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ASYMPTOTIC ANALYSIS OF TODA LATTICE ON DIAGONALIZABLE MATRICES

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1. INTRODUCTION

WHEN studying a nonlinear spring chain composed of finitely many mass points on a line subject to the influence of exponential repulsive forces, one can rewrite the associated Hamiltonian system after Flaschka's transformation as the following matrix equation [4, 7],

$$\dot{L} = [L, B] = LB - BL \tag{1.1}$$

where

$$L = \begin{bmatrix} a_1, b_1 & & & \\ b_1, a_2 & \ddots & & \\ & \ddots & \ddots & \\ & & a_{n-1}, & b_{n-1} \\ & & b_{n-1}, & a_n \end{bmatrix}$$

is a Jacobi matrix (with positive off-diagonal entries) and

$$B = \begin{bmatrix} 0, -b_1 & & & \\ b_1, \ 0 & \ddots & & \\ & \ddots & \ddots & \\ & & 0 & , -b_{n-1} \\ & & b_{n-1}, & 0 \end{bmatrix}$$

is a skew-symmetric matrix. Equation (1.1) is known as the Toda lattice. Among many of its interesting properties which have been studied [2–4, 7, 11], probably the most important features are the isospectral property—starting with any initial value $L(0) = L_0$, the solution flow $L(t)$ of (1.1) has the same spectrum for all t, and the global asymptotic convergence property—the solution flow $L(t)$, while preserving the tridiagonal form for all t, converges to a diagonal matrix.

Recently the significance of this dynamical system was further underscored by the discovery of the close relation between its flow and important QR-algorithm in numerical analysis [2, 3, 11]. Roughly speaking, one step in the QR-algorithm applied to the initial matrix $\exp(L_0)$ gives the same matrix as the Toda flow sampled at integer times.

The equation (1.1) has been generalized to the most extent in a previous paper [2] where the following initial value problem was studied.

$$\begin{cases} \dot{X} = [X, \Pi_0(G(X))] \\ X(0) = X_0. \end{cases} \tag{1.2}$$

In this problem, X is a general complex-valued matrix, $G(X)$ is the matrix-valued contour integral

$$G(X) = \frac{1}{2\pi i}\int_\Gamma G(\lambda)(\lambda I - X)^{-1}\,\mathrm{d}\lambda \tag{1.3}$$

where $G(z)$ is an analytic function defined on a domain Ω containing the spectrum of X, $\Gamma \subset \Omega$ is any contour surrounding the spectrum of X, and $\Pi_0(G(X))$ is the unique skew-Hermitian matrix in the splitting of $G(X)$ as the direct sum of an upper triangular matrix with real diagonal entries and a skew-Hermitian matrix. It is clear from the commutator form of (1.2) that the solution flow $X(t)$ still has the isospectral property. Indeed we have proved the following properties in [2] which are analogous to (but more general than) results in [3, 8].

LEMMA 1.1. The solution $X(t)$ of (1.2) is given by

$$X(t) = Q^*(t)X_0Q(t) \tag{1.4}$$

where $Q(t)$ solves the initial value problem

$$\begin{cases} \dot{Q}(t) = Q(t)\cdot(\Pi_0(G(X(t))) \\ Q(0) = I \end{cases} \tag{1.5}$$

and Q^* means the adjoint of Q.

LEMMA 1.2. The matrix $Q(t)$ in (1.5) is exactly the unitary matrix involved in the QR-decomposition [5, 9, 12] of the matrix $\mathrm{e}^{tG(X_0)}$, namely

$$\mathrm{e}^{tG(X_0)} = Q(t)R(t) \tag{1.6}$$

where $R(t)$ is an upper triangular matrix with real nonnegative diagonal entries.

Furthermore, the Toda flow is related to the QR-algorithm (for general matrices) by the following lemma [2].

LEMMA 1.3. Suppose $X(t)$ solves problem (1.2) and for $k = 0, \pm1, \pm2, \ldots, e^{G(X(k))}$ has the QR-decomposition

$$\mathrm{e}^{G(X(k))} = Q^{(k)}R^{(k)}. \tag{1.7}$$

Then

$$\mathrm{e}^{G(X(k+1))} = R^{(k)}Q^{(k)}. \tag{1.8}$$

In other words, choosing $G(z) = \ln z$, we recover the classical QR-algorithm from the Toda flow. It is also clear that the QR-algorithm with shifts is equivalent to the choice $G(z) = \ln(z - c)$.

Unfortunately, not very much is known about the global asymptotic behavior of $X(t)$ for this general Toda lattice (1.2). For partial results, see e.g. [1–3, 8]. The analysis apparently is much harder than that for (1.1). In this expository paper we shall study the dynamics of $X(t)$ only under the following assumptions:

(A1) $X(0) = X_0 \in \mathbb{R}^{n \times n}$ is diagonalizable;
(A2) $G(z) = z$;
(A3) X_0 is an irreducible upper Hessenberg matrix.

One should note that the assumption (A3) is not restrictive at all, but rather ought to be the way to proceed if one is really interested in numerical work because it can be shown [2] that the resulting $X(t)$ is also irreducible and upper Hessenberg for all t.

By Schur's theorem, there exists a unitary matrix U_0 such that

$$X_0 = U_0^* T U_0 \tag{1.9}$$

where T is an upper triangular matrix. From (1.4) it follows that

$$X(t) = U^*(t) T U(t) \tag{1.10}$$

with

$$U(t) = U_0(Q(t)). \tag{1.11}$$

Suppose also that the matrix T is diagonalized by P, i.e.

$$T = P \Lambda P^{-1} \tag{1.12}$$

where $\Lambda = \operatorname{diag}\{\lambda_1, \ldots, \lambda_n\}$. Our major result is stated as follows.

THEOREM 1.1. If, in addition to assumptions (A1), (A2) and (A3), the matrix X_0 also satisfies

(A4) all eigenvalues are real and $\lambda_1 > \lambda_2 > \ldots > \lambda_n$, then as $t \to \infty$

(1) the matrix $X(t)$ converges to an upper triangular matrix,
(2) the matrix $U(t)$ converges to the matrix obtained by orthonormalizing the columns of P, and
(3) the matrix $P^{-1}U(t)$ converges to an upper triangular matrix.

The case when X_0 is a Jacobi matrix (and hence a general symmetric matrix by a standard tridiagonalization algorithm) has been studied extensively and its asymptotic behavior is well known [3, 8, 11]. In [1] we have shown the global convergence property for normal matrices. All these results are special cases of our current presentation. Although part of the results in this paper can be obtained using standard techniques (as in [3] and [8]), we find that O.D.E. approaches do offer better insight into old results.

This paper is organized as follows. Some preliminary facts are considered in Section 2. The most important one is a new representation of the first column vector of the transformation $U(t)$. This turns out to be crucial in describing the total dynamics. In Section 3 we analyze the dynamics of the transformation $U(t)$ with the aid of the results in Section 2. As will be seen, the idea of invariant subspaces of a certain transformation matrix manifests the whole structure of the ω-limit set of the underlying differential system. Finally, we conclude this paper with a brief discussion when complex-conjugate eigenvalues appear.

2. PRELIMINARIES

Notice that, by (1.5) and (1.11), $U(t)$ solves the problem

$$\begin{cases} \dot{U}(t) = U(t) \cdot \Pi_0 X(t) \\ U(0) = U_0. \end{cases} \tag{2.1}$$

Let us denote the matrix $U(t)$ in (1.11) as

$$U(t) = [u_1(t), \ldots, u_n(t)] \tag{2.2}$$

where $u_i(t)$ is the ith column of $U(t)$. Then (1.10) implies

$$[u_1, \ldots, u_n] \begin{bmatrix} x_{11}, & x_{12}, & \cdots & \cdots & x_{1n} \\ x_{21}, & x_{22}, & \ddots & & \vdots \\ & x_{32}, & \ddots & \ddots & \vdots \\ & & \ddots & \ddots & \vdots \\ \bigcirc & & & x_{n,n-1}, & x_{nn} \end{bmatrix} = T \cdot [u_1, \ldots, u_n]. \tag{2.3}$$

The equality

$$\sum_{i=1}^{k+1} x_{ik} u_i = T u_k \tag{2.4}$$

obviously holds for each $k = 1, \ldots, n$ with the notation $u_{n+1} = x_{n+1,n} = 0$. It is also true that

$$x_{ij} = \langle u_i, T u_j \rangle \tag{2.5}$$

for all i and j where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{C}^n$.

From (2.1), (2.4) and (2.5), it is hard to see

LEMMA 2.1. The first column $u_1(t)$ of $U(t)$ satisfies the equation

$$\dot{u}_1 = T u_1 - \langle u_1, T u_1 \rangle u_1. \tag{2.6}$$

This equation is known as the Moser's formula and was found in [3]. Direct computation also shows

LEMMA 2.2. The solution to (2.6) is given explicitly by

$$u_1(t) = \frac{e^{Tt} u_0}{\|e^{Tt} u_0\|_2}, \tag{2.7}$$

where u_0 is the first column of U_0.

Suppose now the matrix P in (1.12) is written as

$$P = [p_{ij}]_{n\times n} = [p_1, \dots, p_n] \tag{2.8}$$

with each column vector P_i being normalized. Then the ith component $u_{i1}(t)$ of $u_1(t)$ is given by

$$u_{i1}(t) = \frac{\sum_{k=1}^{n} p_{ik}\, e^{\lambda_k t}\rho_k}{\left\{\sum_{j=1}^{n}\left|\sum_{k=1}^{n} p_{jk}\, e^{\lambda_k t}\rho_k\right|^2\right\}^{1/2}} \tag{2.9}$$

where

$$P^{-1}u_0 = [\rho_1, \dots, \rho_n]^T \tag{2.10}$$

are the coordinates of u_0 on the basis of columns of P.

It is really nice to have the explicit expression (2.9) for the exact solution $u_1(t)$. It turns out this is sufficient to determine the matrices $X(t)$ and $U(t)$ completely because of the following important inverse algorithm [9].

THEOREM 2.1. Suppose B is an irreducible upper Hessenberg matrix with positive subdiagonal elements and Q is a unitary matrix, then Q and B are uniquely determined by the first column of Q, provided A is given and $B = Q^*AQ$.

For our application, we shall replace A by T, Q by U and B by X. From (1.10), (2.9) and the above theorem, we know that $X(t)$ and $U(t)$ are completely determined. The detailed analysis is presented in the next section.

3. ASYMPTOTIC ANALYSIS

Primarily we shall be concerned about the case when (A4) is true.

Then from (2.9), we know

$$u_{i1}(t) = \frac{\sum_{k=1}^{n} p_{ik}\, e^{(\lambda_k-\lambda_1)t}\rho_k}{\left\{\sum_{j=1}^{n}\left|\sum_{k=1}^{n} p_{jk}\, e^{(\lambda_k-\lambda_1)t}\rho_k\right|^2\right\}^{1/2}} \to \frac{\rho_1}{|\rho_1|}p_{i1} \tag{3.1}$$

as $t \to \infty$. More precisely we shall write

$$\left\| u_1(t) - \frac{\rho_1}{|\rho_1|}p_1 \right\| = O(e^{(\lambda_2-\lambda_1)t}). \tag{3.2}$$

For simplicity of presentation, we shall denote $\frac{\rho_1}{|\rho_1|}p_1$ by the same letter p_1. Then by (2.5),

$$\begin{aligned}|x_{11} - \lambda_1| &= |\langle u_1, Tu_1 - \lambda_1 u_1\rangle| \le \|Tu_1 - \lambda_1 u_1\| \\ &\le \|T - \lambda_1\|\,\|u_1 - p_1\| = O\,(e^{(\lambda_2-\lambda_1)t}),\end{aligned} \tag{3.3}$$

and by (2.4),

$$|x_{21}| = \|Tu_1 - x_{11}u_1\| \leqslant \|T - x_{11}\| \|u_1 - p_1\| + |x_{11} - \lambda_1| = O(e^{(\lambda_2-\lambda_1)t}). \tag{3.4}$$

From the computational point of view, when $x_{21}(t)$ is small enough, one would perform the obvious deflation and continue the calculation on the resulting submatrix. In this paper, however, we would like to show rigorously the exact dynamic behavior of $X(t)$. From the equality

$$x_{12}u_1 + x_{22}u_2 + x_{32}u_3 = Tu_2 \tag{3.5}$$

we realize that verifying that $x_{32}(t)$ converges to zero is equivalent to verifying that the subspace $\{u_1, u_2\}$ spanned by u_1 and u_2 converges to a subspace invariant under T. To achieve this, we define

$$v_i = P^{-1}u_i \tag{3.6}$$

for each $i = 1, \ldots, n$. Then (2.4) implies

$$x_{11}v_1 + x_{21}v_2 = \lambda v_1. \tag{3.7}$$

Equivalently, on the ith component we have

$$x_{11}v_{i1} + x_{21}v_{i2} = \lambda_i v_{i1}. \tag{3.8}$$

It then follows for each i and j that

$$\frac{v_{i2}}{v_{j2}} = \frac{(\lambda_i - x_{11})v_{i1}}{(\lambda_j - x_{11})v_{j1}} = \frac{(\lambda_i - x_{11})\rho_i}{(\lambda_j - x_{11})\rho_j} \cdot e^{(\lambda_i-\lambda_j)t}. \tag{3.9}$$

Thus for $i, j \geqslant 2$, it is true that

$$\frac{v_{i2}}{v_{j2}} = O(e^{(\lambda_i-\lambda_j)t}) \tag{3.10}$$

as $t \to \infty$. In particular, for all $i \leqslant 3$

$$|v_{i2}| \leqslant O(e^{(\lambda_3-\lambda_2)t}) \tag{3.11}$$

because $v_{22}(t)$ is bounded for all t and $\lambda_2 \neq \lambda_1$. So the vector v_2 has been shown to converge to a vector of the form $[x, x, 0, \ldots, 0]^T$ where the x's represent some values which will be actually determined later. From (3.6), $u_2(t)$ converges to a vector in the subspace $\{p_1, p_2\}$ spanned by eigenvectors p_1 and p_2 of T, which certainly is invariant under T. Furthermore, since u_2 is orthogonal to u_1 (and hence p_1), u_2 must converge to the normalized vector of either $p_2 - \langle p_1, p_2\rangle p_1$ or its negative. This will determine the limits of $v_{12}(t)$ and $v_{22}(t)$ (and hence $x_{12}(t)$ and $x_{22}(t)$) completely. In fact, from (2.5) and (3.11), it is not hard to see that

$$|x_{22} - \lambda_2| = O(e^{\lambda_3-\lambda_2)t}). \tag{3.12}$$

Notice that (3.11) also implies

$$x_{32} = O(e^{(\lambda_3-\lambda_2)t}). \tag{3.13}$$

From (3.8) and (3.4), for $i \geq 2$

$$\frac{x_{12}v_{i1}}{v_{i2}} = \frac{x_{12}x_{21}}{\lambda_i - x_{11}} = O(\mathrm{e}^{(\lambda_2-\lambda_1)t}). \tag{3.14}$$

To apply induction, let us now assume that with a fixed $m \geq 3$ we have shown for all $k \leq m-1$ the following relations

$$\frac{v_{ik}}{v_{jk}} = O(\mathrm{e}^{(\lambda_i-\lambda_j)t}) \quad \text{for} \quad i,j \geq k \tag{3.15}$$

$$v_{ik} = O(\mathrm{e}^{(\lambda_{k-1}-\lambda_k)t}) \quad \text{for} \quad i > k \tag{3.16}$$

$$x_{k+1,k} = O(\mathrm{e}^{(\lambda_{k-1}-\lambda_l)t}) \tag{3.17}$$

$$\frac{\sum_{r=1}^{k-1} x_{rk}v_{ir}}{v_{ik}} = O(\mathrm{e}^{(\lambda_{k+1}-\lambda_k)t}) \quad \text{for} \quad i \geq k \tag{3.18}$$

$$|x_{kk} - \lambda_k| = O(\mathrm{e}^{(\lambda_{k-1}-\lambda_k)t}). \tag{3.19}$$

We want to show how the same relations hold for $k = m$. From (2.7), we have

$$x_{1,m-1}v_1 + \ldots + x_{m-1,m-1}v_{m-1} + x_{m,m-1}v_m = Tv_{m-1}. \tag{3.20}$$

So

$$\frac{v_{im}}{v_{jm}} = \frac{(\lambda_i - x_{m-1,m-1})v_{i,m-1} - \sum_{r=1}^{m-2} x_{r,m-1}v_{ir}}{(\lambda_j - x_{m-1,m-1})v_{j,m-1} - \sum_{r=1}^{m-2} x_{r,m-1}v_{jr}}$$

$$= \frac{v_{i,m-1}}{v_{j,m-1}} \frac{(\lambda_i - x_{m-1,m-1}) - \left(\sum_{r=1}^{m-2} x_{r,m-1}v_{ir}/v_{i,m-1}\right)}{(\lambda_j - x_{m-1,m-1}) - \left(\sum_{r=1}^{m-2} x_{r,m-1}v_{jr}/v_{i,m-1}\right)}. \tag{3.21}$$

It follows from (3.15) and (3.18) that for $i,j \geq m$

$$\frac{v_{im}}{v_{jm}} = O(\mathrm{e}^{(\lambda_i-\lambda_j)t}). \tag{3.22}$$

But then

$$v_{im} = O(\mathrm{e}^{(\lambda_{m-1}-\lambda_m)t}) \tag{3.23}$$

for $i > m$ and also

$$x_{m-1,m} = O(\mathrm{e}^{(\lambda_{m-1}-\lambda_m)t}). \tag{3.24}$$

Now for $i \geq m$, observe

$$\frac{\sum_{r=1}^{m-1} x_{rm} v_{ir}}{v_{im}} = \frac{x_{m,m-1}\left(\sum_{r=1}^{m-1} x_{rm} v_{ir}\right)}{(\lambda_i - x_{m-1,m-1}) v_{i,m-1} - \sum_{r=1}^{m-2} x_{r,m-1} v_{ir}}$$
$$= \frac{x_{m,m-1}\left(\sum_{r=1}^{m-1} x_{rm} v_{ir}/v_{i,m-1}\right)}{(\lambda_i - x_{m-1,m-1}) - \left(\sum_{r=1}^{m-2} x_{r,m-1} v_{ir}/v_{i,m-1}\right)} = O(e^{(\lambda_{m-1}-\lambda_m)t}) \tag{3.25}$$

where we have used facts (3.20), (3.18) and (3.24). The relation (3.23) shows that the subspace $\{u_1, \ldots, u_m\}$ spanned by $u_1, \ldots, u_m$ converges to the invariant subspace $\{p_1, \ldots, p_m\}$ spanned by eigenvectors $p_1, \ldots, p_m$ of T. Hence u_m converges to the vector obtained by orthonormalizing p_m with respect to the limits of $u_1(t), \ldots, u_{m-1}(t)$ as $t \to \infty$. By (2.5) and (3.23), it is not hard to show

$$|x_{mm} - \lambda_m| = O(e^{(\lambda_{k+1}-\lambda_k)t}). \tag{3.26}$$

Thus by mathematical induction, we have established the major result of theorem 1.1.

Remark. The above theorem can be proved alternatively from a well-known result in numerical analysis concerning the convergence of the QR-algorithm together with the fact of continuous dependence of the initial data for the system (1.2), see [2]. But what we have done above is the really interesting point of this paper—we obtained the asymptotic behavior of the flow using O.D.E. techniques. The details that we present here clearly offer certain insights into the dynamics involved in the old results.

To study what can happen when complex-conjugate pairs of eigenvalues appear, we replace (A4) by

(A5) all eigenvalues are real except $\lambda_1 = \bar{\lambda}_2 = a + bi$ with $b \neq 0$ and also $a > \lambda_3 > \ldots > \lambda_n$.
Then we have

$$v_1(t) \sim \left[\frac{e^{ibt}\rho_1}{\alpha(t)}, \frac{e^{-ibt}\rho_2}{\alpha(t)}, 0, \ldots, 0\right]^T \tag{3.27}$$

as $t \to \infty$ where

$$\alpha(t) = \left\{\sum_{j=1}^{n} |p_{j1} e^{ibt}\rho_1 + p_{j2} e^{-ibt}\rho_2|^2\right\}^{1/2}. \tag{3.28}$$

It is clear that the vector $u_1(t)$ keeps rotating in the plane $\{p_1, p_2\}$ and does not converge at all. If X_0 is a normal matrix, then T can be chosen to be a diagonal matrix and the following convergence

$$\begin{bmatrix} x_{11}(t) & x_{12}(t) \\ x_{21}(t) & x_{22}(t) \end{bmatrix} \to \begin{bmatrix} a & \mp b \\ \pm b & a \end{bmatrix}$$

can be shown to exist [1]. If X_0 is a nonnormal, then it may happen that the above block becomes oscillatory instead of convergent. The simplest example can be found in [2] where we showed the existence of such a periodic solution. In either case, however, by using the argument that led to (3.9) and (3.10), we are still able to show (3.11) and, in fact, (3.16) for $k > 2$. In other words, under assumption (A5), we may say that matrix converges essentially (in the sense of [10]) to a quasi-upper triangular matrix which is the real-valued version of Schur's theorem, see [6].

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