SLICES OF MATRICES — A SCENARIO FOR SPECTRAL THEORY

RICARDO S. LEITE AND CARLOS TOMEI

Abstract. Given a real, symmetric matrix $S$, we define the slice $\mathcal{F}_S$ through $S$ as being the connected component containing $S$ of two orbits under conjugation: the first by the orthogonal group, and the second by the upper triangular group. We describe some classical constructions in eigenvalue computations and integrable systems which keep slices invariant — their properties are clarified by the concept. We also parametrize the closure of a slice in terms of a convex polytope.

THE BASIC DEFINITION

Let $S$ be a real $n \times n$ symmetric matrix with simple spectrum $\sigma(S) = \{\lambda_1 > \ldots > \lambda_n\}$. When is a matrix simultaneously an orthogonal and an upper triangular conjugation of $S$? More precisely, we consider the slice $\mathcal{F}_S$ through $S$, defined to be the intersection of the sets $\{Q^T SQ, \text{for arbitrary real orthogonal matrices } Q \text{ with } \det Q = 1\}$ and $\{RSR^{-1}, \text{for arbitrary real upper triangular matrices } R \text{ with } \text{diag } R > 0\}$. How large is a slice? Clearly, if $Q^T SQ = RSR^{-1}$ then $SQR = QRS$, and hence, since $S$ has simple spectrum, $QR = f(S)$, for some (real) polynomial $f$. The matrices $Q$ and $R$ are uniquely determined from $f(S)$ if $f(S)$ is invertible: this is the standard $QR$-factorization of a matrix ([7]). For convenience, we write $f(S) = QR = [f(S)]_Q[f(S)]_R$.

Slices have been appearing in disguised form in the literature of numerical analysis and integrable systems, and questions about the geometry of slices have come up intermittently. By putting these three aspects side by side, we expect to convince the reader that the concept is indeed a natural one.

SLICES AND THE COMPUTATION OF EIGENVALUES

Francis, in his fundamental work on the $QR$ algorithm ([11]) considered the following map between matrices. Take $S$ invertible symmetric, factor $S = QR$ and define the $QR$ step $S' = RQ$. It is clear that $S'$ is symmetric with the same spectrum of $S$, since $S' = Q^T SQ$. But more is true: $S' = RSR^{-1}$. In particular, as Francis had already pointed out, $S$ and $S'$ have the same bandwidth (the reader should compare this argument with the usual one ([13])). Also, $S'$ belongs to the slice through $S$: in the notation for the elements of $\mathcal{F}_S$ presented in the introduction, $S'$ is associated to the function $f(x) = x$.

Date: February 5, 2002.

1991 Mathematics Subject Classification. Primary 58F07, 15A18; Secondary 15A23.

Key words and phrases. Toda flows, $QR$ decompositions.

The authors were supported by CNPq, FINEP and FAPERJ.
Numerical analysts also know well that \( S^{(k)} = [S^k]^T Q S [S_k]^T Q \) equals the matrix obtained by applying \( k \) times the QR step starting from \( S \); in other words, \( S^{(k)} \) is the \( k \)-th step of the QR iteration starting from \( S = S^{(0)} \). Again, \( S^{(k)} \) belongs to \( F_S \), and is associated to \( f(x) = x^k \).

Instead, by taking \( f(x) = x^{1/k} \), the resulting matrix \( S^{(1/k)} \) is, in a precise sense, the \( 1/k \)-th QR step. Taking the limit \((7)\)

\[
\lim_{k \to \infty} (S^{(1/k)} - S^{(0)})k = \lim_{\epsilon \to 0} \frac{S^{(\epsilon)} - S}{\epsilon}
\]
yields a vector field \( \dot{S} = X(S) \), whose solution \( S(t) \) starting at \( S(0) = S \) at time \( k \) equals \( S^{(k)} \)! The computation of this limit appears in a number of arguments in the subject. The expression for \( S^{(\epsilon)} \) is

\[
S^{(\epsilon)} = \left[ S^{\epsilon} \right]^T Q S \left[ S^{\epsilon} \right] Q, \quad \text{where} \quad S^{\epsilon} = \left[ S^{\epsilon} \right]^T Q S \left[ S^{\epsilon} \right] R.
\]

Evaluating the derivatives in \( \epsilon \), we learn that

\[
\frac{d}{d\epsilon} S^{(\epsilon)} = \frac{d}{d\epsilon} \left[ S^{\epsilon} \right]^T Q S \left[ S^{\epsilon} \right] Q + \left[ S^{\epsilon} \right]^T Q \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) \left[ S^{\epsilon} \right] Q,
\]

\[
(\log S) S^{\epsilon} = \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) \left[ S^{\epsilon} \right] Q + \left[ S^{\epsilon} \right]^T Q \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) \left[ S^{\epsilon} \right] R.
\]

From the last equation,

\[
\left[ S^{\epsilon} \right]^T Q (\log S) S^{\epsilon} \left[ S^{\epsilon} \right] Q^{-1} = \left[ S^{\epsilon} \right]^T Q \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) + \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) \left[ S^{\epsilon} \right] R,
\]

which obtains

\[
\left[ S^{\epsilon} \right] R (\log S) \left[ S^{\epsilon} \right] Q \left[ S^{\epsilon} \right] Q^{-1} R = \log S^{(\epsilon)} = \left[ S^{\epsilon} \right]^T Q \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) + \left( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \right) \left[ S^{\epsilon} \right] R.
\]

Now evaluate the derivatives at \( \epsilon = 0 \): we must have \( I = S^0 = I.I = \left[ S^0 \right]^T Q \left[ S^0 \right] R \) and \( S^{(0)} = S \). The equation above yields

\[
\log S = \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \bigg|_{\epsilon=0} + \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] R \bigg|_{\epsilon=0}.
\]

The two terms in the right hand side of the last equation are special matrices: they are respectively skew symmetric and upper triangular. Consider the (unique, linear) decomposition of a matrix \( M = \Pi_a M + \Pi_u M \) as a sum of a skew symmetric and an upper triangular matrix. Then, from the expression for the derivative of \( S^{(\epsilon)} \), \( \frac{d}{d\epsilon} \left[ S^{\epsilon} \right] Q \bigg|_{\epsilon=0} = \Pi_a \log S \). The vector field which interpolates the QR iteration then is \( X(S) = [S, \Pi_a \log S] \).

The iterations and flows defined above lie in \( F_J \). In particular, both preserve the eigenvalues of the initial condition, its symmetry and its bandwidth.

For numerical analysts, the asymptotic behavior of the QR iteration, well known to Francis, is of capital importance. Say, for example, that \( J \) is an arbitrary Jacobi matrix (i.e., a real, tridiagonal matrix whose entries \( J_{k,k+1} = J_{k+1,k}, k = 1, \ldots, n-1 \) are strictly positive). Starting with \( J \), the QR iteration converges to a diagonal matrix \( D \). Not only \( D \) and \( J \) have the same spectrum but \( D \) must lie in the closure of \( F_J \), the slice through \( J \). Steps of QR type related to different functional parameters \( f \) give rise to iterations which, starting from \( J \), always converge to diagonal matrices, with diagonal entries consisting of the (distinct) eigenvalues of \( J \) in an arbitrary order. The closure of the slice \( F_J \) clearly ought to contain additional points. In a nutshell, they correspond to reducible Jacobi matrices, i.e.,
matrices for which some entry $J_{k,k+1} = J_{k+1,k}$ is zero. This will be explained in the sequel.

**Slices and the Toda flows**

We now describe briefly the Toda lattice, which is an integrable system for which slices appear as natural phase spaces. Consider $n$ particles on the line with positions $x_k$ and velocities $y_k$ evolving under the Hamiltonian

$$H = \frac{1}{2} \sum_{k=1}^{n} y_k^2 + \sum_{k=1}^{n-1} e^{(x_k-x_{k+1})/2}.$$ 

This Hamiltonian was introduced as a model of wave propagation in one dimensional crystals \cite{16}. It was Flaschka’s remarkable discovery \cite{5} that this dynamical system is equivalent to the matrix differential equation

$$\dot{J} = [J, \Pi_a J],$$

where $J$ is the Jacobi matrix with nonzero entries

$$J_{k,k} = -y_k/2 \quad \text{and} \quad J_{k,k+1} = J_{k+1,k} = e^{(x_k-x_{k+1})/2}/2.$$

The fact that the differential equation is in the so called Lax pair form \cite{9} implies that the evolution $J(t)$ is actually an orthogonal conjugation of the initial condition $J(0)$. But again more is true: the evolution stays within the set of Jacobi matrices, as we should expect, since there are no other physically significant variables in the problem (velocities essentially are the diagonal entries, and distances between particles with neighboring indices correspond to the off-diagonal entries).

Indeed, it is not hard to check that

$$J(t) = [e^{tJ(0)}]_Q J(0) [e^{tJ(0)}]_Q = [e^{tJ(0)}]_R J(0) [e^{tJ(0)}]_R^{-1},$$

the celebrated solution of the Toda lattice by factorization \cite{14}. To check this formula, proceed as in the computation of the limit of the previous section. Thus, again, the orbit $J(t)$ lies within the slice through $J(0)$.

Moser also computed the asymptotic behavior of the Toda lattice \cite{11}: for $f(x) = x$, the orbit $J(t)$ starting from a Jacobi matrix $J(0)$ converges to a diagonal matrix, with eigenvalues disposed in decreasing order. This is in accordance with the relationship between Toda and $QR$ and has a natural physical interpretation. Diagonal entries are velocities: in the long run, particles move apart and tend to undergo uniform motion, each with speed given by a different eigenvalue. Faster particles move ahead, explaining the ordered outcome of the eigenvalues along the diagonal found in applications of the $QR$ iteration. The remarkable fact that asymptotic speeds both at $-\infty$ and $+\infty$ are the same will not be relevant to us: this is strong evidence of the integrability of the system — each orbit ‘remembers’ this data. Other matrices belonging to the boundary of the slice through $J(0)$ correspond to asymptotic behavior in which the system of particles breaks into essentially disconnected components, the so called clustering.

For a symmetric matrix $S$ and an arbitrary function $g$, the matrix equation

$$\dot{S} = [S, \Pi_a g(S)]$$

admits a similar solution by factorization: conjugate the initial condition by $[e^{tS(0)}]_Q$. It is this last fact which historically was responsible for relating the $QR$ iteration and Toda flows \cite{15,4}: when $g(x) = \log(x)$, the resulting differential equation gives rise to the orbits interpolating the $QR$ iteration.
For applications of these differential equations to numerical analysis, the reader may consult [3].

**Geometric aspects of slices**

Detailed study of variables for which the Toda flow becomes especially simple led Moser ([11]) to a parametrization of Jacobi matrices. It turns out that Jacobi matrices have simple spectrum and its eigenvectors always have nonzero first coordinates — in particular, they can be normalized so as to have (strictly) positive first coordinates. Moser proved that the map taking Jacobi matrices to \( n \)-uples of distinct real numbers (the eigenvalues) and a point in the first octant of the unit sphere in \( \mathbb{R}^n \) (the first coordinates of the normalized eigenvectors) is a diffeomorphism. He then showed that an appropriate choice of Toda flow (i.e., of functional parameter \( g \)) gives rise to orbits joining any two Jacobi matrices with the same spectrum. Thus, given a Jacobi matrix \( J \), \( \mathcal{F}_J \) is the set of all Jacobi matrices with the same spectrum as \( J \). (We remind the reader that Jacobi matrices always have simple spectrum.) From Moser’s parametrization, *Jacobi slices* are diffeomorphic to \( \mathbb{R}^{n-1} \).

More generally, getting back to the definition of slices, we have seen that a matrix \( S' \in \mathcal{F}_S \) is of the form \( S' = Q^T SQ = RSR^{-1} \), where \( f(S) = QR \) for some function \( f \). Keeping account of the requests on \( Q \) and \( R \), one may obtain a simple coordinatization of a slice. A matrix \( S \) is *irreducible* if \( S \) has no invariant subspace generated by a subset of the canonical vectors \( e_1, \ldots, e_n \). Indeed, there is a diffeomorphism between positive polynomials up to scalar multiplication and elements of \( \mathcal{F}_S \), for an irreducible symmetric matrix ([10]).

Which matrices are in the boundary \( \partial \mathcal{F}_J \) of the slice through a Jacobi matrix \( J \)? Numerical analysts knew that the diagonal matrix \( \lambda = (\lambda_1, \ldots, \lambda_n) \) and its permuted counterparts \( \lambda_\pi = (\lambda_\pi(1), \ldots, \lambda_\pi(n)) \). As we shall see, the simplest possible way of combining such \( n! \) points to form a reasonable boundary turns out to be the topological description of \( \partial \mathcal{F}_J \). Let \( \mathcal{P}_\Lambda \) be the *permutohedron*, obtained by taking the convex closure of the points of the form \( \lambda_\pi \in \mathbb{R}^n \). Notice that actually \( \mathcal{P}_\Lambda \) has an interior of dimension \( n-1 \), since the sum of the coordinates of any point in \( \mathcal{P}_\Lambda \) equals the trace of \( J \). The permutohedron \( \mathcal{P}_\Lambda \) is homeomorphic to the closure of \( \mathcal{F}_J \), as was proved in [18] with combinatorial arguments.

The figure below describes the situation for a 3\( \times \)3 Jacobi matrix \( J \) with spectrum \( \sigma(J) = \{4, 2, 1\} \). On the left is a topological representation of the closure of the slice \( \mathcal{F}_J \). Interior points of the hexagon are points in \( \mathcal{F}_J \). The boundary consists of two kinds of points: the six diagonal matrices, corresponding to the vertices, and the matrices which form the edges, which have either entry (1, 2) or (2, 3) equal to zero. On the right, the permutohedron associated to \( \sigma(L) \) is projected on the \((x, y)\) plane. Notice that a map taking vertices to vertices, say, taking \( \text{diag}(1, 2, 4) \) to \( (1, 2, 4) \) and \( \text{diag}(2, 1, 4) \) to \( (2, 1, 4) \) may not behave so naively on all vertices, for continuity reasons.

The permutohedron associated to a Jacobi 4\( \times \)4 matrices is also drawn below. Faces have a clear meaning: there must be four hexagons associated to matrices for which entry (1, 2) equals zero (and hence contained a Jacobi 3\( \times \)3 block of fixed spectrum), six quadrilaterals corresponding to matrices with entry (2, 3) equal to zero, and four more hexagons for matrices with entry (3, 4) equal to zero. There are also 4! vertices.
The permutohedron is familiar to spectral theorists, from the well known Schur-Horn theorem \((12)\). Let \(S\) be a symmetric matrix with simple spectrum \(\sigma(S) = \{\lambda_1, \ldots, \lambda_n\}\), and consider the set \(O_S = \{Q^T S Q, Q \text{ orthogonal}\}\). Then the map \(S \mapsto \text{diag} \ S\) is surjective from \(O_S\) to \(P_\Lambda\). Such a map is highly not injective. Slices are in a sense minimal sets in \(O_S\) in bijection with permutohedra.

The presence of a convex polytope raised the possibility of relating slices to moment maps of symplectic toroidal actions \((1,8)\). Indeed, following this route, Bloch Flaschka and Ratiu obtained an explicit diffeomorphism between the closure of \(\mathcal{F}_J\) and \(P_\Lambda\), which we now describe. Let \(S\) be a symmetric matrix with simple spectrum, and consider the spectral decomposition \(S = Q^T \Lambda Q\), where, as usual, \(Q\) is orthogonal and \(\Lambda\) is diagonal. Now, order the diagonal entries of \(\Lambda\) in descending order: \(Q\) is then defined up to a choice of sign for each column of \(Q^T\) (since they are normalized eigenvectors of \(S\)). Thus, \(S = Q^T D \Lambda Q\), for some diagonal matrix \(D\) of signs. The matrix \(DQ\Lambda Q^T D\) is dependent on \(D\), but its diagonal is not! The
map $S \mapsto \text{diag} (QAQ^T)$ is the BFR map. Its restriction to the closure of a Jacobi slice $\mathcal{F}_J$ is the required diffeomorphism to $\mathcal{P}_\Lambda$.

The proof of the result above makes use of sophisticated machinery. However, once we knew what had to be proved, a simpler argument appeared, yielding a more general result [10]. Let $S$ be an arbitrary real, symmetric, irreducible matrix with simple spectrum. Call the diagonal matrices in the closure of $\mathcal{F}_S$ accessible, and their images under the BFR map the accessible vertices. Now let $\mathcal{P}_S$, the spectral polytope of $S$, be the convex closure of the accessible vertices of $S$.

**Theorem:** The BFR map is a diffeomorphism between the closure of the slice $\mathcal{F}_S$ and the spectral polytope $\mathcal{P}_S$.

Generically, the spectral polytope of a symmetric matrix with simple spectrum is indeed the permutohedron associated to the $n!$ diagonal arrangements of the eigenvalues. But this is not the case in general. A self-contained description of the spectral polytope of an irreducible matrix $S$ is as follows. Consider the spectral decomposition, $S = Q^T \Lambda Q$. We denote by $Q\{r_1, \ldots, r_k\}, \{c_1, \ldots, c_k\}$ the minor of $Q$ consisting of the entries in the intersection of rows with indices $r_1, \ldots, r_k$ with columns with indices in $c_1, \ldots, c_k$. For a permutation $\pi$ in $n$ symbols, let $\Pi$ denote the permutation matrix with entries $\Pi_{i,j} = \delta_{i,\pi(j)}$.

**Theorem:** A diagonal matrix $\Lambda_\pi = \Pi^T \Pi$ is an accessible vertex of the slice $\mathcal{F}_S$ if and only if the minors $Q\{\pi(1), \{1\}, Q\{\pi(1), \pi(2), \{1, 2\}, \ldots, Q\{\pi(1), \ldots, \pi(n)\}, \{1, \ldots, n\}$ have nonzero determinant.

As an example, let $S = Q^T \Lambda Q$ be a $3 \times 3$ matrix with eigenvalues $\Lambda = \text{diag} (4, 2, 1)$, and so that the entry $Q_{1,1}$ equals zero, but no other minor of $Q$ has determinant equal to zero. The slice $\mathcal{F}_S$ and the spectral polytope have only four vertices: diagonal matrices with entry $(1, 1)$ equal to 4 do not belong to $\mathcal{F}_S$, and the vertices of the spectral polytope are $(2, 1, 4), (2, 4, 1), (1, 2, 4)$ and $(1, 4, 2)$. $\mathcal{F}_S$ is a quadrilateral.

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Departamento de Matemática, PUC-Rio, R. Mq. de S. Vicente 225, 22453-900, Rio de Janeiro Brazil,

E-mail address: rsl@mat.puc-rio.br
E-mail address: tomei@mat.puc-rio.br