Lecture 3
Lax Evolution and Its Equivalents

Orthogonal Polynomials, Moments, Determinants, and Measure Deformation

Moody T. Chu

North Carolina State University

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Outline

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Basic Dynamics

- Lax dynamics:

$$\frac{dX(t)}{dt} := [X(t), k_1(X(t))]$$
$$X(0) := X_0.$$

- Parameter dynamics:

$$\frac{dg_1(t)}{dt} := g_1(t)k_1(X(t))$$
$$g_1(0) := I.$$

and

$$\frac{dg_2(t)}{dt} := k_2(X(t))g_2(t)$$
$$g_2(0) := I.$$

- $k_1(X) + k_2(X) = X$.

Similarity Property

$$X(t) = g_1(t)^{-1}X_0g_1(t) = g_2(t)X_0g_2(t)^{-1}.$$

- Define $Z(t) = g_1(t)X(t)g_1(t)^{-1}$.
- Check

$$\begin{aligned}\frac{dZ}{dt} &= \frac{dg_1}{dt}Xg_1^{-1} + g_1\frac{dX}{dt}g_1^{-1} + g_1X\frac{dg_1^{-1}}{dt}\\ &= (g_1k_1(X))Xg_1^{-1} + g_1(Xk_1(X) - k_1(X)X)g_1^{-1}\\ &\quad + g_1X(-k_1(X)g_1^{-1}) = 0.\end{aligned}$$

- Thus $Z(t) = Z(0) = X(0) = X_0$.

Factorization Property

$$exp(tX_0) = g_1(t)g_2(t).$$

- Trivially $exp(X_0 t)$ satisfies the IVP

$$\frac{dY}{dt} = X_0 Y, Y(0) = I.$$

- Define $Z(t) = g_1(t)g_2(t)$.
- Then $Z(0) = I$ and

$$\begin{aligned} \frac{dZ}{dt} &= \frac{dg_1}{dt} g_2 + g_1 \frac{dg_2}{dt} \\ &= (g_1 k_1(X))g_2 + g_1(k_2(X)g_2) = g_1 X g_2 \\ &= X_0 Z \text{ (by Similarity Property).} \end{aligned}$$

- By the uniqueness theorem in ODEs, $Z(t) = exp(X_0 t)$.

Reversal Property

$$exp(tX(t)) = g_2(t)g_1(t).$$

- By Factorization Property,

$$\begin{aligned} g_2(t)g_1(t) &= g_1(t)^{-1}exp(X_0t)g_1(t) \\ &= exp(g_1(t)^{-1}X_0g_1(t)t) \\ &= exp(X(t)t). \end{aligned}$$

Abstract QR-type Factorization

- Arbitrary subspace splitting $gl(n) \Longleftrightarrow$ Factorization of a *one-parameter semigroup* in the neighborhood of I as the product of two nonsingular matrices , i.e.,

$$exp(X_0 t) = g_1(t) g_2(t).$$

  - Lie algebra splitting of $gl(n) \Longleftrightarrow$ Lie group decomposition of $Gl(n)$ in the neighborhood of I.
- The product $g_1(t)g_2(t)$ will be called the *abstract* $g_1 g_2$ *factorization* of $exp(X_0 t)$.

Abstract QR-type Algorithm

- By setting $t = 1$, we have

$$\begin{aligned} exp(X(0)) &= g_1(1)g_2(1) \\ exp(X(1)) &= g_2(1)g_1(1). \end{aligned}$$

- The dynamical system for $X(t)$ is autonomous $\Longrightarrow$ The above phenomenon will occur at every feasible integer time.
- Corresponding to the abstract $g_1 g_2$ factorization, the above iterative process at all feasible integers is regarded as an *abstract $g_1 g_2$ algorithm*.

Toda Flow

- Lie algebra splitting:
  - Write
  $$X = \underbrace{X^- - X^{-\top}}_{\Pi_0(X)} + \underbrace{X^0 + X^+ + X^{-\top}}_{\Pi_1(X)}.$$
  where X^o is the diagonal, X^+ the strictly upper triangular, and X^- the strictly lower triangular part of X.
  - $gl(n) = \{\text{skew symmetric}\} \bigoplus \{\text{upper triangular}\}$.
- The Toda lattice (Symes'82, Deift el al'83):

$$\begin{aligned} \frac{dX}{dt} &= [X, \Pi_0(X)] \\ X(0) &= X_0. \end{aligned}$$

QR Algorithm and Limiting Behavior

- *QR* flows in two Lie subgroups,

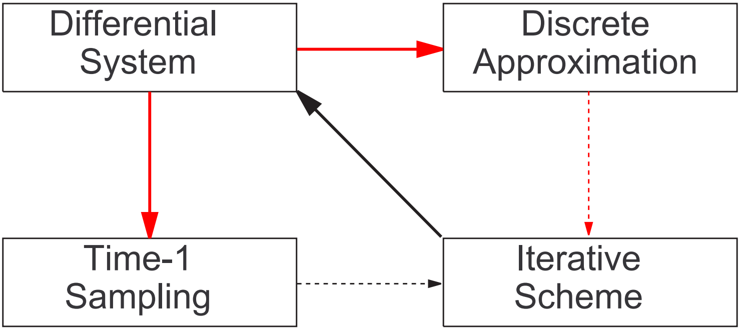
$$\frac{dQ(t)}{dt} := Q(t)\Pi_0(X(t)),\ Q(0) := I \quad \Rightarrow Q(t) \text{ is orthogonal.}$$
$$\frac{dR(t)}{dt} := \Pi_1(X(t))R(t),\ R(0) := I \quad \Rightarrow R(t) \text{ is upper triangular.}$$

- Samples at integer times,
  - $\{X(k)\}$ gives the same sequence as does the *QR* algorithm applied to the matrix $A_0 = exp(X_0)$.
- An isospectral flow starting from X_0,
  - Toda lattice is a Hamiltonian system.
  - Certain physical quantities are kept at constant, i.e., this is a *completely integrable* system.
  - Asymptotic behavior can be analyzed via ODE theory.

Mimicry versus Embedment

- A continuous system that mimics the dynamical behavior of a discrete system is easy to generate.
- The correspondence between the *QR* algorithm and the Toda lattice exhibits a new type of involvement.
  - The result of an iterative scheme is entirely “embedded" in the solution curve of a continuous dynamical system.
  - The solution curve of a differential equation smoothly “interpolates" all points generated by a discrete dynamical system.

Mutual Implications



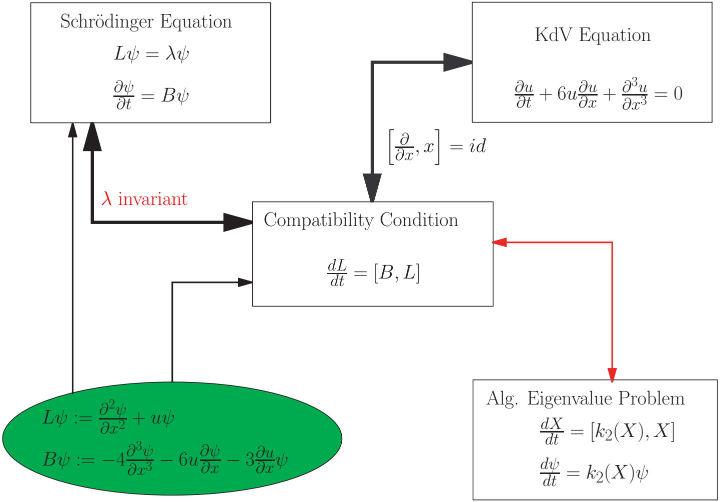
Generalized Toda Lattice

- Pseudo convergence:
  - The *QR* algorithm can be applied to general nonsymmetric matrices.
  - If A_0 has complex eigenvalues, the *QR* iterates do not converge to any fixed limit point, but to a block upper triangular “form" with at most 1×1 or 2×2 blocks along the main diagonal.
  - The *QR* algorithm produces only the upper quasi-triangular form, but not any fixed matrix, in its limiting behavior.
- Limit cycle:
  - The Toda flow applied to a nonsymmetric matrix X_0 does not have any asymptotically stable equilibrium point in general.
  - The flow converges to an upper quasitriangular form where each of the 2×2 blocks actually represents an ω-limit cycle.
  - The limit cycle behavior of the Toda flow offers a theoretical explanation of the pseudo-convergence behavior of the *QR* algorithm.

Informal Definitions

- A differential system is said to be *completely integrable*
  - $\Leftrightarrow$ It enjoys infinitely many conservation laws.
  - $\Leftrightarrow$ It can be expressed in terms of a Lax pair.
- The existence of a Lax pair allows to apply (at least formally) inverse scattering techniques to solve a completely integrable equation.

KdV and Schrödinger Equations



Time Invariant Eigenvalues

- Suppose L and B are general time-dependent operators satisfying

$$\begin{aligned} L\psi &= \lambda\psi \\ \frac{\partial\psi}{\partial t} &= B\psi. \end{aligned}$$

- If λ is time invariant, then

$$\frac{dL}{dt}\psi + L\underbrace{\frac{\partial\psi}{\partial t}}_{B\psi} = \lambda\underbrace{\frac{\partial\psi}{\partial t}}_{B\psi}.$$

- The Lax dynamics:

$$\frac{dL}{dt} = BL - LB.$$

  - Regardless how B and L are defined.

Schrödinger Operator

$$L := \frac{\partial^2}{\partial x^2} + u.$$

- $\frac{dL}{dt} = \frac{\partial u}{\partial t}$ is but a multiplication.
- Fundamental operation:

$$\underbrace{\left[\frac{\partial}{\partial x}, x\right]}_{\textit{identity}} \psi = \left(\frac{\partial}{\partial x} x - x \frac{\partial}{\partial x}\right) \psi = \frac{\partial}{\partial x}(x\psi) - x \frac{\partial}{\partial x} \psi = \psi.$$

Searching Operator B

- Try $B_0 = \frac{\partial}{\partial x} \Rightarrow \frac{\partial u}{\partial t} = [B_0, L] = \frac{\partial u}{\partial x}$.
  - This is a trivial translation.
- Try $B_1 = \frac{\partial^3}{\partial x^3} + b\frac{\partial}{\partial x} + \frac{\partial}{\partial x}b$.

$$[B_1, L] = \frac{\partial^3 u}{\partial x^3} + 3\frac{\partial^2 u}{\partial x^2}\frac{\partial}{\partial x} + 3\frac{\partial u}{\partial x}\frac{\partial^2}{\partial x^2} + 2b\frac{\partial u}{\partial x} - 4\frac{\partial b}{\partial x}\frac{\partial^2}{\partial x^2} - 4\frac{\partial^2 b}{\partial x^2}\frac{\partial}{\partial x} - \frac{\partial^3 b}{\partial x^3}$$

  - Choose $b = \frac{3}{4}u \Rightarrow [B_1, L] = \frac{1}{4}\frac{\partial^3 u}{\partial x^3} + \frac{3}{2}u\frac{\partial u}{\partial x}$.
- Choose $B := -4B_1 \Rightarrow$
  - $B = -\frac{\partial^3}{\partial x^3} - 3u\frac{\partial}{\partial x} - 3\frac{\partial}{\partial x}u$
  - $\frac{dL}{dt} = BL - LB$ (Lax Dynamics) $\Leftrightarrow \frac{\partial u}{\partial t} + 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0$ (KdV equation).

Some Basic Notions about Computation

- Central theme in the game.
  - Engage dynamical systems such as the Lax dynamics.
  - Maintain isospectrality.
- Most conventional numerical ODE methods, in particular the linear multi-step and the Runge-Kutta schemes, cannot preserve isospectral flows (Calvo, Iserles & Zanna, ’97).

One Quick Remedy

- Bypass the isospectrality.
  - Perform numerical integration over the parameter dynamical system.
  - Employ the similarity property to reclaim $X(t)$.
- Solving the parameter dynamical system still requires the preservation of some structures, but can be handled more easily.
  - Orthogonal integrators (Dieci, Russell & Van Vleck, '94).
  - Projections.

Two (Three) Avenues of Attack

- Follow the paradigm of discretization from the classical numerical analysis prospective.
- Geometric integrator.
  - Numerical schemes that preserve geometric properties, such as properties of the exact flow of a differential equation.
    - Symplectic integrators.
    - Lie group integrators.
    - Volume preserving integrators.
    - Energy preserving integrators.
    - Integrators preserving first integrals and Lyapunov functions.
    - Integrators preserving coadjoint orbits and Casimirs.
    - Lagrangian and variationial integrators.
    - Integrators respecting Lie symmetries.
    - Integrators preserving contact structures.
  - Very active reserach subject at the moment.
- Integrable discretization.
  - Can be considered as a special geometric integrator.
  - Few research results.

Orthogonal Polynomials

- Orthogonal polynomials with respect to a given a measure $\mu(x)$,

$$\int p_k(x)p_\ell(x)\,d\mu(x) = \delta_{k,\ell}, \quad k,\ell = 0,1,\dots.$$

- Three-term recurrence relationship.

$$xp_k(x) = a_k p_{k+1}(x) + b_k p_k(x) + a_{k-1}p_{k-1}(x), \quad k = 1,2,\dots,$$

  with $p_{-1}(x) \equiv 0$ and $p_0(x) \equiv 1$.
- Corresponding monic polynomials $\{\tilde{p}_k(x)\}_k$,

$$x\tilde{p}_k(x) = \tilde{p}_{k+1} + b_k\tilde{p}_k(x) + a_{k-1}^2\tilde{p}_{k-1}(x).$$

Hankel Determinants

$$H_k := \det \begin{bmatrix} s_0 & s_1 & \dots & s_{k-1} \\ s_1 & s_2 & & s_k \\ \vdots & & & \vdots \\ s_{k-1} & s_k & \dots & s_{2k-2} \end{bmatrix}.$$

- s_j are *moments* with respect to μ,

$$s_j := \int x^j \, d\mu(x), \quad j = 0, 1, \dots .$$

Classical Moment Problem

- $\tilde{p}_k(x)$ is given by (Akhiezer'65,Szegö'75),

$$\tilde{p}_k(x) = \frac{1}{H_k}\det\begin{bmatrix} s_0 & s_1 & \dots & s_k \\ s_1 & s_2 & & s_{k+1} \\ \vdots & & & \vdots \\ s_{k-1} & s_k & \dots & s_{2k-1} \\ 1 & x & \dots & x^k \end{bmatrix},$$
$$= x^k + c_1^{(k)}x^{k-1} + \dots + c_{k-1}^{(k)}x + c_k^{(k)},$$

- $$c_j^{(k)} = \frac{(-1)^j}{H_k}\det\begin{bmatrix} s_0 & \dots & s_{k-j-1} & s_{k-j+1} & \dots & s_k \\ s_1 & & & & & s_{k+1} \\ \vdots & & \vdots & \vdots & & \vdots \\ s_{k-1} & \dots & s_{2k-j-2} & s_{2k-j} & \dots & s_{2k-1} \end{bmatrix}.$$

Polynomials in Moments

- By comparing the corresponding coefficients,

$$\begin{aligned} a_k^2 &= \frac{H_k H_{k+2}}{H_{k+1}^2}, \\ b_k &= c_1^{(k)} - c_1^{(k+1)}. \end{aligned}$$

- A classical result.

$$\mu(x) \rightsquigarrow s_j \leftrightsquigarrow H_k \rightsquigarrow p_k(x) \leftrightsquigarrow \{a_{k-1}, b_k\}.$$

Measure Deformation

- Rewrite orthogonality in matrix form,

$$\underbrace{\begin{bmatrix} b_0 & a_0 & 0 & & & \\ a_0 & b_1 & a_1 & 0 & & \\ 0 & a_1 & b_2 & a_2 & 0 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}}_{J} \begin{bmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{bmatrix} = x \begin{bmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{bmatrix}.$$

- What can be said about

$$\mu(x;t) \leftrightsquigarrow J(t),$$

if the measure is time dependent?

  - This is a hard inverse moment problem.

Semi-infinite Toda Lattice

- If $J(t)$ follows the Toda flow, that is, if

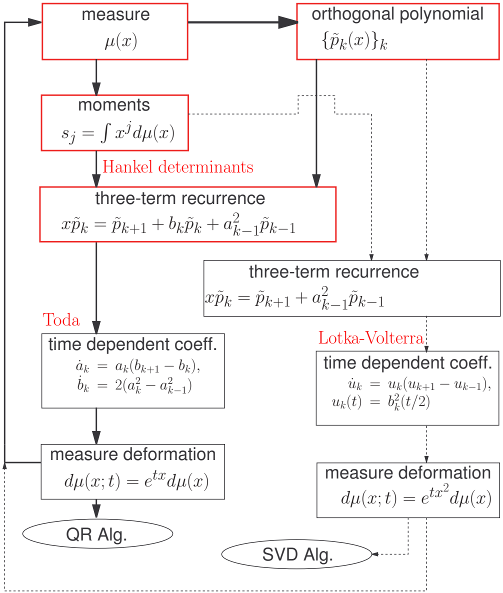
$$\begin{aligned} \frac{da_k}{dt} &= a_k(b_{k+1} - b_k), \\ \frac{db_k}{dt} &= 2(a_k^2 - a_{k-1}^2), \end{aligned}$$

with $a_{-1} \equiv 0$, then (Moser'75)

$$d\mu(x;t) := e^{tx} d\mu(x;0).$$

Moment Generator for Toda Lattice

$$s_{\ell+1} = \frac{ds_\ell}{dt}, \quad \ell = 0, 1, \ldots$$


measure
$\mu(x)$
orthogonal polynomial
$\{\tilde{p}_k(x)\}_k$
moments
$s_j = \int x^j d\mu(x)$
Hankel determinants
three-term recurrence
$x\tilde{p}_k = \tilde{p}_{k+1} + b_k\tilde{p}_k + a_{k-1}^2\tilde{p}_{k-1}$
three-term recurrence
$x\tilde{p}_k = \tilde{p}_{k+1} + a_{k-1}^2\tilde{p}_{k-1}$
Toda
time dependent coeff.
$\dot{a}_k = a_k(b_{k+1} - b_k),$
$\dot{b}_k = 2(a_k^2 - a_{k-1}^2)$
Lotka-Volterra
time dependent coeff.
$\dot{u}_k = u_k(u_{k+1} - u_{k-1}),$
$u_k(t) = b_k^2(t/2)$
measure deformation
$d\mu(x;t) = e^{tx}d\mu(x)$
measure deformation
$d\mu(x;t) = e^{tx^2}d\mu(x)$
QR Alg.
SVD Alg.

Finite-Dimensional Eigenvalue Problem

- Truncation.

$$\underbrace{\begin{bmatrix} b_0 & a_0 & 0 & & & \\ a_0 & b_1 & a_1 & 0 & & \\ 0 & a_1 & b_2 & a_2 & 0 & \\ & & \ddots & \ddots & \ddots & \\ & & & & & a_{n-2} \\ & & & 0 & a_{n-2} & b_{n-1} \end{bmatrix}}_{L} \begin{bmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \\ \\ p_{n-1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \\ a_{n-1}p_n(x) \end{bmatrix} = x \begin{bmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \\ \\ p_{n-1}(x) \end{bmatrix}.$$

- λ is a root of the polynomial $p_n(x)$ if and only if λ is an eigenvalue of the finite-dimensional tridiagonal matrix L.

Genius Change of Variables
(Kadomtsev-Petviashvili or Hirota-Miwa Hierarchies)

- Redefine the off-diagonal elements by

$$c_k(t) := a_k^2\left(\frac{t}{2}\right), \quad k = 0, 1, \ldots .$$

- Reduce the Toda lattice into a self-contained second-order system:

$$\frac{d^2 \ln c_k}{dt^2} = c_{k+1} - 2c_k + c_{k-1}.$$

- Diagonal elements can be obtained from

$$\frac{d \ln c_k}{dt} = b_{k+1}\left(\frac{t}{2}\right) - b_k\left(\frac{t}{2}\right).$$

τ Functions

- Introduce new variables $\{\tau_k(t)\}_k$ implicitly via

$$c_k = \frac{\tau_{k+1}\tau_{k-1}}{\tau_k^2},$$

so that

$$\ln c_k = \ln \tau_{k+1} - 2 \ln \tau_k + \ln \tau_{k-1}.$$

- Compatibility condition:

$$c_k = \frac{d^2 \ln \tau_k}{dt^2},$$

Solving for τ_k

- Hirota bilinear form:

$$\tau_k \frac{d^2\tau_k}{dt^2} - \left(\frac{d\tau_k}{dt}\right)^2 = \tau_{k-1}\tau_{k+1}, \tag{1}$$

  - $\tau_0 \equiv 1$.

- Starting with $\tau_1 = \phi(t)$, then

$$\begin{aligned}
\tau_2(t) &= \phi\frac{d^2\phi}{dt^2} - \left(\frac{d\phi}{dt}\right)^2, \\
\tau_3(t) &= -\left(\frac{d^2\phi}{dt^2}\right)^3 + \phi\left(\frac{d^2\phi}{dt^2}\right)\frac{d^4\phi}{dt^4} - \left(\frac{d\phi}{dt}\right)^2\frac{d^4\phi}{dt^4} \\
&\quad +2\left(\frac{d\phi}{dt}\right)\left(\frac{d^2\phi}{dt^2}\right)\frac{d^3\phi}{dt^3} - \phi\left(\frac{d^3\phi}{dt^3}\right)^2, \\
&\vdots
\end{aligned}$$

Hankel Determinant, again!

- From a given $\phi(t)$, define

$$\hat{H}_k(t) := \det \begin{bmatrix} \phi & \phi^{(1)} & \dots & \phi^{(k-1)} \\ \phi^{(1)} & \phi^{(2)} & & \phi^{(k)} \\ \vdots & & & \vdots \\ \phi^{(k-1)} & \phi^{(k)} & \dots & \phi^{(2k-2)} \end{bmatrix},$$

  - For abbreviation,

$$\phi^{(\ell)} = \frac{d^\ell \phi}{dt^\ell}, \quad \ell = 1, 2, \dots.$$

Matrix Calculus

- Define $\hat{H}_k \begin{bmatrix} i \\ j \end{bmatrix} :=$ the determinant of the submatrix by deleting the ith row and the jth column from the matrix defining $\hat{H}_k$.
- Observe that

$$\begin{aligned} \frac{d\hat{H}_k}{dt} &= \hat{H}_{k+1} \begin{bmatrix} k+1 \\ k \end{bmatrix}, \\ \frac{d^2\hat{H}_k}{dt^2} &= \hat{H}_{k+1} \begin{bmatrix} k \\ k \end{bmatrix}. \end{aligned}$$

- Recall the Sylvester determinant identity

$$\hat{H}_{k+1}\hat{H}_{k-1} = \det \begin{bmatrix} \hat{H}_{k+1} \begin{bmatrix} k+1 \\ k+1 \end{bmatrix} & \hat{H}_{k+1} \begin{bmatrix} k+1 \\ k \end{bmatrix} \\ \hat{H}_{k+1} \begin{bmatrix} k \\ k+1 \end{bmatrix} & \hat{H}_{k+1} \begin{bmatrix} k \\ k \end{bmatrix} \end{bmatrix}.$$

Determinantal Solution

- $\hat{H}_k(t)$ satisfies precisely the Hirota bilinear form.
- Toda lattice is finally solved.

$$\tau_k(t) = \det \begin{bmatrix} \phi & \phi^{(1)} & \dots & \phi^{(k-1)} \\ \phi^{(1)} & \phi^{(2)} & & \phi^{(k)} \\ \vdots & & & \vdots \\ \phi^{(k-1)} & \phi^{(k)} & \dots & \phi^{(2k-2)} \end{bmatrix}.$$

- Perhaps some smart integrable discretization? (Iwasaki & Nakamura, ’06)

Conclusion

- The Toda lattice governs the evolution of a certain class of orthogonal polynomials whose orthogonality is determined by a specific time-dependent measure.
- Since the measure deformation is explicitly known, moments can be calculated which, when properly assembled, lead to the conclusion abstractly, but literally, that the iterates of the *QR* algorithm can be expressed in closed-form!
- Hankel determinantal solutions are too complicated to be useful. Would a “smart" integrability-preserving discretization of the Toda lattice yield a useful algorithm for eigenvalue computation?