Toda and QR flows on tridiagonal matrices

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The Toda and QR flows on the space of symmetric, tridiagonal matrices are described, as are the connections to Cayley graphs and the symmetric eigenvalue problem. The primary reference is [1], from which the figures appearing here were copied and modified, and to which the reader is referred for the details omitted below.

The equations of motion of the 1-dimensional Toda lattice lead us to consider the system

$$\frac{dL}{dt} = [A, L] = AL - LA, \tag{1}$$

where L is an $n \times n$, real, symmetric, tridiagonal matrix with diagonal $(b_1, \cdots, b_n)$ and off-diagonal $(a_1, \ldots, a_{n-1})$, and $A = (L)_{>0} - (L)_{<0}$, that is, the skew-symmetric matrix with zero diagonal and upper off-diagonal $(a_1, \ldots, a_{n-1})$. Consider the following facts.

    i. If M is a symmetric, tridiagonal matrix with positive entries on the off-diagonal, then M has distinct eigenvalues and the first coordinate of each of its eigenvectors is non-zero.

    ii. The positivity of the a_i's is preserved under the flow (1).

    iii. The flow (1) is isospectral.

If we fix a spectrum $\Lambda = \{\lambda_1 > \cdots > \lambda_n\}$ and let T_Λ denote the space of $n \times n$, real, symmetric, tridiagonal matrices with each $a_i > 0$ and spectrum Λ, then the facts above give us the following.

Proposition 1 *The equation $\frac{dL}{dt} = [A, L]$ yields a flow on T_Λ.*

The next step is to understand the space T_Λ.

Proposition 2 *The space T_Λ is diffeomorphic to $S_{>0}^{n-1} = \{x \in \mathbb{R}^n \mid \sum x_i^2 = 1, \ x_i > 0\}$.*

Proof (sketch). By the spectral theorem, write $L \in T_\Lambda$ as $L = U\Lambda U^T$ where, by an abuse of notation, Λ is a diagonal matrix with diagonal Λ, $U = (u_{ij})$ is orthogonal, and for each i, $(u_{ij})_j$ is the eigenvector corresponding to the eigenvalue λ_i, normalized so that $u_{i1} > 0$. Define $\varphi : T_\Lambda \longrightarrow S_{>0}^{n-1}$ by $\varphi(L) = (u_{11}, u_{21}, \ldots, u_{n1})$, that is, φ sends matrices to the first coordinates of their appropriately normalized eigenvectors.

Writing the eigenvalue equation $LU = U\Lambda$ and using the orthogonality of U, we may conclude that the first coordinates of the eigenvectors are enough (along with the eigenvalues) to recover L. Indeed, the a_i's, b_i's, and u_{ij}'s may be computed inductively from the u_{i1}'s via

$$b_i = \sum_{j=1}^n \lambda_j u_{ij}^2, \quad a_i^2 = \sum_{j=1}^n \left((\lambda_j - b_i)u_{ij} - a_{i-1}u_{i-1,j}\right)^2, \quad u_{i+1,j} = \left((\lambda_j - b_i)u_{ij} - a_{i-1}u_{i-1,j}\right)/a_i, \tag{2}$$

where $a_0 = a_n = u_{0j} = 0$. $\qquad\qquad\square$

To understand the Toda flow on $S_{>0}^{n-1}$, let us analyze the form of the matrices corresponding to the boundaries of the space. We take $n = 3$ as an example. Using (2) and the orthogonality of U, we find that as (x_1, x_2, x_3) limits to a point $(u_1, u_2, 0)$, $u_1, u_2 \neq 0$, in $S_{>0}^2$, the corresponding matrices $\varphi^{-1}(x_1, x_2, x_3)$ limit to a matrix of the form $\begin{pmatrix} b_1 & a_1 & 0 \\ a_1 & b_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$. The same holds for the matrices corresponding to points in $S_{>0}^2$ limiting to $(u_1, 0, u_3)$, $u_1, u_3 \neq 0$, and $(0, u_2, u_3)$, $u_2, u_3 \neq 0$, with λ_3 replaced by λ_2 and λ_1, respectively (see *Figure 1*).

As (x_1, x_2, x_3) approaches one of $(1, 0, 0)$, $(0, 1, 0)$, or $(0, 0, 1)$, the corresponding matrices $\varphi^{-1}(x_1, x_2, x_3)$ have a limit if and only if the ratio of the two terms tending to zero has a limit in $[0, \infty]$. By blowing up each of the three vertices $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ by parameterizing lines of different slopes through those points, we arrive topologically at a hexagon (see *Figure 2*).
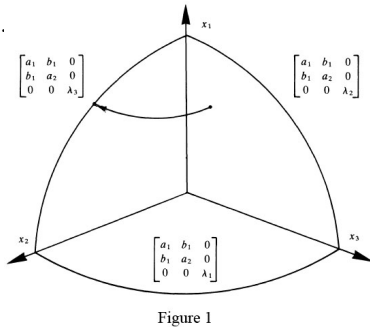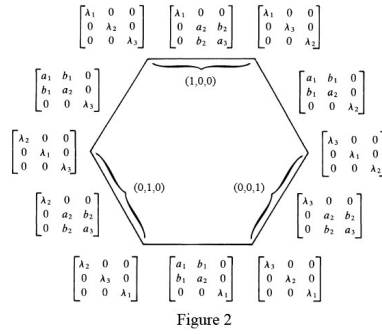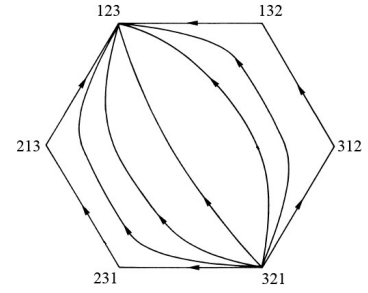
Figure 1

Figure 2

Figure 3

The Toda flow, or at least a topologically equivalent one, may now be realized on the hexagon, where the labels on the vertices and sides indicate the limiting form of the corresponding matrices. Note that this hexagon corresponds to the Cayley graph of S_3 with generators (12) and (23). In general, after the appropriate topological modifications, the homeomorphism between $S_{>0}^{n-1}$ and the interior of the Cayley graph of S_n generated by $(12), (23), \ldots, ((n-1)n)$ with its usual embedding in R^{n-1} reveals the correspondence with T_Λ.

Now that we have an understanding of the space $S_{>0}^{n-1}$ with respect to its association with T_Λ, our goal is to describe the Toda flow (1) on $S_{>0}^{n-1}$.

Proposition 3 *Let M be an $n \times n$, real, symmetric matrix. Then $\frac{dx}{dt} = Mx - \langle Mx, x \rangle x$ is a flow on $S_{>0}^{n-1}$. Given $x(0) = x_0$, it has unique solution $x(t) = \frac{e^{Mt}x(0)}{||e^{Mt}x(0)||}$. Moreover, the case $M = \Lambda$ corresponds to the Toda flow on T_Λ under the aforementioned diffeomorphism.*

It follows easily from Proposition 3 that regardless of the initial condition x_0, $x(t) \to (1, 0, \ldots, 0)$ as $t \to \infty$. From the study of the matrices associated to the boundaries of $S_{>0}^{n-1}$, this gives that $L(t) \longrightarrow \Lambda$ as $t \to \infty$. We have seen this eigenvalue sorting property of the Toda flow before. With some effort, Proposition 3 also yields that the rate of convergence is exponential. When $n = 3$, Proposition 3 allows us to visualize the Toda flow on the hexagon (see *Figure 3*).

Next we present another flow on T_Λ related to the symmetric eigenvalue problem and QR factorization. The following is Francis' algorithm to compute the eigenvalues of a matrix $L \in T_\Lambda$ by repeated QR factorization. Suppose for convenience that each $\lambda_i > 0$. Factorize $L = L_0 = Q_0 R_0$ where Q_0 is orthogonal and R_0 is upper triangular. Let $L_1 = R_0 Q_0 = Q_0^T L_0 Q_0$, then factorize $L_1 = Q_1 R_1$. Let $L_2 = R_1 Q_1 = Q_1^T L_1 Q_1$, and factorize $L_2 = Q_2 R_2$. Continuing in this manner, we obtain inductively a sequence of tridiagonal matrices $(L_k)_k \subseteq T_\Lambda$.

Theorem *The sequence $(L_k)_k$ converges to Λ as $k \to \infty$. Moreover, the convergence is exponential.*

Proof. We may prove the first statement of the theorem by realizing $(L_k)_k$ as the positive integer times of a flow on $S_{>0}^{n-1}$ and utilizing Proposition 3. To accomplish this, by the spectral theorem, write $L_k = U_k \Lambda U_k^T$ and set $u_k = U_k^T e_1$, that is, the vector consisting of the first coordinates of each normalized eigenvector of L_k. Since $L_1 = Q_0^T L_0 Q_0 = Q_0^T U_k \Lambda U_k^T Q_0$, $U_1^T = U_0^T Q_0$. Since Q_0 is orthogonal and R_0 is upper triangular, $Q_0 e_1 = \frac{L_0 e_1}{||L_0 e_1||}$. Finally,

$$u_1 = U_1^T e_1 = U_0^T Q_0 e_1 = U_0^T \left(\frac{L_0 e_1}{||L_0 e_1||} \right) = \frac{U_0^T L_0 e_1}{||U_0^T L_0 e_1||} = \frac{\Lambda U_0^T e_1}{||\Lambda U_0^T e_1||} = \frac{\Lambda u_0}{||\Lambda u_0||}.$$

It follows by an easy induction that $u_k = \frac{\Lambda^k u_0}{||\Lambda^k u_0||}$ for $k = 0, 1, 2, \ldots$. This corresponds exactly to the positive integer times of the flow in Proposition 3 with $M = \log \Lambda$, and so $L_k \to \Lambda$ as $k \to \infty$. $\square$

References

[1] P. Deift, T. Nanda, and C. Tomei. Ordinary differential equations and the symmetric eigenvalue problem. *SIAM J. Numer. Anal.*, 20(1):1–22, 1983.