = 0,1,2,\dots.$$

Proof. Substituting $\hat{B}$ for x in (40), summing from 1 to m, and taking exponents, we find that, for $m = 1,2,3,\dots$,

$$\exp\left(\int_0^m f(s,\hat{B})\,ds\right) = p_1(\hat{A})\cdots p_m(\hat{A}). \tag{41}$$

Then by (39) and (34)

$$F(m)G(m) = F_m G_m, \qquad m = 1,2,3,\dots.$$

By the uniqueness of the FG decomposition, $F(m) = F_m$ and $G(m) = G_m$. Thus $A_m = F_m^{-1}\hat{A}F_m = F(m)^{-1}\varphi(\hat{B})F(m) = \varphi(B(m))$. ■

Example 9.4. Define f to be the step function

$$f(t,x) = \log p_i(\varphi(x)), \quad i-1 \leqslant t < i, \qquad i = 1,2,3,\dots.$$

This f certainly satisfies (40), so it gives rise to a flow of the desired type. Since f is constant on each interval $[i-1,i)$, this flow is just a patchwork of segments of flows of the type discussed in earlier sections. At each integer time the flow is changed to correspond to a new shift.

Example 9.5. A slightly less crude example is obtained by requiring that $f(t,x)$ be piecewise linear and continuous in t. For $0 \leqslant t < 1$ define $f(t,x) = 2t\log p_1(\varphi(x))$. Then $f(0,x) = 0$ and

$$\int_0^1 f(t,x)\,dt = \log p_1(\varphi(x)). \tag{42}$$

Now suppose f has been defined for $i-1 \leqslant t < i$, and let $a_i(x) = \lim_{t\to i-} f(t,x)$. The conditions of continuity at $t = i$ and linearity in t force the form

$$f(t,x) = a_i(x) + m_i(x)(t-i), \qquad i \leqslant t < i+1, \tag{43}$$

for some $m_i(x)$. In addition (40) requires

$$\log p_{i+1}(\varphi(x)) = \int_i^{i+1} \{ a_i(x) + m_i(x)(t-i) \} \, dt = a_i(x) + \tfrac{1}{2} m_i(x).$$

Thus

$$m_i(x) = 2 \log p_{i+1}(\varphi(x)) - 2a_i(x). \tag{44}$$

Noting that $a_{i+1}(x) = \lim_{t \to i+1-} f(t,x)$, we get a recursion formula for a_i:

$$a_{i+1}(x) = a_i(x) + m_i(x). \tag{45}$$

Equations (42)–(45) specify the desired flow.

Example 9.6. Clearly the technique of the previous example can be generalized to yield a flow satisfying the conditions of Theorem 9.3 for which $f(t,x)$ is piecewise quadratic in t and C^1 at integer values of t or, more generally, piecewise a polynomial of degree j and C^{j-1} at integer times. There is no point in writing down the formulas here. The choices $j = 0$ and 1 give the flows of Examples 9.4 and 9.5, respectively.

Example 9.7. From Example 9.6 we see that there are flows of the desired type for which f is a C^j function of t, where j can be made arbitrarily large. Now we construct a flow which is C^∞ in t. Let $\psi(t) \in C_0^\infty(0,1)$ have the property $\int_0^1 \psi(t)\, dt = 1$. Define

$$f(t,x) = \psi(t-i) \log p_{i+1}(\varphi(x)), \quad i \leqslant t < i+1, \qquad i = 0,1,2,\dots.$$

Then f satisfies (40) and is a C^∞ function of t. This flow is stationary on a neighborhood of each integer.

10. FLOWS FOR WHICH $\mathcal{F} \cap \mathcal{G} \neq \{I\}$

There is at least one important situation in which the Lie-group and Lie-algebra decompositions are not unique.

Example 10.1. Let $\mathcal{F}$ and $\mathcal{G}$ denote the Lie groups of nonsingular lower and upper triangular matrices, respectively. Then $\mathcal{F} \cap \mathcal{G}$ is nontrivial;

it consists of the nonsingular diagonal matrices. It is nevertheless possible to specify uniquely a decomposition

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

where $\rho(C) \in \Lambda(\mathscr{F})$ and $\sigma(C) \in \Lambda(\mathscr{G})$, provided that we make the additional requirement

$$\operatorname{diag}\{\rho(C)\} = \operatorname{diag}\{\sigma(C)\}.$$

This decompostion leads to the Cholesky flows introduced in [32].

It is natural to ask to what extent the theorems which we have established extend to this and similar situations. It turns out that practically everything carries over. Let us suppose we have Lie groups $\mathscr{F}$ and $\mathscr{G}$ for which $\Lambda(\mathscr{F}) \cap \Lambda(\mathscr{G}) \neq \{0\}$ but $\Lambda(\mathscr{F}) + \Lambda(\mathscr{G}) = \mathbf{F}^{n\times n}$. Suppose in addition that there exist locally Lipschitz continuous functions $\rho : \mathbf{F}^{n\times n} \to \Lambda(\mathscr{F})$ and $\sigma : \mathbf{F}^{n\times n} \to \Lambda(\mathscr{G})$ such that for all $M \in \mathbf{F}^{n\times n}$

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

(This is certainly the case in Example 10.1.) Then the initial-value problem

$$\dot{B} = [B, \rho(f(B))] = [\sigma(f(B)), B], \qquad B(0) = \hat{B}$$

has a unique solution on some interval $[0, \hat{t})$ because the right-hand side of the differential equation is locally Lipschitz. By part (a) of Theorems 2.1 and 2.1′ this solution satisfies

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

where F and G are the solutions of

$$\dot{F} = F\rho(f(B)), \qquad F(0) = I,$$

$$\dot{G} = \sigma(f(B))G, \qquad G(0) = I.$$

Differentiating FG, we find as in (14) that FG satisfies the initial-value problem $\dot{K} = f(\hat{B})K$, $K(0) = I$. Thus

$$e^{f(\hat{B})t} = F(t)G(t). \tag{46}$$

While $F(t) \in \mathcal{F}$ and $G(t) \in \mathcal{G}$, it is no longer true that these conditions together with (46) specify F and G uniquely. Thus the equation (46) cannot be used to continue the flow after singularities, unless some additional condition is placed on the decomposition. In the case of the Cholesky flows such a condition exists: $\operatorname{diag}\{F(t)\} = \operatorname{diag}\{G(t)\}$.

11. PRESERVATION OF STRUCTURE

A matrix $C = (c_{ij})$ is *lower k-banded* if $c_{ij} = 0$ whenever $i - j > k$. C is *upper k-banded* if C^T is lower k-banded. C is *k-banded* if it is both upper and lower k-banded.

THEOREM 11.1. *Let $B(t)$ be the solution of an FG flow with initial condition $B(0) = \hat{B}$. If all elements of either $\mathcal{F}$ or $\mathcal{G}$ are upper (lower) triangular, and $\hat{B}$ is lower (upper) k-banded, then $B(t)$ is lower (upper) k-banded for all t.*

Proof. Without loss of generality suppose that all matrices in $\mathcal{F}$ are upper triangular, and $\hat{B}$ is lower k-banded. It is obvious that the product of a lower k-banded matrix with an upper triangular matrix in either order is lower k-banded. Since $B(t) = F(t)^{-1}\hat{B}F(t)$, and $F(t)^{-1}$ and $F(t)$ are upper triangular, $B(t)$ must be lower k-banded for all t. ■

THEOREM 11.2. *Let $B(t)$ be the solution of an FG flow with initial condition $B(0) = \hat{B}$. If $\hat{B} \in \Lambda(\mathcal{F})$ $(\Lambda(\mathcal{G}))$, then $B(t) \in \Lambda(\mathcal{F})$ $(\Lambda(\mathcal{G}))$ for all t.*

Proof. Assume $\hat{B} \in \Lambda(\mathcal{G})$. We use the equation $B(t) = G(t)\hat{B}G(t)^{-1}$. Fix t, and write $B = G\hat{B}G^{-1}$ for simplicity. Since $\hat{B} \in \Lambda(\mathcal{G})$, there exists a differentiable function $Y(s)$ defined for s near zero, such that $Y(s) \in \mathcal{G}$ for all s, $Y(0) = I$, and $\dot{Y}(0) = \hat{B}$. Let $Z(s) = GY(s)G^{-1}$. Then $Z(s) \in \mathcal{G}$ for all s, $Z(0) = I$, and $\dot{Z}(0) = G\hat{B}G^{-1} = B$. Thus $B(t) = B \in \Lambda(\mathcal{G})$. ∎

COROLLARY 11.3. *In an SR flow, if $\hat{B}$ is Hamiltonian, then $B(t)$ is Hamiltonian for all t.*

COROLLARY 11.4. *In a QR flow, if $\hat{B}$ is skew-Hermitian, then $B(t)$ is skew-Hermitian for all t.*

COROLLARY 11.5. *In an HR flow, if $\hat{B}$ is J-skew-Hermitian, $B(t)$ is J-skew-Hermitian for all t.*

COROLLARY 11.6. *In any flow for which the members of either $\mathcal{F}$ or $\mathcal{G}$ are upper (lower) triangular, if $\hat{B}$ is upper (lower) triangular, then $B(t)$ upper (lower) triangular for all t.*

Of course Corollary 11.6 also follows from Theorem 11.1.

THEOREM 11.7. *In an HR flow, if $\hat{B}$ is J-Hermitian, then $B(t)$ is J-Hermitian for all t.*

Proof. $B(t) = H(t)^{-1}\hat{B}H(t)$, where $H(t)$ is J-unitary. A similarity transformation by a J-unitary matrix preserves the J-Hermitian property. ∎

Taking $J = I$ in Theorem 11.7, we get the known result that the QR flows preserve Hermitian matrices.

COROLLARY 11.8. *In an HR flow, if $\hat{B}$ is k-banded and J-Hermitian or J-skew-Hermitian, then $B(t)$ is k-banded for all t.*

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