THE TODA LATTICE, OLD AND NEW

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Abstract. Originally a model for wave propagation on the line, the Toda lattice is a wonderful case study in mechanics and symplectic geometry. In Flaschka's variables, it becomes an evolution given by a Lax pair on the vector space of Jacobi matrices, with a very special asymptotic behavior. It is a completely integrable system on the coadjoint orbit of the upper triangular group, for which the Liouville-Arnold tori are parameterized in terms of norming constants (which play the role of discrete inverse variables in analogy to the solution by inverse scattering of KdV) and the more recent bidiagonal coordinates (which parameterize also non-Jacobi tridiagonal matrices and reduce asymptotic questions to local theory). Larger phase spaces for the Toda lattice lead to the study of isospectral manifolds and different coadjoint orbits. Moreover, the time one map of the associated flow is computed by a familiar algorithm in numerical linear algebra.

The text is mostly expositive and quite self contained, presenting alternative formulations of familiar results and a few applications to numerical analysis.

1. **Introduction.** The Toda lattice is a beautiful mathematical object: mathematical miracles and serendipity are abundant. Somehow, everybody has something to say about it, and this extends way beyond mathematicians: there are abundant connections with physics and numerical analysis which are fruitful and clarifying. Moreover, the formalism is versatile, accomodating a number of interesting dynamical systems.

In this text, we present some of these many aspects of the Toda lattice. After more than thirty years of amazing discoveries, the subject is not exhausted even in its most elementary formulation. We aim at concrete examples, and provide occasional pointers to more abstract approaches.

In Section 2, the differential equation is presented as the physical system introduced by Toda and converted into an evolution on Jacobi matrices, after Flaschkas remarkable change of variables. The two basic properties are discussed: the conservation of eigenvalues and the very simple asymptotic behavior. A comparison with the archetypical Lax pair, the Korteweg-de Vries equation, motivates the introduction of Mosers inverse variables on Jacobi matrices, given by eigenvalues and (discrete) norming constants.

The change of variables taking the original mechanical system in $\mathbb{R}^{2n}$ to the set of Jacobi matrices with a fixed trace $\mathcal{J}_0$ leads to a brief description of the general setup for the Hamiltonian formalism. After a brief description of completely integrable systems and coadjoint orbits as symplectic spaces, we interpret the Toda equation as a Hamiltonian system on coadjoint orbits (in particular $\mathcal{J}_0$), as done by Adler and Kostant. We then consider larger phase spaces: generic coadjoint orbits, isospectral manifolds of tridiagonal matrices.

Section 4 is another geometric approach to the Toda lattice, which might have anticipated its discovery by decades. It leads very naturally to the solutions by factorization by Symes. Section 5 is dedicated to an interpolation theorem which connects the subject to numerical analysis: one Hamiltonian in the completely integrable collection associated to the Toda equation gives rise to a flow which, at integer times, consists of matrices obtained by the so called QR algorithm, extensively used in algorithms to compute eigenvalues.

Norming constants have a drawback: they do not extend to the boundary of the set of Jacobi matrices, which is where the fine asymptotic properties of the flows have to be studied. Section 6 describes bidiagonal coordinates, which provide charts for the full isospectral manifold of tridiagonal matrices. A brief interlude on QR algorithms with shifts is provided as an example of the versatility of this new instrument.

2. **Physical origins and Flaschka's variables.** In the mid sixties, the Japanese physicist M. Toda [36] proposed a model for wave propagation along n particles in a line by the Hamiltonian

$$H(x,y) = \frac{1}{2} \sum_1^n y_k^2 + \sum_1^{n-1} \exp(x_k - x_{k+1}).$$

As usual, positions x_k and velocities y_k vary as

$$\dot{x}_k = \frac{\partial H}{\partial y_k} = y_k, \quad \dot{y}_k = -\frac{\partial H}{\partial x_k} = \exp(x_{k-1} - x_k) - \exp(x_k - x_{k+1}), \; i = 1, \ldots, n.$$

Here, $x_0 = -\infty, x_{n+1} = +\infty$ — this is the *non-periodic* case of the *Toda lattice*. The particles are labeled and from a mathematical viewpoint, there is nothing wrong with occasional collisions: they simply pass each other.

Clearly, the energy $H(x(t), y(t))$ is a conserved quantity. The invariance under translation in configuration space (i.e., the fact that $H(x,y) = H(x+c, y)$, for any fixed $c \in \mathbb{R}^n$) implies that the center of mass of the system moves uniformly (i.e., the linear momentum of the system is preserved).

Following Flaschka[18], shift to center of mass coordinates (i.e., work with differences $x_k - x_{k+1}$), get rid of exponentials and adjust constants,

$$a_k = -\frac{y_k}{2}, \quad k = 1, \ldots, n, \quad b_k = \frac{1}{2} e^{(x_k - x_{k+1})/2}, \quad k = 1, \ldots, n-1$$

and the evolutions for $x(t)$ and $y(t)$ become

$$a_k' = 2(b_k^2 - b_{k-1}^2), \, k = 1, \ldots, n, \quad b_k' = b_k(a_{k+1} - a_k), \, k = 1, \ldots, n-1$$

which, surprisingly, can be cast as the matrix differential equation

$$\dot{J} = [J, \Pi_{sk} J] = J(\Pi_{sk} J) - (\Pi_{sk} J)J. \tag{J}$$

Here, J is a Jacobi matrix with diagonal entries a_k and principal off-diagonal entries b_k. A *Jacobi matrix* J is a real $n \times n$ symmetric matrix which is tridiagonal (i.e., $J_{ij} = 0$ if $|i - j| > 1$) and such that the principal off-diagonal entries (those for which $|i - j| = 1$) is a positive number. The matrix $\Pi_{sk} M$ is skew-symmetric, with the same lower triangular part as M.

There is nothing wrong in considering equation (J) for arbitrary real symmetric matrices (and even non-symmetric matrices). Explicitely, consider the differential equation on real symmetric matrices $S(t)$ given by

$$S'(t) = [S(t), \Pi_a S(t)], \quad S(0) = S_0. \qquad (S)$$

2.1. **Lax pairs, asymptotic behavior.** We present two fundamental facts. The first one is a question about differential equations. What kind of differential equation on matrices gives rise to an evolution $M(t)$ which preserves the eigenvalues? More precisely, what kind of vector field gives rise to a flow of the form $M(t) = (P(t))^{-1} M(0) P(t)$? Simply take derivatives,

$$M'(t) = -(P(t))^{-1} P'(t) (P(t))^{-1} M(0) P(t) + (P(t))^{-1} M(0) P'(t)$$
$$= -(P(t))^{-1} P'(t) M(t) + M(t)(P(t))^{-1} P'(t) = [M(t), (P(t))^{-1} P'(t)].$$

In words, equations given by *Lax pairs* $M'(t) = [M(t), X(t)]$ are solved by conjugating the initial condition. In particular, if the initial condition is a real, symmetric matrix $S(0)$, and we require P to be an orthogonal matrix (so that symmetry, together with spectrum, is preserved along the orbit $S(t)$), one should consider a Lax pair of the form $S'(t) = [S(t), A(t)]$, where $A(t)$ is a real, skew symmetric matrix (this follows from the standard computation — take the derivative at 0 of a curve of orthogonal matrices $Q(t)$ with $Q(0) = I$).

Proposition 1. *The solution $S(t)$ of (S) starting from a real, symmetric matrix $S(0)$ is of the form $S(t) = Q(t)^* S(0) Q(t)$: it is well defined for all $t \in \mathbb{R}$.*

The explicit form of $Q(t)$ is given in Section 4.2.

Proof. We are left with showing global existence: the matrix norm $||S||^2 = \operatorname{tr} S^T S$ is conserved along an orbit. $\square$

We now consider the asymptotic behavior for $S(t)$ and $J(t)$, the orbits starting from arbitrary symmetric and Jacobi matrices. In the Jacobi case, we may get information from the physical interpretation: informally, minimizing the potential energy (the second term in the Hamiltonian) leads to the particles spreading itself, so that one might expect $x_k - x_{k+1} \to -\infty$. Thus, for $t \to \infty$, particles should be essentially independent from each other and undertake uniform motion. In Flaschkas variables, the orbit $J(t)$ converges to a diagonal matrix.

Proposition 2. *The limits for $t \to \pm\infty$ of $S(t)$ are diagonal matrices. When $t \to \infty$ (resp. $t \to -\infty$), $J(t)$ converges to a diagonal matrix with strictly decreasing (resp. increasing) entries along the diagonal.*

Proof. The differential equations for the diagonal entries of $S(t)$ are given by

$$S'_{11} = 2(S_{12} + S_{13}^2 + \ldots + S_{1n}^2),$$
$$S'_{22} = 2(-S_{21} + S_{23}^2 + \ldots + S_{2n}^2),$$

and, in general, $S'_{kk} = -\sum_{j<k} S^2_{kj} + \sum_{j>k} S^2_{kj}$. The equation for S'_{11} indicates that it is nondecreasing in time. The same is true not for S'_{22} but for $S'_{11} + S'_{22}$, and in general the partial traces $\sum_{j=1}^{k} S_{jj}$ are nondecreasing. Since the norm of $S(t)$ is constant, all entries S_{ij} and the partial traces (and their derivatives) are uniformly bounded. In particular, the derivatives of the partial traces are integrable, Lipschitz functions on $\mathbb{R}$ and hence all entries $S_{ij}, i \neq j$ must go to zero. This implies the diagonal convergence of $S(t)$ (and hence of $J(t)$) at $\pm\infty$.

From equation $b'_k = b_k(a_{k+1} - a_k)$, the entries $b_k(t)$ of $J(t)$ are always positive (indeed, if $b_k = 0$ at some time, it is always zero). When $t \to \infty$, we must then have $a_{k+1} - a_k < 0$, so that the diagonal limit matrix has entries in strictly decreasing order (the fact that the eigenvalues of a Jacobi matrix are all distinct is proved in Lemma 2.1). A similar argument obtains the result for $t \to -\infty$. $\qquad\square$

As a side remark, notice that the above proposition proves the spectral theorem (only in finite dimensions: the presence of continuous spectrum brings up new issues to the asymptotics of the Toda flow [13]). The interested reader might enjoy a proof of the *Wielandt-Hoffman* theorem along similar lines ([15]).

2.2. Scattering and inverse variables.

Flaschka was certainly inspired by P. Lax's casting of the Korteweg-de Vries (KdV) equation into *Lax pair* form. Briefly, the evolution

$$u_t(t,x) = 6u(t,x)u_x(t,x) - u_{xxx}(t,x), \qquad t \geq 0, \ x \in \mathbb{R}$$

is equivalent to the operator evolution

$$L'(t) = [L(t), H(t)],$$

where

$$L(t)f(x) = -f''(x) + u(t,x)f(x), \ H(t)f(x) = 4f'''(x) - 6u(t,x)f'(x) - 3u_x(t,x)f(x).$$

Lax then reproved the seminal discovery of Gardner, Greene, Kruskal and Miura ([20]) that the the evolution of KdV varies the operator L preserving its eigenvalues. Analogous computations replacing L by higher order operators lead to the *Gelfand-Dickey flows*, which include the Boussinesq equation and more ([4]).

The connection between differential equations like KdV and the *inverse scattering method* discovered in the late sixties ([20], [2]) led to intense research on integrable systems. Originally as a formalism, inverse data provided (infinite dimensional) action-angle variables for the KdV equation.

Similarly, inverse variables for Jacobi matrices were pervasive in the early approaches to the Toda flows, starting with Moser ([29]). The theorem below, that he attributed to Stieltjes, provides inverse variables for the Toda equation (J).

Lemma 2.1. *Jacobi matrices always have distinct real eigenvalues. The first and last coordinate of each eigenvector is a nonzero number.*

Proof. Suppose $Jv = \lambda v$ and $v[1] = 0$: equating the first coordinates in the equation obtains $v[2] = 0$, and successively — so the extreme entries of eigenvectors are nonzero. Now, two independent eigenvectors associated to the same eigenvalue would yield an eigenvector with first coordinate equal to zero. $\qquad\square$

Theorem 2.2. *The set of Jacobi matrices is diffeomorphic to the product*

$$\{(\lambda_1, \lambda_2, \ldots, \lambda_n)\, ; \lambda_1 < \lambda_2 < \ldots < \lambda_n\} \times \{(v_1, v_2, \ldots, v_n\, ; v_i > 0, \sum_i v_i^2 = 1\}.$$

More precisely, the diffeomorphism takes J to its ordered eigenvalues and to the first coordinates of its associated eigenvectors, normalized to be positive.

Rather ironically, Parlett ([32]) remarked that this algorithm is used by numerical analysts to obtain a tridiagonal matrix from a full symmetric matrix, not from a diagonal matrix.

Proof. We sketch a procedure to invert this map presented in [14]. Define the matrix Λ and the vector v as

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) \quad , \quad v = (v_1, v_2, \ldots, v_n)$$

and consider the sequence of vectors $v, \Lambda v, \ldots, \Lambda^{n-1} v$. The vectors $q_1 = v, q_2, \ldots, q_n$ obtained from this sequence by applying the Gram-Schmidt method are the columns of an orthogonal matrix Q for which $J = Q^T \Lambda Q$. □

The entries of the vector v are the *norming constants* associated to J. Still in analogy with KdV, as $J(t)$ solves equation (J), the eigenvalues stay put, as Flaschka knew, and Moser showed that the norming constants $v(t)$ varied in a simple fashion: simply normalize (under the Euclidean norm) the vector $exp(t\Lambda)v(0)$.

From Proposition 2, a Jacobi orbit $J(t)$ converges to diagonal matrices with ordered eigenvalues along the diagonal entries. Using norming constants, Moser computed the *scattering map* of the Toda flow. Particles group in pairs with the same asymptotic velocity at extreme times: the quantity of interest is the *shift*, the distance between the two straight lines tangent to the asymptotic motion at $\pm\infty$ of particles in the same pair.

Norming constants, alas, do not parameterize the limit matrices of the flows. Actually, they degenerate on a large part of the boundary of the set of Jacobi matrices. This will be circumvented by *bidiagonal coordinates* in section 6.

There is a basic issue which has not been handled carefully so far: the fact that equation (J) is given in terms of skew symmetric matrices $A(t)$ yielded that the solution is an orthogonal conjugation of the initial condition $J(0)$ — thus, in particular, $J(t)$ is always real, symmetric, and eigenvalues are preserved. But why should the evolution preserve the tridiagonal form? This has to happen, if Flaschkas change of variable preserves the physical meaning of the variables. Also, this fits with the solution by inverse variables of (J). A more conceptual argument showing that $J(t)$ is always a Jacobi matrix will be presented in the next section. Yet another argument will come up in Section 4.2.

3. **Some symplectic geometry.** From its physical description in terms of positions x_i and velocities y_i, it is clear the Toda lattice admits a Hamiltonian formulation in $\mathbb{R}^{2n}$. By Flaschka's change of variables, after removal of the (trivial) evolution of the center of mass, the phase space for the differential equation becomes the set of Jacobi matrices with trace equal to zero, a cone of dimension $2n-2$, from Theorem 2.2. Somehow, one should be able to transfer the original Hamiltonian formulation to the new variables, and still proceed with the study of the Toda lattice within the new phase as a problem in mechanics. This leads to build up a more

general context, the starting point of a vast field, *symplectic geometry*. In the next subsection, we outline some basic requisites for this project.

3.1. **Complete integrability.** We start with a brief description of a more general definition of *Hamiltonian formulation* of a vector field. Take a differential equation with phase space M, or more precisely, consider the associated vector field Z defined on the tangent bundle TM. First equip M with a closed, nondegenerate, 2-form ω: the pair (M, ω) is a *symplectic manifold*, necessarily of even dimension, say $2n$ (excellent sources for symplectic geometry are [3], [21]).

Each *Hamiltonian* $H : M \to \mathbb{R}$ gives rise to a vector field X_H as follows: the contraction of ω with X_H should obtain the 1-form dH. Said differently, for every vector field Y in M, we must have at each $m \in M$

$$\omega_m(X_H(m), Y(m)) = dH(Y(m)) = Y(H)(m),$$

where $Y(H)(m)$ is the derivative of H along Y at m. The vector field Z admits a Hamiltonian formulation if $Z = X_H$ for an appropriate choice of ω and H.

The simplest example is the standard 2-form in $\mathbb{R}^{2n} = \{(x, y); \, x, y \in \mathbb{R}^n\}$ given by $\omega = \sum_k x_k \wedge y_k$. Let us find the vector field $X_H = \sum_k A_k \partial_{x_k} + \sum_k B_k \partial_{y_k}$ associated to the Hamiltonian $H : \mathbb{R}^{2n} \to \mathbb{R}$ (here, ∂_z is the partial derivative in the variable z, and $H_z = \partial_z H$). For an arbitrary vector field $Y = \sum_k a_k \partial_{x_k} + \sum_k b_k \partial_{x_k}$,

$$\omega(X_H, Y) = \sum_k -a_k A_k + \sum_k b_k B_k = \sum_k a_k H_{x_k} + \sum_k b_k H_{y_k} = dH(Y),$$

and, as expected, $X_H = \sum_k H_{y_k} \partial_{x_k} - \sum_k H_{x_k} \partial_{y_k}$.

When is a Hamiltonian vector field X_H *completely integrable*? Complete integrability requires n *commuting* Hamiltonians $H_k : M \to \mathbb{R}$ (i.e., their induced vector fields $X_k = X_{H_k}$ commute, or equivalently, such that $\{H_i, H_j\} = 0$ for the *Poisson bracket* induced by the 2-form ω, $\{H_i, H_j\} = \omega(X_{H_i}, X_{H_j})$) among themselves and with H itself. Finally, the Hamiltonians H_k should be *functionally independent* (i.e., their gradients should be linearly independent on a dense set of M).

Very few dynamical systems are completely integrable, but these are especially important for being situations in which explicit computations may be performed. Indeed, one can make precise the idea that a generic Hamiltonian vector field does not have a second conserved quantity (recall that H itself is conserved along orbits). But this is just the opposite of what we expect from certain iterations in numerical analysis: to compute eigenvalues, for example, we expect to change something (an original matrix, an approximation of an eigenvector) without varying the objects being computed (the eigenvalues themselves).

The *Liouville-Arnold-Jost theorem* for completely integrable equations states that, under appropriate hypothesis, phase space foliates into invariant tori (i.e., products of lines and circles), given by levels of the conserved quantities H_k (frequently called the *action variables* in this context). In each torus, in *angle variables*, the evolution is just straight line motion. The angles vary smoothly among neighboring tori, and the global dynamics is mostly dependent on the arithmetic properties of the many angular velocities.

3.2. **Toda flows in coadjoint orbits.** Using Flaschka's change of variables, one might push forward the standard 2-form in $\mathbb{R}^{2n}$ to $\mathcal{J}_0$, the cone of Jacobi matrices with zero trace, thus converting it into a symplectic manifold. The surprising fact is that the resulting 2-form comes up from another construction of great interest, which we now describe briefly.

A large class of symplectic manifolds is given by *coadjoint orbits*, equipped with the *Lie-Kirillov-Poisson* 2-form. Let G be a (finite dimensional) Lie group, $\mathfrak{G}$ its Lie algebra, and identify $\mathfrak{G}^*$, the dual of the Lie algebra, by means of a *nondegenerate coupling*

$$(\alpha, A) \in \mathfrak{G}^* \times \mathfrak{G} \to \langle \alpha, A \rangle \in \mathbb{R}.$$

The coupling is bilinear and nondegeneracy means that the restrictions $\langle \alpha, . \rangle$ and $\langle ., A \rangle$, for $\alpha, A \neq 0$, give rise to nonzero functionals respectively on $\mathfrak{G}^*$ and $\mathfrak{G}$. Thus, all linear functionals in $\mathfrak{G}$ are of the form $A \mapsto \langle \alpha, A \rangle$ for some $\alpha \in \mathfrak{G}^*$.

For the Toda flow, start with $G = U^+$, the group of $n \times n$ upper triangular real matrices with positive diagonal entries. Then $\mathfrak{G} = \mathfrak{U}$ is the vector space of real upper triangular matrices and we may identify $\mathfrak{G}^*$ with $\mathcal{S}$, the vector space of real, symmetric matrices, through the pairing $\langle S, A \rangle = \operatorname{tr} SA$.

The group G acts on itself by conjugation and on its Lie algebra $\mathcal{G}$ by its derivative at the origin, *the adjoint action*. For $G = U^+$, the adjoint action is given by $(g, U) \in G \times \mathfrak{G} \mapsto Ad_g(U) = gUg^{-1} \in \mathfrak{G}$. The *coadjoint action* from $G \times \mathfrak{G}^*$ to $\mathfrak{G}^*$ satisfies the natural duality,

$$\langle Ad_g^*(\alpha), A \rangle = \langle \alpha, Ad_{g^{-1}}(A) \rangle, \quad \forall \alpha \in \mathfrak{G}^*, \forall A \in \mathfrak{G}.$$

Back to Toda, one has

$$\forall \alpha \in \mathcal{S}, \forall A \in \mathfrak{U} \langle, Ad_g^*\alpha, A \rangle = \langle \alpha, Ad_{g^{-1}}(A) \rangle = \operatorname{tr} \alpha g^{-1} A g = \operatorname{tr}(g \alpha g^{-1})A.$$

The bad news is that $g \alpha g^{-1}$ is not a symmetric matrix. Denote by $\mathfrak{sU}$ the vector space of real, strictly upper triangular matrices. Clearly, for $E \in \mathfrak{sU}$ and $A \in \mathfrak{U}$ we have $\operatorname{tr} EA = 0$. Consider the (unique) splitting

$$M = S + E = \Pi_{\mathcal{S}}M + \Pi_{\mathfrak{sU}}M, \quad S \in \mathcal{S}, E \in \mathfrak{sU}.$$

We clearly have

$$\forall A \in \mathfrak{U} \langle Ad_g^*\alpha, A \rangle = \operatorname{tr}(g \alpha g^{-1})A = \operatorname{tr} \Pi_{\mathcal{S}}(g \alpha g^{-1})A,$$

from which we finally obtain $Ad_g^*\alpha = \Pi_{\mathcal{S}}(g \alpha g^{-1})$.

By definition, M and $\Pi_{\mathcal{S}}M$ have the same lower triangular part (and this includes the diagonal). In particular, all matrices in the coadjoint of a Jacobi matrix J are also Jacobi, with the same trace of J: indeed, M. Adler [1] and B. Kostant [22] realized that Jacobi matrices with fixed trace form a *coadjoint orbit*.

The celebrated Lie-Kirillov-Poisson 2-form on a coadjoint orbit is given as follows. Let $\mathcal{O}_\alpha$ be the coadjoint orbit through α. To obtain two vectors a and b in the tangent space of $\mathcal{O}_\alpha$ at α, take two elements of the Lie algebra $A, B \in \mathfrak{G}$, draw two curves in $\mathcal{O}_\alpha$, $Ad_{exp(tA)}^*\alpha$ and $Ad_{exp(tB)}^*\alpha$ and compute their derivatives at zero. Set

$$\omega_\alpha(a, b) = -\langle \alpha, [A, B] \rangle.$$

The minus sign is rather innocuous, still there is so much to prove here. First, it is not clear that ω is well defined: other elements in $\mathfrak{G}$ might give rise to the same tangent vectors at α. More, ω has to be proven nondegenerate and closed. We will take all those issues for granted.

Instead, we continue with the computations related to the Toda flow. In this case, the curve $Ad^*_{exp(tA)}\alpha = \Pi_{\mathcal{S}}e^{tA}\alpha e^{-tA}$ has the tangent vector $\Pi_{\mathcal{S}}[A, S]$ at α. The 2-form is given by

$$\omega_S(\Pi_{\mathcal{S}}[A, S], \Pi_{\mathcal{S}}[B, S]) = -\operatorname{tr} S[A, B].$$

A simple comoputation shows that the initial Hamiltonian $H(x, y)$ for the Toda lattice in physical variables converts to $H(S) = \operatorname{tr} S^2/2$ in Flaschka' s variables.

Proposition 3. *The Toda lattice is the vector field X_H associated to the Hamiltonian $H(S) = \operatorname{tr} S^2/2$ defined on a coadjoint orbit $\mathcal{O}_S$.*

Proof. We search for a vector field $X_H = \Pi_{\mathcal{S}}[U, S]$ for which, given any vector field $Y = \Pi_{\mathcal{S}}[V, S]$, we must have

$$\omega_S(X_H, Y) = -\operatorname{tr} S[U, V] = Y(H) = -\operatorname{tr} S\Pi_{\mathcal{S}}[V, S].$$

Let $\mathfrak{A}$ be the vector space (Lie algebra!) of real, skew symmetric matrices. We consider another splitting,

$$M = A + U = \Pi_{sk} M + \Pi_{up}M, \quad A \in \mathfrak{A}, U \in \mathfrak{U}$$

and make use of the orthogonalities $\mathfrak{A} \perp \mathcal{S}$ and $\mathfrak{U} \perp \mathfrak{s}\mathfrak{U}$:

$$\operatorname{tr} S\ [U, V] = \operatorname{tr} S\ \Pi_{\mathcal{S}}[V, S] = \operatorname{tr} \Pi_{up}S\ \Pi_{\mathcal{S}}[V, S]$$

$$= \operatorname{tr} \Pi_{up}S\ [V, S] = \operatorname{tr}[\ S,\ \Pi_{up}S]\ V = -\operatorname{tr}[\ S,\ \Pi_{sk}\ S],$$

so that $-\operatorname{tr}[S, U]\ V = \operatorname{tr}[\ S,\ \Pi_{sk}\ S]\ V$, for all $V \in \mathfrak{U}$, which is equivalent to say that $[S, U] = [\ S,\ \Pi_{sk}\ S] + E$, for some $E \in \mathfrak{s}\mathfrak{U}$, so that

$$X_H = \Pi_{\mathcal{S}}[S, U] = \Pi_{\mathcal{S}}[\ S,\ \Pi_{sk}\ S] = [\ S,\ \Pi_{sk}\ S].$$

$\square$

We are thus led to a very geometric explanation for the fact that the solution of the equation (J), $J'(t) = [J(t), B(J(t))] = [J(t), \Pi_{sk}\ J(t)]$, is always a Jacobi matrix, if $J(0)$ is: it simply does not leave the coadjoint orbit $\mathcal{O}_{J(0)}$.

A similar computation obtains the commutativity of the Hamiltonians $H_k(J) = \operatorname{tr} J^k, k = 1, \ldots, n)$. Indeed, the computation above generalize to yield the *Adler-Kostant-Symes* theorem ([**?**]), a criterion to identify families of commuting Hamiltonians. For the Toda lattice on Jacobi matrices with trace given by the initial condition $J(0)$, the H_k's form a family of $n - 1$ commuting flows which are functional independent throughout $\mathcal{O}_{J(0)}$, since Jacobi matrices have simple spectrum from Lemma 2.1. Thus, the original Toda vector field and any other vector field given by a Hamiltonian of the form $H_f(J) = \operatorname{tr} f(J)$ are completely integrable.

From Theorem 2.2, the related invariant Liouville-Arnold tori, given by sets of $n \times n$ Jacobi matrices with fixed spectrum, is diffeomorphic to the set of possible choices for norming constants — the positive octant of the unit sphere in $\mathbb{R}^{n-1}$.

3.3. **Toda flows in larger phase spaces.** From the computations above, the same Hamiltonian $H = \operatorname{tr} S^2/2$ induces equation (S) on larger coadjoint orbits and the proof of complete integrability on these phase spaces requires many more conserved quantities. The problem was considered in two cases. In [10], the authors consider the orbits of maximal dimension given by $2[n^2/4]$ in $\mathcal{S}$. The new commuting Hamiltonians $H(S)$ are obtained by *chopping*: they are the (symmetric functions of the) roots of the determinants of the matrices obtained by removing the first k rows and last k columns of the matrix $S - \lambda I$. In analogy to Mosers computations in

the Jacobi orbit, angle variables are essentially the first components of (generalized) eigenvectors.

The generic phase space for real, nonsymmetric matrices is handled in [11]. First, one need to interpret the Toda equation as a Hamiltonian on an appropriate phase space, which in this case is a maximal (coadjoint) orbit of dimension $n^2 - n$ of a certain semidirect product. At a matrix M, the new commuting Hamiltonians are the coefficients of the polynomial $p(z, \lambda) = \det(M - zM^T - \lambda)$, so a Riemann surface $p(z, \lambda) = 0$ is associated to M and is invariant under the Toda flow. Such additional structure was around has been known since the first studies of the *periodic* Toda flow, where the particles move on a circle instead of in the line ([38], [?]). For non-symmetric matrices, the additional angle variables are obtained from an extension of the Abel-Jacobi map, by integrating a set of explicit meromorphic 1-forms on the surface along specific divisors, related again by generalized eigenvectors.

3.4. **The isospectral manifold of tridiagonal matrices.** The set $\mathcal{J}_\Lambda$ of Jacobi matrices with a given simple spectrum

$$\lambda_1 < \lambda_2 < \ldots < \lambda_n, \qquad \Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

is diffeomorphic to $\mathbb{R}^{n-1}$. There is a natural enlargement of this set — define $\mathcal{T}_\Lambda$, the set of real, symmetric tridiagonal matrices with spectrum Λ. This set is actually a compact manifold ([37]).
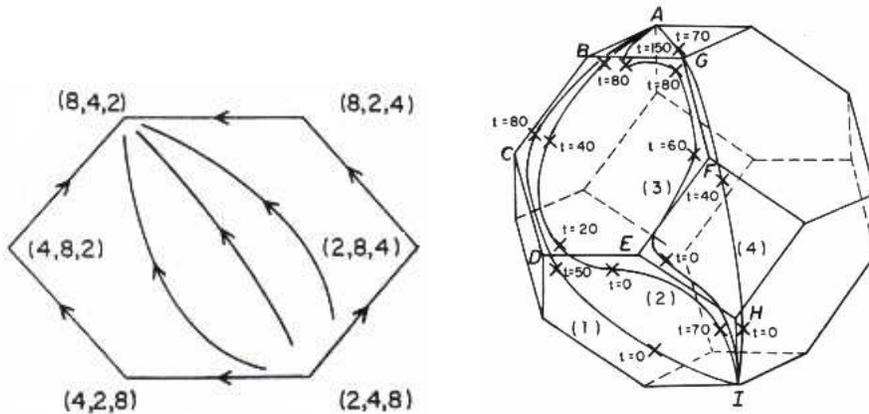

FIGURE 1. $\bar{\mathcal{J}}_\Lambda$, for $n = 3$ and 4

The first step in the understanding of $\mathcal{T}_\Lambda$ is taking the closure (within the space of real,symmetric matrices) of $\mathcal{J}_\Lambda$. It turns out that $\bar{\mathcal{J}}_\Lambda$ has an interesting combinatorial structure, which we now describe.

For matrix dimensions $n = 3$ and $n = 4$ (and any choices of different eigenvalues) this set is homeomorphic to the polytopes in the figure. The vertices correspond to the $n!$ diagonal matrices with the same spectrum as Λ. For $n = 3$, edges correspond to matrices having a single zero in the main off-diagonal entries. Thus, for example, the top edge consists of matrices with $(1, 2)$ entry equal to zero; the eigenvalue 8 is trapped at entry $(1, 1)$ and the bottom 2×2 block consists of Jacobi matrices with eigenvalues 4 and 2, whose closure is homeomorphic to the whole edge. Edges are

invariant under the Toda flow, and arrows indicate the sense of the flow. Notice that all interior points have the same α and ω limits.

For $n = 4$ the boundary still consists of points with zero off-diagonal entries, which split the matrix in two kinds of sets, eight of which are homeomorphic to the 3×3 case (hexagons), and six which are homeomorphic to the product of two 2×2 blocks with fixed spectrum, the quadrilaterals. Again, the curves represent some orbits of the Toda flow. For the general case ([37]), [?]), define the *permutohedron* $\mathcal{P}_\Lambda = \mathrm{conv}_{\pi \in S_n} \{(\lambda_{\pi(1)}, \ldots, \lambda_{\pi(n)})\}$.

Theorem 3.1. *The map from $\bar{\mathcal{J}}_\Lambda$ to the permutohedron $\mathcal{P}_\Lambda$*

$$J = Q^T \Lambda Q \mapsto diag(Q \Lambda Q^T) \in \mathcal{P}_\Lambda\}$$

is a homeomorphism.

The existence of a homeomorphism in [37] led Bloch, Flaschka and Ratiu ([?]) to search for a proof of the statement in terms of Atiyah's celebrated theorem on the convexity of the image of Hamiltonian torus actions ([?]). Their proof starts with the identification of the homeomorphism as a moment map, given by the formula above. A simple proof was later presented in [28].
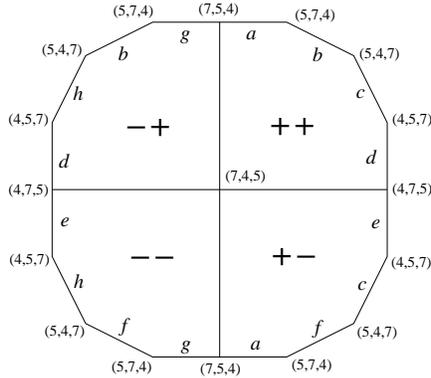

FIGURE 2. Gluing four copies of $\bar{\mathcal{J}}_\Lambda$

From $\bar{\mathcal{J}}_\Lambda$ to the full isospectral manifold $\mathcal{T}_\Lambda$, its a game of mirrors (or, more precisely, the construction of an appropriate *Coxeter group* ([37]). In a nutshell, dropping the signs of the off-diagonal entries of a real, symmetric tridiagonal matrix (preserving its symmetry!) does not change the eigenvalues — this is something that numerical analysts use systematically: to compute eigenvalues of a matrix in $\mathcal{T}_\Lambda$, it suffices to handle Jacobi matrices. in particular, the sets of matrices in $\mathcal{T}_\Lambda$ with non zero entries split into 2^{n-1} connected components, all isomorphic to $\mathcal{J}_\Lambda$. to get $\mathcal{T}_\Lambda$, one takes the closure of these components and glues them along faces which are naturally identified. For $n = 3$ and $\Lambda = \{7, 5, 4\}$, Figure 2 shows some edges already glued. All edges along the boundary have to be identified: boundary vertices must be the same, together with a sign (which?). The resulting bitorus is drawn so as to emphasize the boundaries of the hexagons (for more on this picture, see Section 6).

The universal cover of $\mathcal{T}_\Lambda$ is $\mathbb{R}^{n-1}$ and the homology groups are torsion free, with computable Betti numbers ([37], [19]).
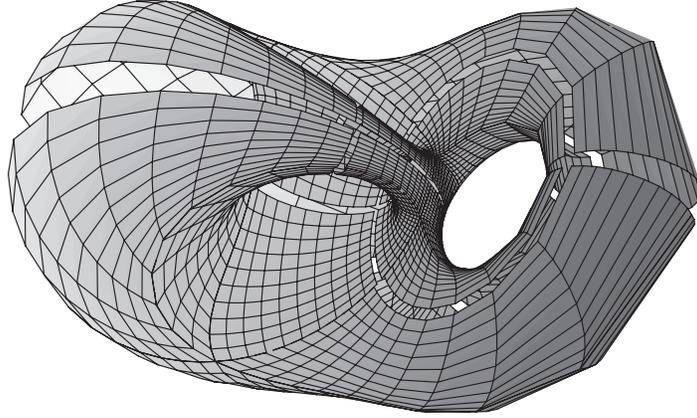
FIGURE 3. For $n = 3$, $\mathcal{T}_\Lambda$ is a bitorus

4. **A missed opportunity.** We present another trail ([28]) leading to the Toda equation: it might have anticipated the study of these equations by fifty years.

We fix notation. Let $\mathcal{M}(n)$ consist of the $n \times n$ real matrices, $SO(n) \subset \mathcal{M}(n)$ be the set of orthogonal matrices with positive determinant and $\mathcal{U}^+(n) \subset \mathcal{M}(n)$ be the set of upper triangular matrices with positive diagonal entries.

Clearly, both (Lie) groups act on $\mathcal{M}(n)$ by conjugation. For $M \in \mathcal{M}(n)$, set

$$\mathcal{O}_M^O = \{Q^T M Q, Q \in SO(n)\}, \quad \mathcal{O}_M^U = \{Q^T M Q, Q \in \mathcal{U}^+(n)\}$$

be respectively the *orthogonal* and *upper triangular* orbit through M. Clearly $\mathcal{O}_M^O$ and $\mathcal{O}_M^U$ are connected manifolds of matrices with the same eigenvalues as M.

For convenience, let M have (strictly) positive simple spectrum (i.e., positive distinct eigenvalues) — what is the *slice* $\mathcal{S}$ through M, defined as the connected component $\mathcal{C}_M$ of $\mathcal{O}_M^O \cap \mathcal{O}_M^U$?

The dimension count might suggest that such intersection is trivial, but this is not the case. Indeed, for a matrix $X \in \mathcal{S}$, there are $Q \in SO(n)$ and $R \in \mathcal{U}(n)$ such that

$$X = Q^T M Q = R M R^{-1} \;\Rightarrow\; (QR)\, M = M\, (QR)$$

.

In words, the matrix QR commutes with M. Since M has simple spectrum, QR is a function of M, in the sense that there exists $f : \mathbb{R} \to \mathbb{R} - \{0\}$ such that $QR = f(M)$. Notice that that Q and R are real invertible). This is the QR *factorization* of $f(M)$ (see Appendix 1 for details). In general, a real matrix X with positive determinant admits a unique factorization $X = [M]_Q [M]_R$, where $[M]_Q \in SO(n)$ and $[M]_R \in \mathcal{U}^+(n)$.

Adding up, given $f : \mathbb{R} \to \mathbb{R}^+$, we obtain a matrix $\phi(f, M) \in \mathcal{C}_M$,

$$\phi(f, M) = [\, f(M)\,]_Q^T\, M\, [\, f(M)\,]_Q = [\, f(M)\,]_R\, M\, [\, f(M)\,]_R^{-1} \; .$$

4.1. **Parameterizing the slice with commuting flows.** The notation $\phi(f, M)$ was introduced to suggest that we are close to a flow on $\mathcal{C}_M$.

Proposition 4. *Let $f, g : \mathbb{R} \to \mathbb{R}^+$ and M be a real matrix with real, simple spectrum. Then*

$$\phi(fg, M) = \phi(gf, M) = \phi(g, \phi(f, M)).$$

Proof. It suffices to show that

$$[\, f(M)\, g(M)\,]_Q = [\, f(M)\,]_Q\, [\, g(\phi(f, M))\,]_Q.$$

Now, from the uniqueness of the QR decomposition, for X with $\det X > 0$,

$$[\, QX\,]_Q = Q[\, X\,]_Q \text{ and } [\, XR\,]_Q = [\, X\,]_Q, \text{ for any } Q \in SO(n),\ R \in \mathcal{U}^+(n).$$

Using that $f(PXP^{-1}) = Pf(X)P^{-1}$ and the first equality just above,

$$[\, g(\phi(f, M))\,]_Q = [\, g\big([\, f(M))\,]_Q^T\, M\, [\, f(M))\,]_Q\big)\,]_Q =$$

$$\Big[\, [\, f(M)\,]_Q^T\, g(M)\, [\, f(M)\,]_Q\, \Big]_Q = [\, f(M)\,]_Q^T \Big[\, g(M)\, [\, f(M)\,]_Q\, \Big]_Q.$$

Go back to the beginning and use the second equality:

$$[\, f(M)\,]_Q\, [\, g(\phi(f, M))\,]_Q = \Big[\, g(M)\, [\, f(M)\,]_Q\, \Big]_Q =$$

$$\Big[\, g(M)\, [\, f(M)\,]_Q\, [\, f(M)\,]_R\, \Big]_Q = \Big[\, g(M)\, f(M)\Big]_Q = [\, (fg)(M)]_Q.$$

$\square$

Corollary 1. *Let M, f and g as above. Then the map*

$$(t, \tilde{M}) \in \mathbb{R}\ \times \mathcal{O}_M \mapsto \phi(tf, \tilde{M}) \in \mathcal{O}_M$$

is a globally defined flow in $\mathcal{O}_M$. The maps associated to f and g commute. The slice $\mathcal{S}$ through M is

$$\{[\exp f(M)]_Q^T\, M\, [\exp f(M)]_Q\, ,\, f \sim g \Leftrightarrow f = g + const\}.$$

In particular, it is diffeomorphic to $\mathbb{R}^{n-1}$:

$$(t_1, \ldots, t_{n-1}) \in \mathbb{R}^{n-1} \mapsto \phi(t_1 x + \ldots, t_{n-1} x^{n-1}, M) \in \mathcal{O}_M\ .$$

At this point, the reader might ask the relevance of writing $g = \exp f$. This is done to make explicit the presence of an underlying flow.

4.2. **Diferential equations for the flows.**
We obtain the standard equation for the flow $\phi(t, M)$ associated to f given above — let's take derivatives. For $Q(t) = [\, e^{f(M)}\,]_Q$ and $R(t) = [\, e^{f(M)}\,]_R$ and $M(0) = M$,

$$M(t) = \phi(tf\ , M) = Q(t)^T\, M(0)\, Q(t) = R(t)\, M(0)\, R^{-1}(t)\quad (*)$$

where $e^{tf(M(0))} = Q(t)\, R(t)$, so that, dropping time dependence,

$$M' = (Q^T)'M(0)\, Q + Q^T M(0)\, Q'\, ,\ f(M(0))e^{tf(M(0))} = f(M(0))\, Q\, R\ = Q'R + Q\, R'.$$

To get a differential equation, eliminate $M(0) = Q(t)M(t)(Q(t))^T$. Now, M, Q and R depend on t:

$$M' = (Q^T)'QM + MQ^T\, Q'\quad \text{and}\quad Q\, f(M(0))\, R\ = Q'R + Q\, R'.$$

Since $Q(t)$ is a curve of orthogonal matrices, $A(t) = Q^T\, Q'$ is a curve of skew symmetric matrices. Thus

$$M' = -AM + MA = [M, A]\quad \text{and}\quad f(M)\ = Q^T\, Q' +\ R'R^{-1}.$$

We are almost done: the matrix $f(M)$ in the last equation is a sum of a skew symmetric $Q^T Q'$ and and upper triangular $R'R^{-1}$, which bring to mind the factorization $M = \Pi_{sk} M + \Pi_{up}M$ from Section 3.2. Here $\Pi_{sk} M$ and M have the same strictly lower triangular part, which determines $\Pi_{sk} M$. Adding up,

$$M'(t) = [M(t), A(t)] = [M(t), \Pi_{sk} \ f(M(t))] .$$

The case $f(x) = x$ is the Toda lattice after Flaschka's change of variables. Equation (∗) is Symes's *solution by factorization* to the differential equation ([33]).

The fact that the Toda flow admits two different formulas by factorization, given by orthogonal and upper triangular conjugation of the initial condition, immediately implies that the evolution preserves the real tridiagonal symmetric form of the initial condition. Indeed, orthogonal conjugations preserve symmetry, and upper triangular conjugations preserve the upper Hessenberg form (i.e., the only nonzero entries below the diagonal lie in the subdiagonal of entries $(i + 1, i)$).

5. **Toda, QR and other algorithms.** In the fifties, Francis [19] came up with the QR algorithm to compute eigenvalues of symmetric matrices. Say $S = S_0$ is a real, symmetric matrix of positive simple spectrum. Consider the alternation of QR decompositions and reorderings,

$$S_0 = Q_0 R_0, \quad S_1 \ = \ R_0 Q_0 \ = \ Q_0^T S_0 \, Q_0 \ = \ R_0 \, S_0 \, R_0^{-1}.$$

Clearly, $S_1 \in \mathcal{O}_{S_0}$, so S_0 and S_1 are both symmetric with a common spectrum: the QR *step* is a diffeomorphism from $\mathcal{O}_{S_0}$ to itself. The remarkable thing about it is that iteration of this map converges to a diagonal matrix Λ — since a QR step clearly preserves spectrum, the diagonal entries of Λ are the eigenvalues of S_0!

It was Moser, again, who drew Percy Deift's attention to Symes's beautiful connection between the Toda flow and the QR algorithm [34]: at integer times n, the solution $J(t)$ of the Toda differential equation satisfies $exp\, J(n) = E_n$, where E_n is the n-th term in the QR sequence starting from $E_0 = expJ_0$. Since the Toda equation is one within a family of flows of the kind $\dot{J} = [f, \Pi_{skew}f(J)]$, one might fudge with the functional parameter ([14]):

Theorem 5.1. *The flow associated to $\dot{J} = [f, \Pi_{skew} \ln J]$ interpolates the QR sequence J_n.*

Proof. From Section 4.2, the solution of the equation is given by

$$J(t) = Q^*(t)J(0)Q(t), \quad \text{where } \exp t \ln J(0) = Q(t)R(t).$$

Thus, $J_0 = J(0) = Q(1)R(1)$ and $J(1) = Q^*(1)J(0)Q(1) = J_1$, the matrix obtained from J_0 from a QR step. □

The result holds, with the same proof, for arbitrary symmetric matrices S_0.

The fact that a Toda flow interpolates the QR iteration implies that the convergence properties of Toda flows are also satisfied by the iteration. The vocabulary of dynamical systems clarifies certain eigenvalue computations. The right side of Figure 1 represents $\bar{\mathcal{J}}_\Lambda$, the closure of the set of 4×4 Jacobi matrices with eigenvalues $1, 2, 3$ and 4. The vertices correspond to diagonal matrices, which are equilibria for the Toda vector field. The vertex I is a repulsor, A is an attractor and the remaining vertices are saddles with different signatures (i.e., dimensions of the unstable manifold). The presence of saddles explains why orbits bifurcate close to

some vertices (say, H, E and F) in the neighborhood of which an orbit spends long times (i.e., many QR iterations), a fact that was known in the numerical literature as *root disorder*.

Numerical analysts might have realized a long time ago that the QR algorithm is the integer evaluation of a flow. Indeed, it has been known for decades that one can obtain directly the matrix S_n of the QR iteration starting with a symmetric matrix S_0 is given by $S_n = Q_n^* S_0 Q_n = R_n S_0 R_n^{-1}$ where Q_n and R_n are obtained from the QR factorization $S_0^n = Q_n R_n$. Morally (and indeed, true), the step

$$S_{1/n} = Q_{1/n}^* S_0 Q_{1/n} = R_{1/n} S_0 R_{1/n}^{-1}, \quad S_0^{1/n} = Q_{1/n} R_{1/n}$$

is an n-th root of the usual QR step (in the sense that n such steps yield the usual QR step). Now, to obtain the interpolating flow (which belongs to the Toda family, as we saw) simply compute

$$\lim_{n \to \infty} n(S_{1/n} - S_0) = \lim_{n \to \infty} n(Q_{1/n}^* S_0 Q_{1/n} - S_0).$$

Up to order $1/n$,

$$S_0^{1/n} \simeq I + \ln S_0, \quad I + \ln S_0 \simeq (\Pi_{sk} \ln S_0)(\Pi_{up}(I + \ln S_0))$$

and thus $Q_{1/n} \simeq I + \Pi_{sk} \ln S_0$. The interpolating flow, for which $f = \ln(x)$, is

$$S'(t) = [\, S, \Pi_{sk} \ln S \,].$$

5.1. **Toda, Choleski and SVD.** There is nothing special about QR factorizations: other factorizations give rise to flows which are very similar to the Toda lattice.

A *Cholesky* factorization $M = M_L M_U$ decomposes a matrix M as a product of lower and upper triangular matrices M_L and M_U with the same positive diagonal. The factorization can be performed (uniquely) for matrices in G_+, having upper principal minors with positive determinant. Now ([11]), on G_+ define the product $g * h = h_L g h_U$. For an appropriate coupling, the induced dual Lie algebra is the phase space which accommodates the Cholesky iteration,

$$M_n = L_n U_n, \quad M_{n+1} = U_n L_n, \quad n = 0, 1, \ldots$$

and its continuous interpolation (notice that blowups may happen). The Lie bracket associated to this group structure is an example of the so called *R-matrix formalism* applied to the standard matrix Lie bracket, but this is another story.

Given a real matrix M, its *singular values* are the (nonnegative) lengths of the semi-axis of the ellipsoid obtained by applying M to the unit (Euclidean) sphere. The *singular value decomposition* of M is the product $M = Q\Sigma U$, where Q and U are orthogonal matrices and Σ is a diagonal matrix having the singular values as diagonal entries.

There is an efficient algorithm, similar to QR, to compute singular values of tridiagonal matrices, which was shown by J. Demmel and XXXX Kahan to have remarkable stability properties with respect to relative errors. In [9], these properties were considered from a symplectic setup: the appropriate phase space is chosen taking into account the specific concern with relative errors. The Jacobian $M(i, j)$ of the map sending a matrix at step i to its (discrete) evolution at time j is studied using Krein's perturbation theory for symplectic matrices. A number of properties arise, which are responsible for the good performance of the algorithm: for large i, the spectrum of $M(i, j)$ is simple, lies in the unit circle and $M(i, j)$ converges

to a limit, explicitly computed. The agreement between theoretical estimates and experiments was remarkable: the rate between computed and estimated error was never larger than 8, independent of dimension.

6. **Bidiagonal coordinates.** Norming constants in Section 2.2 have a drawback: they do not cover the limit points of algorithms which converge to reduced matrices (i.e., tridiagonal matrices with some main off-diagonal entries equal to zero), like the Toda flows and QR type algorithms. This problem has been circumvented by the introduction of *bidiagonal coordinates* ([25]). As an extra bonus, bidiagonal coordinates provide an atlas for $\mathcal{T}_\Lambda$. The construction goes as follows.

Let $\mathcal{L}^1(n)$ denote the group of lower triangular matrices with unit diagonal entries. For $M \in \mathcal{M}(n)$, the *LU positive factorization*, when it exists, is given by $M = LU$, where $L \in \mathcal{L}^1(n)$ and $U \in \mathcal{U}^+(n)$. Clearly, this happens if and only if the determinants of the upper principal minors of M are positive.

Let S_n be the symmetric group on the set $\{1, 2, \ldots, n\}$. For $\pi \in S_n$, define

$$\Lambda_\pi = \mathrm{diag}(\lambda_{\pi(1)}, \lambda_{\pi(2)}, \ldots, \lambda_{\pi(n)}).$$

Bidiagonal coordinates provide a chart of $\mathcal{T}_\Lambda$ for each permutation π, having for domain the set $\mathcal{U}_\Lambda^\pi \subset \mathcal{T}_\Lambda$ consisting of matrices $T = Q_\pi^* \Lambda_\pi Q_\pi$ for which there exists an orthogonal matrix Q_π admitting an LU positive factorization $Q_\pi = L_\pi U_\pi$. This is not as restrictive as it looks: if $T = Q_\pi^* \Lambda_\pi Q_\pi$, another spectral decomposition is given by $T = Q_\pi^* E \Lambda_\pi E Q_\pi$, where E is a diagonal matrix with entries equal to ± 1 along the diagonal: one may use E to force the positivity of the determinants of the principal minors of EQ_π, provided that the corresponding determinants of Q_π are nonzero. Notice that the request that Q_π admits an LU positive factorization gives rise to a *unique* spectral decomposition $T = Q_\pi^* \Lambda_\pi Q_\pi$. We then have

$$T = Q_\pi^* \Lambda_\pi Q_\pi = (L_\pi U_\pi)^{-1} \Lambda_\pi L_\pi U_\pi = U_\pi^{-1} B_\pi U_\pi$$

where

$$B_\pi = L_\pi^{-1} \Lambda_\pi L_\pi = U_\pi T U_\pi^{-1}.$$

Theorem 6.1. *The matrix B_π is lower bidiagonal with diagonal Λ_π. The principal off-diagonal entries $\beta_k^\pi = (B_\pi)_{k+1,\, k}$ define a diffeomorphism $\psi_\pi : \mathcal{U}_\Lambda^\pi \to \mathbb{R}^{n-1}$. The signs of β_k^π and $T_{k+1,k}$ are equal and their quotient goes to one, when one of them goes to zero. Each domain $\mathcal{U}_\Lambda^\pi$ is an open, dense set $\mathcal{U}_\Lambda^\pi$, containing one diagonal matrix. The charts $\{\psi_\pi : \mathcal{U}_\Lambda^\pi \to \mathbb{R}^{n-1}, \pi \in S_n\}$ form an atlas for $\mathcal{T}_\Lambda$.*

Proof. Since $B_\pi = L_\pi^{-1} \Lambda_\pi L_\pi$, it is a lower triangular matrix and from $B_\pi = U_\pi T U_\pi^{-1}$, it is upper Hessenberg. This implies that B_π is lower bidiagonal, with the same spectrum as Λ_π.

To show that the chart is a diffeomorphism to $\mathbb{R}^{n-1}$, consider the following naive inverse algorithm. Build B_π out of off-diagonal entries β_j^π and (distinct) eigenvalues $\lambda_{\pi(i)}$. Diagonalize, $B_\pi = L_\pi^{-1} \Lambda_\pi L_\pi$, and get Q_π out of the QR factorization $L_\pi = Q_\pi R_\pi$ (notice that, automatically, Q_π admits an LU positive factorization). Finally set $T = Q_\pi^* \Lambda_\pi Q_\pi$. Clearly Q_π admits an LU factorization, so $Q_\pi \in \mathcal{U}_\Lambda^\pi$.

Since $U \in \mathcal{U}^+(n)$, the equation $B_\pi = U_\pi T U_\pi^{-1}$ gives that the signs of β_k^π and $T_{k+1,k}$ are equal.

The remaining statements are left to the reader. $\qquad \square$

Figure 2 is an example for $n = 3$: here $\Lambda_\pi = \mathrm{diag}(7, 4, 5)$ and $\mathcal{U}_\Lambda^\pi$ is the interior of the polygon with boundary given by the unglued edges (the glued edges belong to $\mathcal{U}_\Lambda^\pi$). Figure 3 was obtained using such charts: the standard norming constants would distort too much the picture (and degenerate completely) at boundaries of (signed) Jacobi matrices. Once eigenvalues are fixed, the bitorus $\mathcal{T}_\lambda$ lies in the intersection of a hyperplane (constant $\mathrm{tr}\, S$) and a sphere (constant $\mathrm{tr}\, S^2$), and the figure is the image of a conformal projection of $\mathcal{T}_\lambda$ in $\mathbb{R}^2$.

Another remarkable property of bidiagonal coordinates is that their evolution under the Toda equations manages to be even simpler that the evolution of the standard inverse variables. We consider the Toda vector fields on real, symmetric, tridiagonal matrices,

$$T'(t) = [T(t), \Pi_{sk}\,(f(T(t)))]. \tag{T}$$

Proposition 5. *Fix π, take $T(0) \in \mathcal{U}_\Lambda^\pi$. The chart domain $\mathcal{U}_\Lambda^\pi$ is invariant under equation (T). The evolution of the bidiagonal coordinates is*

$$B_\pi'(t) = [B_\pi(t), -f(\Lambda_\pi)], \ \ i.e., \ (\beta_i^\pi)'(t) = (f(\lambda_{\pi(i+1)}) - f(\lambda_{\pi(i)}))\ \beta_i^\pi(t)\ .$$

Proof. We first prove that (T) leaves $\mathcal{U}_\Lambda^\pi$ invariant. Take $T(0) \in \mathcal{U}_\Lambda^\pi$: omitting the permutation π, we have $T(0) = Q_0^* \Lambda Q_0$, where Q_0 has an LU positive decomposition. Solve (T) as in Section 4.2: for $\exp(tf(T(0))) = Q(t)\,R(t)$,

$$T(t) = Q(t)^*\, T(0)\, Q(t) = Q(t)^*\, Q_0^*\, \Lambda\, Q_0\, Q(t)$$

We want to prove that $\tilde{Q}(t) = Q_0\, Q(t)$ admits an LU positive factorization:

$$\tilde{Q}(t) = Q_0\, \exp(tf(T(0)))\, R^{-1}(t) = Q_0\, \exp(tf(T(0)))\, Q_0^*\, Q_0\, R^{-1}(t)$$

$$= Q_0\, \exp(tf(Q_0^*\, \Lambda\, Q_0))\, Q_0^*\, Q_0\, R^{-1}(t) = \exp(tf(\Lambda))\, Q_0\, R^{-1}(t).$$

The upper principal minors of $\tilde{Q}(t)$ and Q_0 have the same signs, since $\exp(tf(\Lambda))$ is a positive diagonal matrix and $R^{-1}(t) \in \mathcal{U}^+(n)$.

We now consider bidiagonal coordinates. Clearly

$$T(t) = Q^*(t)Q_0^*\, \Lambda\, Q_0 Q(t) = \tilde{Q}^*(t)\, \Lambda\, \tilde{Q}(t), \quad \tilde{Q}^*(t)\, \tilde{Q}'(t) = Q^*(t)Q'(t).$$

Now, $B(t) = L^{-1}(t)\, \Lambda\, L(t)$ and we obtain $B'(t) = [B(t), L^{-1}(t)\, L'(t)]$ by now familiar computations. The matrix L is obtained by the LU positive factorization $\tilde{Q}(t) = L(t)\, U(t)$, so that, dropping the time dependence, $\tilde{Q}' = L'U + LU'$ yields

$$L^{-1}\tilde{Q}'U^{-1} = L^{-1}L' + U'U^{-1}.$$

Consider the split $M = \Pi_{sl}\, M + \Pi_u M$ of a matrix M into strictly lower and upper triangular parts. Since L has a diagonal of ones, $L^{-1}L'$ is strictly lower triangular. The solution by factorization in Section 4.2 gives $\tilde{Q}^*\, \tilde{Q}' = \Pi_{sk}\,(f(T))$, so that

$$L^{-1}L' = \Pi_{sl}\, L^{-1}\tilde{Q}'U^{-1} = \Pi_{sl}\, U\left(\Pi_{sk}\, f(T)\right) U^{-1}.$$

Now, the matrices M and $\Pi_{sk}\, M$ have the same strictly lower triangular part and U is upper triangular, so

$$L^{-1}L' = \Pi_{sl}\, U f(T)U^{-1} = \Pi_{sl}\, f(UTU^{-1}) = \Pi_{sl}\, f(B).$$

Adding up,

$$B' = [B, L^{-1}L'] = [B, \Pi_{sl}\, f(B)] = [B, f(B) - f(\Lambda)] = [B, -f(\Lambda)]$$

$\square$

The proof requires interpretation in the case $f(x) = \ln x$, which is of relevance for QR interpolation: we need $\exp(tf(\Lambda))$ to be a positive diagonal matrix — in this case, the diagonal entries must be equal to $|\lambda_k|$.

Bidiagonal coordinates are especially convenient to study asymptotic behavior of Toda flows. As an application, [25] computes their scattering map, described in Section 2.2, by filling up the following inevitable outline. Recall from Figure 1 that Toda flows starting from Jacobi matrices have for ω and α limits the diagonal matrices associated to $\pi_\omega(i) = i$ and $\pi_\alpha(i) = n - i + 1$. On each chart, the Toda evolution in bidiagonal coordinates is simple. The change of charts required to keep track of both extremes of an orbit is equally simple.

An appropriate extension of this formalism provides charts on isospectral manifolds of real and complex matrices with given *profile*, a natural extension of the concept of tridiagonality — a text is under preparation ([35]).

6.1. QR steps with shifts.

Numerical analysts have clever ways to accelerate the convergence of QR steps. The original QR step is just the choice $f(x) = \ln x$ in the family

$$S_n \mapsto S_{n+1} = [\exp f(S_0)]_Q^* \, S_0 \, [\exp f(S_0)]_Q = [\exp f(S_0)]_R \, S_0 \, [\exp f(S_0)]_R^{-1}.$$

Bidiagonal coordinates may be used to indicate interesting alternatives: interpret a step as a time 1 map for a differential equation and integrate the trivial flow which describe evolutions in Proposition 5. For $f(x) = \ln g(x)$, taking into account the caveat after its proof, the change of the bidiagonal coordinates of a matrix $T \in \mathcal{U}_\Lambda^\pi$ under a step is

$$(\beta_1^\pi, \ldots, \beta_{n-1}^\pi) \mapsto \left(\left| \frac{g(\lambda_{\pi(2)})}{g(\lambda_{\pi(1)})} \right| \beta_1^\pi, \ldots, \left| \frac{g(\lambda_{\pi(n)})}{g(\lambda_{\pi(n-1)})} \right| \beta_{n-1}^\pi \right).$$

We are interested in functions g for which some β_k^π becomes small — in this case, the corresponding matrix essentially decouples in two smaller tridiagonal matrices, for which the computation of eigenvalues is simpler. Taking into account the denominators in the formula, a natural possibility is a function g which equals zero at $\lambda_{\pi(n)}$ but does not vanish at the other eigenvalues. Keep in mind that, unfortunately, we do not know the eigenvalues. In particular, it is especially hard to obtain such a g which would reduce drastically a centrally located β_k^π (i.e., $k \sim n/2$).

Notice that, from Theorem 6.1, the matrix T is Jacobi if and only if its bidiagonal coordinates β_k^π are positive, and the sign is preserved under general QR steps. On the other hand, removing the absolute values in the formula shows that one can replace iterations lying within Jacobi matrices to iterations on tridiagonal matrices without changing their asymptotic properties: only the off-diagonal entries eventually have different signs. The new iteration is *smooth* on the isospectral manifold $\mathcal{T}_\Lambda$, and convergence rates may be obtained using Taylor expansions.

Typically, along an iteration of an algorithm searching for eigenvalues, one has good approximations s for one of them. Numerical analysts then use $g(x) = x - s$, the iteration with *shift s*. The bidiagonal coordinates, in this case, change as follows:

$$(\beta_1^\pi, \ldots, \beta_{n-1}^\pi) \mapsto \left(\left| \frac{\lambda_2^\pi - s}{\lambda_1^\pi - s} \right| \beta_1^\pi, \ldots, \left| \frac{\lambda_n^\pi - s}{\lambda_{n-1}^\pi - s} \right| \beta_{n-1}^\pi \right).$$

Numerical analysts frequently do not wait until they get a good approximation s. There are different shift strategies ([31]), we consider the *Rayleigh quotient shift*,

for which $s = T_{n,n}$, and the *Wilkinson shift*: compute the eigenvalues of $\hat{T}$, the bottom 2×2 principal minor of T, and take for s the one which is closer to $T_{n,n}$.

Under the Rayleigh shift, once iteration approaches convergence, a simple Taylor expansion shows that the bottom entry $b = \beta_{n-1}^{\pi}$ converges cubically to zero, in the sense that $b^{m+1} = O((b^m)^3)$ for bottom entries at consecutive iterations. Once b is small enough, the matrix undergoes *deflation*: $T_{n,n}$ is declared a good approximation of an eigenvalue and the algorithm proceed with the top $(n-1) \times (n-1)$ block. There is one catch however: for some initial conditions, the Rayleigh shift gives rise to periodic orbits.

This does not happen for the Wilkinson shift. The dynamics in this case is richer: we describe the results but may only indicate [26] and [27] for proofs.

Theorem 6.2. *For the generic initial condition, a Wilkinson iteration leads to cubic convergence of $b = \beta_{n-1}^{\pi} \sim T_{n,n-1}$. If the original matrix T has no three eigenvalues in arithmetic progression, this is always the case. Otherwise, there may be a Cantor-like set of initial conditions for which iteration is quadratic.*

In a nutshell, there are discontinuities in the choice of s, at points where $T_{n,n}$ is equidistant from the eigenvalues of the block $\hat{T}$. The Cantor-like set in the statement of the theorem consists of matrices all of whose iterations lie in this situation. Typically, this never happens or happens just at few steps and convergence is cubic.

7. **Lax pairs beyond Toda.** Forty years of contributions from a large community greatly increased our understanding of the Toda flow, which sometimes is undistinguishable from the more general Lax pair evolution. Mutations are abundant: for a beautiful starting point about different representations of the Toda flow (and yet other geometric issues which may studied through them), the reader should refer to [**?**].

In this text, we emphasized examples over theory. In order to indicate the versatility of the concepts which have been presented, we close with a final example.

7.1. **The billiard on an ellipsoid.** Moser and Veselov [30] came up with an very interesting formulation of the elliptic billiard. In the ellipsoid $E = \{x : (x, C^{-2}x) \leq 1\}$, a ball moves along a direction y_0 (a unit vector), hits the boundary ∂E at x_0, and leaves with direction y_1 until it hits x_1. They presented the *billiard map* $\Psi(x_0, y_0) = (x_1, y_1)$ in the following fashion. Write the (matrix) polynomial

$$L_0(\lambda) = y_0 \otimes y_0 + \lambda x_0 \wedge y_0 - \lambda^2 C^2$$

and factor in linear terms,

$$L_0(\lambda) = (\lambda C + y_0 \otimes \xi_0)(-\lambda C + \xi_0 \otimes y_0), \quad \xi_0 = C^{-1}x_0, \|\xi_0\| = 1,$$

intertwine factors as in the QR algorithm and factor again,

$$L_0'(\lambda) = (-\lambda C + \xi_0 \otimes y_0)(\lambda C + y_0 \otimes \xi_0) = (\lambda C + y_0' \otimes \xi_0')(-\lambda C + \xi_0' \otimes y_0'),$$

with $y_0' = \psi_0, \|\xi_0'\| = 1$. Set $\phi(x_0, y_0) = (-Cy_1, C^{-1}x_0)$: then $\Psi = -\phi^2$.

In [12], the analogy of the Moser-Veselov formalism to the QR iteration — better still, to the Cholesky iteration [11] — is taken literally. The relevant group now is G_+, consisting of loops $\gamma : i\mathbb{R} \to GL(n, \mathbb{C})$ which are smooth at ∞, contract to the identity loop, are positive diagonal at ∞, satisfy the reality condition $\gamma(\bar{\lambda}) = \overline{\gamma(\lambda)}$ and admit a (unique) Riemann-Hilbert factorization $\gamma = \gamma_L \gamma_R$, where γ_L and γ_R have analytic continuations to the left and right side of the imaginary axis

respectively, and same diagonal values at ∞. The group operation is $\gamma * \delta = \delta_L \gamma \delta_R$. Take an initial data for the billiard evolution and construct the rational matrix function $A_0(\lambda) = L_0(\lambda)/(1 - \lambda^2)$.

One has to circumvent a technical difficulty: $A_0(0)$ is not invertible — it is a rank one matrix! Still, as in the finite dimensional cases, the evolution is interpolated by a differential equation. This time, the solution formula by factorization involves a *Riemann-Hilbert problem*, with a mild singularity at $\lambda = 0$.

8. **Appendix 1: the QR and LU factorizations.** Let M an invertible, real matrix. Then there is a unique $Q \in SO(n)$ and $R \in \mathcal{U}(n)$ for which $M = QR$, the *QR factorization of M*. Indeed, let $e_i, i = 1, \ldots, n$ be the canonical vectors: the reader should have no difficulty in showing that the subspaces generated by Me_i and Qe_i, for $i = 1, \ldots, k$ (k arbitrary) should be the same, if such a decomposition exists. Since the columns of Q are orthonormal, they must be the vectors obtained by applying the Gram-Schmidt orthogonalization procedure to the columns of M sequentially. The entries of R are the coefficients used in the representation of Me_i in terms of the columns $Qe_1, \ldots, Qe_i$. Since M is invertible, the process is feasible, and appropriate normalizations give rise to positive diagonal entries of R.

Similarly, the (unique) LU decomposition of M is $M = LU$, where $L \in \mathcal{L}^1(n)$ and $U \in \mathcal{U}^+(n)$. This decomposition exists if and only if the principal diagonal minors of M (i.e., the determinants of the $k \times k$ submatrices M_k with entries in the intersection of the first k rows and columns, $k = 1, \ldots, n$) are strictly positive. In a nutshell, from $M_k = L_k U_k$, it is clear that an inductive construction is at hand: the details are left to the reader or in standard texts ([**?**], [**?**]).

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