Conserved quantities of the discrete finite Toda equation and lower bounds of the minimal singular value of upper bidiagonal matrices

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Abstract

Some numerical algorithms are known to be related to discrete-time integrable systems, where it is essential that quantities to be computed (for example, eigenvalues and singular values of a matrix, poles of a continued fraction) are conserved quantities. In this paper, a new application of conserved quantities of integrable systems to numerical algorithms is presented. For an $N \times N$ ($N \geq 2$) real upper bidiagonal matrix $\boldsymbol{B}$ where all the diagonals and the upper subdiagonals are positive, conserved quantities $\mathrm{Tr}(((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1})$ ($M = 1, 2, \cdots$) of the discrete finite Toda equation give a sequence of lower bounds of the minimal singular value of $\boldsymbol{B}$. Recurrence relations for computing higher order conserved quantities $\mathrm{Tr}(((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1})$ are also derived.

Key words. discrete Toda equation, conserved quantities, minimal singular value

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1 Introduction

As a numerical method for non-linear differential equations which possess conserved quantities, we can use 1) the well-known Runge-Kutta method, 2) symplectic integrators (see [3], for example,) to Hamiltonian systems, or 3) energy preserving methods (see [7], for example). In the methods 1) and 2), conserved quantities can be used as an indicator for precision of difference schemes. Namely, a difference scheme is regarded as a better scheme if deviation of conserved quantities from the correct value during time evolution is smaller than those of other schemes. On the other hand, in the method 3), a difference scheme is designed so as to preserve a conserved quantity such as an energy function. Therefore, conserved quantities are important in design of difference schemes or verification of their precision.

There are some examples where a special type of difference scheme of an integrable system becomes not only a numerical method but also a recurrence relation of a particular numerical algorithm. The resulting discrete-time dynamical systems have a sufficient number of conserved quantities. We can give a few examples of such sets of a nonlinear integrable system and a numerical algorithm as follows: (i) The discrete finite Toda equation [5] and the qd (quotient difference) algorithm [12] for computing of matrix eigenvalues and so on. This relationship is pointed out by Sogo [14]. (ii) The discrete potential KdV (Korteweg-de Vries) equation [1] and the ϵ-algorithm [16] which is used to accelerate convergence of a sequence. This relationship is pointed out by Papageorgiou *et al*. [10]. (iii) From a discrete-time Lotka-Volterra equation [4], the dLV (discrete Lotka-Volterra) algorithm which is used in computation of singular values of a matrix is presented by Tsujimoto *et al*. [15]. Applications of integrable systems to numerical algorithm are based on the fact that quantities to be computed, for example, eigenvalues and singular values of a matrix and poles of a continued fraction, are conserved under the time evolution of the corresponding discrete integrable system.

In this paper, a new application of conserved quantities of the discrete finite Toda equation of the qd form, which is shown in Section 2, to numerical algorithm is presented. Let $\boldsymbol{B} = (B_{i,j})$ denote an $N \times N$ ($N \geq 2$) real upper bidiagonal matrix where all the diagonals and the upper subdiagonals are positive. Let the suffix T of a matrix denote its transpose. Let the trace of inverse powers of the positive definite matrix $\boldsymbol{B}^T\boldsymbol{B}$ be denoted by

$$J_M(\boldsymbol{B}) \equiv \mathrm{Tr}(((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}) \qquad (M = 1, 2, \cdots). \tag{1}$$

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Note that it holds

$$J_M(\boldsymbol{B}) = \sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M}} \qquad (M = 1, 2, \cdots). \tag{2}$$

It is shown in Section 2 that $J_M(\boldsymbol{B})$ are conserved quantities of the discrete finite Toda equation of the qd form.

Let singular values of $\boldsymbol{B}$ be $\sigma_1(\boldsymbol{B}), \cdots, \sigma_N(\boldsymbol{B})$ such that $\sigma_1(\boldsymbol{B}) > \cdots > \sigma_N(\boldsymbol{B}) > 0$. Since all the subdiagonals of $\boldsymbol{B}$ are nonzero, the singular values are simple [9, p.124].

In this paper, we present two results. The first is as follows. It is shown that the quantities

$$\theta_M(\boldsymbol{B}) \equiv (J_M(\boldsymbol{B}))^{-\frac{1}{2M}} \qquad (M = 1, 2, \cdots) \tag{3}$$

give a sequence of lower bounds of the minimal singular value $\sigma_N(\boldsymbol{B})$ of $\boldsymbol{B}$. Therefore, from the conserved quantities $J_M(\boldsymbol{B})$, a sequence of lower bounds of the minimal singular value of $\boldsymbol{B}$ can be obtained. The bound $\theta_M(\boldsymbol{B})$ is named the generalized Newton lower bound of order M in Section 3. These lower bounds are shown to increase monotonically, that is, $\theta_1(\boldsymbol{B}) < \theta_2(\boldsymbol{B}) < \cdots < \sigma_N(\boldsymbol{B})$ and converges to $\sigma_N(\boldsymbol{B})$ as M goes to infinity.

The second result is as follows. A simple recurrence formula is derived for computing diagonals of the inverses $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$ and $((\boldsymbol{B}\boldsymbol{B}^T)^M)^{-1}$ for a fixed positive integer M. This formula is useful for computing the higher order conserved quantities $J_M(\boldsymbol{B})$ and the sequence of increasing lower bounds.

This paper is organized as follows. In Section 2, as a preliminary, we give a Lax form and conserved quantities of the discrete finite Toda equation of the qd form. In Section 3, we present a sequence of lower bounds of the minimal singular value of an upper bidiagonal matrix $\boldsymbol{B}$. In Section 4, for a fixed positive integer M, a formula for computation of the diagonals of $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$ and $((\boldsymbol{B}\boldsymbol{B}^T)^M)^{-1}$ which enables us to compute the conserved quantity $J_M(\boldsymbol{B})$ is given in a form of recurrence relations. Derivation of these recurrence relations is also described. Moreover, computational complexity for the conserved quantity $J_M(\boldsymbol{B})$ is estimated. In Section 5, concluding remarks are presented.

2 The discrete Lax form of the discrete finite Toda equation of the qd form: Preliminary

Let us consider the discrete finite Toda equation [5]

$$\begin{aligned} &I_i(t+\delta) - I_i(t) = \delta^2(V_i(t) - V_{i-1}(t+\delta)) && (i = 1, \cdots, N), \\ &I_i(t+\delta)V_i(t+\delta) = I_{i+1}(t)V_i(t) && (i = 1, \cdots, N-1), \\ &V_0(t) = V_N(t) = 0. \end{aligned} \tag{4}$$

The Lax form and conserved quantities of the discrete finite Toda equation (4) are given as follows in [5]. Let matrices $L(t)$ and $R(t)$ denote

$$L(t) \equiv \begin{pmatrix} 1 & & & & O \\ \delta V_1(t) & 1 & & & \\ & \delta V_2(t) & 1 & & \\ & & \ddots & \ddots & \\ O & & & \delta V_{N-1}(t) & 1 \end{pmatrix},$$

$$R(t) \equiv \begin{pmatrix} I_1(t) & \delta & & O \\ & I_2(t) & \delta & \\ & & I_3(t) & \ddots & \\ & & & \ddots & \delta \\ O & & & & I_N(t) \end{pmatrix},$$

respectively. Eq. (4) is expressed as

$$R(t)L(t) = L(t+\delta)R(t+\delta).$$

Let us introduce matrices $A(t)$ defined as

$$A(t) \equiv L(t)R(t).$$

Then, we have a discrete Lax form of Eq. (4) as

$$A(t+\delta) = L(t+\delta)R(t+\delta) = R(t)L(t) = (L(t))^{-1}A(t)L(t). \tag{5}$$

Thus, since eigenvalues of $A(t)$ are conserved under the time evolution $t \to t+\delta$, $\mathrm{Tr}((A(t))^m)$ for an arbitrary positive integer m is independent of time t and is a conserved quantity of Eq. (4).

The cases where the integer m is positive are usually considered. For example, $\mathrm{Tr}(A(t))$ and $\mathrm{Tr}((A(t))^2)$ are corresponding to momentum and energy conservation laws, respectively. However, note that in the case where the integer m is negative, these traces are also conserved quantities. Namely, traces $\mathrm{Tr}(((A(t))^{m'})^{-1})$ ($m' = 1, 2, \cdots$) are conserved.

Similarly to [8, 11], let us consider the following transformation

$$\begin{aligned} I_i(n\delta) &= q_i^{(n)} && (i = 1, \cdots, N), \\ V_i(n\delta) &= \frac{e_i^{(n)}}{\delta^2} && (i = 0, \cdots, N) \end{aligned}$$

for $n = 0, 1, 2, \cdots$. By this transform to Eq. (4), We then obtain recurrence relations

$$\begin{aligned} & q_1^{(n+1)} = q_1^{(n)} + e_1^{(n)}, \\ & q_i^{(n+1)} e_i^{(n+1)} = q_{i+1}^{(n)} e_i^{(n)} && (i = 1, \cdots, N-1), \\ & q_i^{(n+1)} + e_{i-1}^{(n+1)} = q_i^{(n)} + e_i^{(n)} && (i = 2, \cdots, N), \\ & e_N^{(n)} = 0 \end{aligned} \tag{6}$$

of the qd algorithm by Rutishauser [12]. See also [5, 14]. Let us call Eq. (6) the discrete finite Toda equation of the qd form. In this paper, let us consider cases where all the $q_i^{(0)}$ ($i = 1, \cdots, N$) and $e_i^{(0)}$ ($i = 1, \cdots, N-1$) are positive. For all $n = 0, 1, 2, \cdots$, all the quantities $q_i^{(n)}$ ($i = 1, \cdots, N$) and $e_i^{(n)}$ ($i = 1, \cdots, N-1$) obtained from the recurrence relations (6) are positive [13]. Let us consider symmetric positive definite tridiagonal matrix

$$\boldsymbol{H}^{(n)} = \begin{pmatrix} q_1^{(n)} & \sqrt{q_1^{(n)} e_1^{(n)}} & & & O \\ \sqrt{q_1^{(n)} e_1^{(n)}} & q_2^{(n)} + e_1^{(n)} & \sqrt{q_2^{(n)} e_2^{(n)}} & & \\ & \sqrt{q_2^{(n)} e_2^{(n)}} & \ddots & \ddots & \\ & & \ddots & \ddots & \sqrt{q_{n-1}^{(n)} e_{n-1}^{(n)}} \\ O & & & \sqrt{q_{n-1}^{(n)} e_{n-1}^{(n)}} & q_n^{(n)} + e_{n-1}^{(n)} \end{pmatrix}$$

for $n = 0, 1, 2, \cdots$. The matrix $\boldsymbol{H}^{(n)}$ is decomposed as

$$\boldsymbol{H}^{(n)} = (\boldsymbol{B}^{(n)})^T \boldsymbol{B}^{(n)}, \tag{7}$$

where $\boldsymbol{B}^{(n)}$ is

$$\boldsymbol{B}^{(n)} = \begin{pmatrix} \sqrt{q_1^{(n)}} & \sqrt{e_1^{(n)}} & & & O \\ & \sqrt{q_2^{(n)}} & \sqrt{e_2^{(n)}} & & \\ & & \ddots & \ddots & \\ & & & \ddots & \sqrt{e_{N-1}^{(n)}} \\ O & & & & \sqrt{q_N^{(n)}} \end{pmatrix}.$$

Let us introduce a diagonal matrix $\boldsymbol{D}^{(n)}$ and a lower bidiagonal matrix $\boldsymbol{G}^{(n)}$ defined as

$$\boldsymbol{D}^{(n)} \equiv \mathrm{diag}(d_1^{(n)}, \cdots, d_N^{(n)}) \qquad \left(d_i^{(n)} \equiv \begin{cases} 1 & (i = 1), \\ \displaystyle\prod_{k=1}^{i-1} \sqrt{\frac{e_k^{(n)}}{q_k^{(n)}}} & (2 \le i \le N), \end{cases} \right),$$

$$\boldsymbol{G}^{(n)} \equiv \begin{pmatrix} q_1^{(n)} & & & & O \\ e_1^{(n)} & q_2^{(n)} & & & \\ & e_2^{(n)} & \ddots & & \\ & & \ddots & \ddots & \\ O & & & e_{N-1}^{(n)} & q_N^{(n)} \end{pmatrix},$$

respectively, for $n = 0, 1, 2, \cdots$. Moreover, let us introduce a diagonal matrix $\tilde{\boldsymbol{D}}^{(n)}$ defined as

$$\tilde{\boldsymbol{D}}^{(n)} \equiv \mathrm{diag}(\tilde{d}_1^{(n)}, \cdots, \tilde{d}_N^{(n)}) \qquad \left(\tilde{d}_i^{(n)} \equiv \sqrt{\frac{q_1^{(n)}}{q_i^{(n)}}} \cdot d_i^{(n)} \quad (i = 1, \cdots, N) \right)$$

for $n = 0, 1, 2, \cdots$. Let $\boldsymbol{U}^{(n)}$ be

$$\boldsymbol{U}^{(n)} \equiv (\boldsymbol{D}^{(n)})^{-1} \boldsymbol{G}^{(n)} \tilde{\boldsymbol{D}}^{(n)} \qquad (n = 0, 1, 2, \cdots).$$

Then, time evolution of Eq. (6) is expressed as the form of similarity transform,

$$\boldsymbol{H}^{(n+1)} = (\boldsymbol{U}^{(n)})^{-1} \boldsymbol{H}^{(n)} \boldsymbol{U}^{(n)} \qquad (n = 0, 1, 2, \cdots).$$

This gives a Lax form of Eq. (6). We have the following remark.

Remark 2.1

The traces $\mathrm{Tr}(((\boldsymbol{B}^{(n)})^T \boldsymbol{B}^{(n)})^m)$ $(m = \pm 1, \pm 2, \cdots)$ are conserved quantities of the discrete finite Toda equation of the qd form for the initial values $q_i^{(0)}$ $(i = 1, \cdots, N)$ and $e_i^{(0)}$ $(i = 1, \cdots, N-1)$.

On the discussion of conserved quantities, the case where m is positive has been usually considered. In this paper, we focus on the case where m is negative.

3 Conserved quantities of the discrete finite Toda equation of the qd form and lower bounds of the minimal singular value

First, in this paper, for a fixed positive integer M, we show that the conserved quantity $J_M(\boldsymbol{B}^{(n)}) = \mathrm{Tr}((((\boldsymbol{B}^{(n)})^T \boldsymbol{B}^{(n)})^M)^{-1})$ gives a lower bound of the minimal singular value of $\boldsymbol{B}^{(n)}$. Note that arbitrary upper bidiagonal matrix $\boldsymbol{B}$ where all the diagonals and the upper subdiagonals are positive can be used as the initial matrix $\boldsymbol{B}^{(0)}$. Therefore, we write $\boldsymbol{B} = \boldsymbol{B}^{(0)}$. Let us consider characteristic equation of the positive definite matrix $(\boldsymbol{B}^T \boldsymbol{B})^M$,

$$\det((\boldsymbol{B}^T \boldsymbol{B})^M - \lambda \boldsymbol{I}) = 0, \tag{8}$$

where $\boldsymbol{I}$ is the $N \times N$ unit matrix, for a fixed positive integer M. Applying once iteration of the well-known Newton method to Eq. (8) starting from $\lambda = 0$, we have $(J_M(\boldsymbol{B}))^{-1}$. Note that $(J_M(\boldsymbol{B}))^{-1}$ gives a lower bound of the minimal eigenvalue $\lambda_N^{(M)}(\boldsymbol{B})$ of the matrix $(\boldsymbol{B}^T \boldsymbol{B})^M$. Since $\lambda_N^{(M)}(\boldsymbol{B}) = (\sigma_N(\boldsymbol{B}))^{2M}$, where $\sigma_N(\boldsymbol{B})$ is the minimal singular value of $\boldsymbol{B}$, we obtain a lower bound $\theta_M(\boldsymbol{B}) = (J_M(\boldsymbol{B}))^{-\frac{1}{2M}}$ of $\sigma_N(\boldsymbol{B})$. Namely,

$$\theta_M(\boldsymbol{B}) < \sigma_N(\boldsymbol{B}). \tag{9}$$

In numerical analysis, $\theta_1(\boldsymbol{B})$ is presented in the preceding works as a lower bound of $\sigma_N(\boldsymbol{B})$. The lower bound $\theta_1(\boldsymbol{B})$ is presented by Fernando and Parlett [2]. Since the lower bounds $\theta_M(\boldsymbol{B})$ $(M = 1, 2, \cdots)$ are obtained from Eq. (8) by the Newton method and this argument is a generalization of those in [2], we name these bounds "the generalized Newton lower bound of order M". These lower bounds have the following properties.

Theorem 3.1
The generalized Newton lower bounds increase monotonically, that is,

$$\theta_1(\boldsymbol{B}) < \theta_2(\boldsymbol{B}) < \cdots < \sigma_N(\boldsymbol{B}). \tag{10}$$

The generalized Newton lower bounds converge to $\sigma_N(\boldsymbol{B})$, the minimal singular value of $\boldsymbol{B}$, as M goes to infinity, namely,

$$\lim_{M\to\infty} \theta_M(\boldsymbol{B}) = \sigma_N(\boldsymbol{B}). \tag{11}$$

The properties in Theorem 3.1 can readily be proved. For an arbitrary positive integer M, $\theta_{M+1}(\boldsymbol{B})/\theta_M(\boldsymbol{B}) > 1$ holds from

$$\begin{aligned}\left(\frac{\theta_{M+1}(\boldsymbol{B})}{\theta_M(\boldsymbol{B})}\right)^{2M(M+1)} &= \frac{\left(\displaystyle\sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M}}\right)^{M+1}}{\left(\displaystyle\sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M+2}}\right)^{M}} \\ &> \frac{\left(\displaystyle\sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M}}\right)^{M+1}}{\left(\displaystyle\frac{1}{(\sigma_N(\boldsymbol{B}))^2}\sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M}}\right)^{M}} = \frac{\displaystyle\sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M}}}{\displaystyle\frac{1}{(\sigma_N(\boldsymbol{B}))^{2M}}} > 1\end{aligned}$$

with consideration of Eqs. (2) and (3). Therefore, we have the inequality (10). Next, for an arbitrary positive integer M, it holds

$$\theta_M(\boldsymbol{B}) = \left(\sum_{i=1}^{N} \frac{1}{(\sigma_i(\boldsymbol{B}))^{2M}}\right)^{-\frac{1}{2M}} = \sigma_N(\boldsymbol{B})\left(1 + \sum_{i=1}^{N-1}\left(\frac{\sigma_N(\boldsymbol{B})}{\sigma_i(\boldsymbol{B})}\right)^{2M}\right)^{-\frac{1}{2M}}$$

from Eqs. (2) and (3). Then, we obtain Eq. (11) by taking the limit of $M \to \infty$ for this equation. □

4 Recurrence relations for diagonals of required inverse

In the previous section, we show that a sequence of lower bounds of the minimal singular value of $\boldsymbol{B} = \boldsymbol{B}^{(0)}$, where $\boldsymbol{B}^{(0)}$ gives an initial value of the discrete finite Toda equation (6) of the qd form, is given as $\theta_M(\boldsymbol{B}) = (J_M(\boldsymbol{B}))^{-\frac{1}{2M}}$ $(M = 1, 2, \cdots)$. Considering that $\mathrm{Tr}(((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}) = \mathrm{Tr}(((\boldsymbol{B}\boldsymbol{B}^T)^M)^{-1})$ $(M = 1, 2, \cdots)$, if all the diagonals of $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$ or $((\boldsymbol{B}\boldsymbol{B}^T)^M)^{-1}$ are obtained, we can compute the conserved quantities $J_M(\boldsymbol{B})$ of Eq. (6). A simple way to compute the diagonals of $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$ or $((\boldsymbol{B}\boldsymbol{B}^T)^M)^{-1}$ for higher order M is required since higher order conserved quantity $J_M(\boldsymbol{B})$ gives a better estimation of the minimal singular value of $\sigma_N(\boldsymbol{B})$ of $\boldsymbol{B}$ from Theorem 3.1.

Here we fix the notations used in the next theorem. Let the diagonal element and the upper subdiagonal element in the i−th row of $\boldsymbol{B}$ be denoted by b_i and c_i, respectively. That is,

$$\begin{cases} b_i \equiv B_{i,i} > 0 & (1 \le i \le N), \\ c_i \equiv B_{i,i+1} > 0 & (1 \le i \le N-1). \end{cases}$$

For a fixed positive integer M, let us set

$$\begin{cases} \boldsymbol{V}^{(m)} = (V_{i,j}^{(m)}) \equiv ((\boldsymbol{B}^T\boldsymbol{B})^m)^{-1}, \\ \boldsymbol{W}^{(m)} = (W_{i,j}^{(m)}) \equiv ((\boldsymbol{B}\boldsymbol{B}^T)^m)^{-1}, \\ \boldsymbol{X}^{(q)} = (X_{i,j}^{(q)}) \equiv (\boldsymbol{B}(\boldsymbol{B}^T\boldsymbol{B})^q)^{-1} = ((\boldsymbol{B}\boldsymbol{B}^T)^q\boldsymbol{B})^{-1}, \\ \boldsymbol{Y}^{(q)} = (Y_{i,j}^{(q)}) \equiv (\boldsymbol{X}^{(q)})^T \end{cases} \tag{12}$$

for integers m $(0 \leq m \leq M)$ and q $(0 \leq q \leq M-1)$, respectively. For simplicity, we write $v_i^{(m)} = V_{i,i}^{(m)}$, $w_i^{(m)} = W_{i,i}^{(m)}$, $x_i^{(q)} = X_{i,i}^{(q)}$ and $y_i^{(q)} = Y_{i,i}^{(q)}$ for $1 \leq i \leq N$. Let $z_i^{(q)}$ be defined by

$$z_i^{(q)} \equiv b_i(x_i^{(q)} + y_i^{(q)}) \tag{13}$$

for $1 \leq i \leq N$ and $0 \leq q \leq M-1$. Note that we have

$$z_i^{(q)} = 2b_i x_i^{(q)} = 2b_i y_i^{(q)} \qquad (1 \leq i \leq N) \tag{14}$$

from the definition (13) since $x_i^{(q)} = y_i^{(q)}$ $(1 \leq i \leq N)$.

Then, the following theorem which is useful for computing the higher order conserved quantities of the discrete finite Toda equation of the qd form holds.

Theorem 4.1

Let M be a fixed positive integer. All the diagonal elements $v_i^{(M)}$ and $w_i^{(M)}$ of inverse matrices $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$ and $((\boldsymbol{B}\boldsymbol{B}^T)^M)^{-1}$, respectively, are obtained through a finite number of arithmetics by using the following simple recurrence relations. The recurrence relations are

$$v_i^{(0)} = 1 \qquad (1 \leq i \leq N), \tag{15}$$

$$w_i^{(0)} = 1 \qquad (1 \leq i \leq N), \tag{16}$$

$$v_N^{(p)} = \frac{1}{b_N^2} w_N^{(p-1)}, \tag{17}$$

$$v_i^{(p)} = \frac{1}{b_i^2}(c_i^2 v_{i+1}^{(p)} + z_i^{(p-1)} - w_i^{(p-1)}) \qquad (1 \leq i \leq N-1), \tag{18}$$

$$w_1^{(p)} = \frac{1}{b_1^2} v_1^{(p-1)}, \tag{19}$$

$$w_i^{(p)} = \frac{1}{b_i^2}(c_{i-1}^2 w_{i-1}^{(p)} + z_i^{(p-1)} - v_i^{(p-1)}) \qquad (2 \leq i \leq N), \tag{20}$$

$$z_1^{(q)} = 2v_1^{(q)}, \tag{21}$$

$$z_i^{(q)} = z_{i-1}^{(q)} + 2(v_i^{(q)} - w_{i-1}^{(q)}) \qquad (2 \leq i \leq N), \tag{22}$$

for integers p and q such that $1 \leq p \leq M$ and $0 \leq q \leq M-1$. Instead of Eqs. (21) and (22), the following relations can be used.

$$z_N^{(q)} = 2w_N^{(q)}, \tag{23}$$

$$z_i^{(q)} = z_{i+1}^{(q)} + 2(w_i^{(q)} - v_{i+1}^{(q)}) \qquad (1 \leq i \leq N-1). \tag{24}$$

for integers q such that $0 \leq q \leq M-1$. □

As preparation for proof of Theorem 4.1, we show some properties of the inverse of $\boldsymbol{B}$ and present four lemmas. For convenience, let us write $\boldsymbol{S} = (S_{i,j}) \equiv \boldsymbol{B}^{-1}$. Since $\boldsymbol{B}\boldsymbol{S} = \boldsymbol{I}$, we obtain

$$\begin{cases} S_{i+1,j} = -\dfrac{b_i}{c_i} S_{i,j} & (1 \leq i < j \leq N), \\ S_{i,j} = \dfrac{1}{b_i} & (1 \leq i = j \leq N), \\ S_{i,j} = 0 & (1 \leq j < i \leq N). \end{cases} \tag{25}$$

Since $\boldsymbol{SB} = \boldsymbol{I}$, the (i, j) element of the matrix product $\boldsymbol{SB}$ is zero if $i < j$. Then, we have

$$S_{i,j} = -\frac{c_{j-1}}{b_j} S_{i,j-1} \quad (1 \leq i < j \leq N). \tag{26}$$

Considering that $(\boldsymbol{B}^T)^{-1} = \boldsymbol{S}^T$, we have

$$\begin{cases} \boldsymbol{V}^{(p)} = \boldsymbol{X}^{(p-1)}\boldsymbol{S}^T = \boldsymbol{S}\boldsymbol{Y}^{(p-1)} = \boldsymbol{S}\boldsymbol{W}^{(p-1)}\boldsymbol{S}^T, \\ \boldsymbol{W}^{(p)} = \boldsymbol{Y}^{(p-1)}\boldsymbol{S} = \boldsymbol{S}^T\boldsymbol{X}^{(p-1)} = \boldsymbol{S}^T\boldsymbol{V}^{(p-1)}\boldsymbol{S}, \\ \boldsymbol{X}^{(q)} = \boldsymbol{V}^{(q)}\boldsymbol{S} = \boldsymbol{S}\boldsymbol{W}^{(q)}, \\ \boldsymbol{Y}^{(q)} = \boldsymbol{W}^{(q)}\boldsymbol{S}^T = \boldsymbol{S}^T\boldsymbol{V}^{(q)} \end{cases} \tag{27}$$

from the definition (12).

Let $\boldsymbol{P} = (P_{i,j})$ and $\boldsymbol{Q} = (Q_{i,j})$ be $N \times N$ $(N \geq 2)$ matrices having some special relationship to $\boldsymbol{S}$. We have the following useful four lemmas.

Lemma 4.2

If $\boldsymbol{P} = \boldsymbol{SQ}$ holds between $\boldsymbol{P}$ and $\boldsymbol{Q}$ through $\boldsymbol{S}$, then the elements of $\boldsymbol{P}$ and $\boldsymbol{Q}$ satisfy

$$P_{i+1,j} + \frac{b_i}{c_i} P_{i,j} = \frac{1}{c_i} Q_{i,j} \quad (1 \leq i \leq N-1 \text{ and } 1 \leq j \leq N). \ \square \tag{28}$$

Proof.

Let j be an integer such that $1 \leq j \leq N$. The element $P_{i,j}$ is expressed with $\alpha_{i,j}$ as

$$\begin{aligned} P_{i,j} &= \sum_{k=1}^{N} S_{i,k} Q_{k,j} = \sum_{k=i}^{N} S_{i,k} Q_{k,j} = S_{i,i} Q_{i,j} + S_{i,i+1} Q_{i+1,j} + \alpha_{i,j} \\ &= \frac{1}{b_i} Q_{i,j} + \left(-\frac{c_i}{b_{i+1}} S_{i,i} \right) Q_{i+1,j} + \alpha_{i,j} \\ &= \frac{1}{b_i} Q_{i,j} - \frac{c_i}{b_{i+1} b_i} Q_{i+1,j} + \alpha_{i,j} \quad (1 \leq i \leq N-1), \end{aligned} \tag{29}$$

where each $\alpha_{i,j}$ is defined by

$$\alpha_{i,j} \equiv \begin{cases} \displaystyle\sum_{k=i+2}^{N} S_{i,k} Q_{k,j} & (N \geq 3,\ 1 \leq i \leq N-2), \\ 0 & (N \geq 2,\ i = N-1). \end{cases}$$

The element $P_{i+1,j}$ is also expressed with $\alpha_{i,j}$. If $N \geq 3$ and $1 \leq i \leq N-2$, it holds

$$\begin{aligned} P_{i+1,j} &= \sum_{k=i+1}^{N} S_{i+1,k} Q_{k,j} = S_{i+1,i+1} Q_{i+1,j} + \sum_{k=i+2}^{N} \left(-\frac{b_i}{c_i} S_{i,k} \right) Q_{k,j} \\ &= \frac{1}{b_{i+1}} Q_{i+1,j} - \frac{b_i}{c_i} \alpha_{i,j}. \end{aligned} \tag{30}$$

If $N \geq 2$ and $i = N-1$, it holds

$$P_{i+1,j} = \sum_{k=i+1}^{N} S_{i+1,k} Q_{k,j} = S_{i+1,i+1} Q_{i+1,j} = \frac{1}{b_{i+1}} Q_{i+1,j} - \frac{b_i}{c_i} \alpha_{i,j}. \tag{31}$$

From Eqs. (29), (30) and (31), we obtain

$$\begin{aligned} P_{i+1,j} + \frac{b_i}{c_i} P_{i,j} &= \frac{1}{b_{i+1}} Q_{i+1,j} - \frac{b_i}{c_i} \alpha_{i,j} + \frac{1}{c_i} Q_{i,j} - \frac{1}{b_{i+1}} Q_{i+1,j} + \frac{b_i}{c_i} \alpha_{i,j} \\ &= \frac{1}{c_i} Q_{i,j} \quad (1 \leq i \leq N-1 \text{ and } 1 \leq j \leq N). \end{aligned}$$

$\square$

Lemma 4.3

If $\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{S}^T$ holds between $\boldsymbol{P}$ and $\boldsymbol{Q}$ through $\boldsymbol{S}$, then the elements of $\boldsymbol{P}$ and $\boldsymbol{Q}$ satisfy

$$P_{i,j+1} + \frac{b_j}{c_j} P_{i,j} = \frac{1}{c_j} Q_{i,j} \quad (1 \le i \le N \text{ and } 1 \le j \le N-1). \ \square$$

Lemma 4.4

If $\boldsymbol{P} = \boldsymbol{S}^T\boldsymbol{Q}$ holds between $\boldsymbol{P}$ and $\boldsymbol{Q}$ through $\boldsymbol{S}$, then the elements of $\boldsymbol{P}$ and $\boldsymbol{Q}$ satisfy

$$P_{i-1,j} + \frac{b_i}{c_{i-1}} P_{i,j} = \frac{1}{c_{i-1}} Q_{i,j} \quad (2 \le i \le N \text{ and } 1 \le j \le N). \ \square$$

Lemma 4.5

If $\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{S}$ holds between $\boldsymbol{P}$ and $\boldsymbol{Q}$ through $\boldsymbol{S}$, then the elements of $\boldsymbol{P}$ and $\boldsymbol{Q}$ satisfy

$$P_{i,j-1} + \frac{b_j}{c_{j-1}} P_{i,j} = \frac{1}{c_{j-1}} Q_{i,j} \quad (1 \le i \le N \text{ and } 2 \le j \le N). \ \square$$

Lemmas 4.3, 4.4 and 4.5 can be proved along the same way as in Lemma 4.2.

Now we prove Theorem 4.1.

Eqs. (15) and (16) hold since $\boldsymbol{V}^{(0)} = \boldsymbol{I}$ and $\boldsymbol{W}^{(0)} = \boldsymbol{I}$ hold from the definition (12).

Let us derive the recurrence relation (18) on $v_i^{(p)}$. In the following derivation, i is an integer such that $1 \le i \le N-1$. The element $V_{i,i+1}^{(p)}$ is expressed in two ways from Lemmas 4.2 and 4.3. Using the lemmas, we obtain

$$V_{i,i+1}^{(p)} = -\frac{c_i}{b_i} v_{i+1}^{(p)} + \frac{1}{b_i} Y_{i,i+1}^{(p-1)}, \tag{32}$$

$$V_{i,i+1}^{(p)} = -\frac{b_i}{c_i} v_i^{(p)} + \frac{1}{c_i} x_i^{(p-1)}. \tag{33}$$

Since the right hand sides of Eqs. (32) and (33) are equal to each other, we have

$$v_i^{(p)} = \frac{c_i^2}{b_i^2} v_{i+1}^{(p)} + \frac{1}{b_i} x_i^{(p-1)} - \frac{c_i}{b_i^2} Y_{i,i+1}^{(p-1)} \tag{34}$$

on the diagonals $v_i^{(p)}$. On $Y_{i,i+1}^{(p-1)}$ in the right hand side of Eq. (34), we obtain

$$Y_{i,i+1}^{(p-1)} = -\frac{b_i}{c_i} y_i^{(p-1)} + \frac{1}{c_i} w_i^{(p-1)} \tag{35}$$

from Lemma 4.3. Substituting Eq. (35) into Eq. (34), finally we derive

$$v_i^{(p)} = \frac{1}{b_i^2} (c_i^2 v_{i+1}^{(p)} + z_i^{(p-1)} - w_i^{(p-1)})$$

on the diagonals $v_i^{(p)}$ of the inverse matrix $((\boldsymbol{B}^T\boldsymbol{B})^p)^{-1}$. This gives Eq. (18) in Theorem 4.1.

Next, let us derive the recurrence relations (20) on $w_i^{(p)}$ and (22) on $z_i^{(q)}$ in similar ways to $v_i^{(p)}$. In the following derivation, i is an integer such that $2 \le i \le N$. From Lemmas 4.4 and 4.5, we have

$$W_{i,i-1}^{(p)} = -\frac{c_{i-1}}{b_i} w_{i-1}^{(p)} + \frac{1}{b_i} X_{i,i-1}^{(p-1)} = -\frac{b_i}{c_{i-1}} w_i^{(p)} + \frac{1}{c_{i-1}} y_i^{(p-1)}.$$

From Lemma 4.5, we have

$$X_{i,i-1}^{(p-1)} = -\frac{b_i}{c_{i-1}} x_i^{(p-1)} + \frac{1}{c_{i-1}} v_i^{(p-1)}.$$

Then, we obtain Eq. (20) in Theorem 4.1. From Lemmas 4.2 and 4.5, we have

$$X_{i,i-1}^{(q)} = -\frac{b_{i-1}}{c_{i-1}} x_{i-1}^{(q)} + \frac{1}{c_{i-1}} w_{i-1}^{(q)} = -\frac{b_i}{c_{i-1}} x_i^{(q)} + \frac{1}{c_{i-1}} v_i^{(q)}.$$

That is,

$$b_i x_i^{(q)} = b_{i-1} x_{i-1}^{(q)} + v_i^{(q)} - w_{i-1}^{(q)}.$$

Doubling both hand sides, we obtain Eq. (22) in Theorem 4.1 with consideration of Eq. (14).

Next, let us consider the values of $v_N^{(p)}, w_1^{(p)}$ and $z_1^{(q)}$ which are the end points of the sequence $v_i^{(p)}, w_i^{(p)}$ and $z_i^{(q)}$ for $1 \leq i \leq N$ on each p or q, respectively. From Eq. (27), we derive

$$\begin{cases} v_N^{(p)} = \sum_{k=1}^{N} \sum_{l=1}^{N} S_{N,k} W_{k,l}^{(p-1)} S_{l,N}^T = (S_{N,N})^2 W_{N,N}^{(p-1)} = \frac{1}{b_N^2} w_N^{(p-1)}, \\ w_1^{(p)} = \sum_{k=1}^{N} \sum_{l=1}^{N} S_{1,k}^T V_{k,l}^{(p-1)} S_{l,1} = (S_{1,1})^2 V_{1,1}^{(p-1)} = \frac{1}{b_1^2} v_1^{(p-1)}. \end{cases} \tag{36}$$

This is because the matrix $\boldsymbol{S}$ is upper triangular. These are Eqs. (17) and (19) in Theorem 4.1. By a manner which is similar to Eq. (36), we obtain

$$x_1^{(q)} = \sum_{k=1}^{N} V_{1,k}^{(q)} S_{k,1} = V_{1,1}^{(q)} S_{1,1} = \frac{1}{b_1} v_1^{(q)}$$

from Eq. (27). Thus, we have

$$z_1^{(q)} = 2 b_1 x_1^{(q)} = 2 v_1^{(q)}$$

from Eq. (14). This is Eq. (21) in Theorem 4.1.

Finally, we derive Eqs. (23) and (24). From Eq. (22), we have

$$z_{i+1}^{(q)} = z_i^{(q)} + 2(v_{i+1}^{(q)} - w_i^{(q)}) \qquad (1 \leq i \leq N-1).$$

Therefore, it is obvious that Eq. (24) holds. Similarly to the derivation of Eq. (21), it holds

$$y_N^{(q)} = \sum_{k=1}^{N} W_{N,k}^{(q)} S_{k,N}^T = \sum_{k=1}^{N} W_{N,k}^{(q)} S_{N,k} = W_{N,N}^{(q)} S_{N,N} = \frac{1}{b_N} w_N^{(q)}.$$

Thus, we have

$$z_N^{(q)} = 2 b_N y_N^{(q)} = 2 w_N^{(q)}$$

from Eq. (14). This gives Eq. (23) in Theorem 4.1.

Now all the recurrence relations in Theorem 4.1 have been derived. This completes the proof of Theorem 4.1. □

On the recurrence relations from (17) through (20) in Theorem 4.1, let us consider the recurrence relations for $p = 1$. Substituting $q = 0$ into the recurrence relations (21) and (22), and using Eqs. (15) and (16), we can readily derive $z_i^{(0)} = 2$ for $1 \leq i \leq N$. Then, substituting $p = 1$ into the recurrence relations from (17) through (20) and using Eqs. (15) and (16), we have the following remark.

Remark 4.6

The recurrence relations from (17) through (20) in Theorem 4.1 for $p = 1$ are simplified to the recurrence relations

$$v_N^{(1)} = \frac{1}{b_N^2}, \tag{37}$$

$$v_i^{(1)} = \frac{1}{b_i^2}(c_i^2 v_{i+1}^{(1)} + 1) \qquad (1 \le i \le N-1), \tag{38}$$

$$w_1^{(1)} = \frac{1}{b_1^2}, \tag{39}$$

$$w_i^{(1)} = \frac{1}{b_i^2}(c_{i-1}^2 w_{i-1}^{(1)} + 1) \qquad (2 \le i \le N). \tag{40}$$

Theorem 4.1 for $M = 1$ is reduced to these recurrence relations. □

In numerical analysis, there exist some preceding works on some limited cases.

Remark 4.7

A formula related to Eqs. from (37) to (40) for computing diagonals of the inverse $(\boldsymbol{B}\boldsymbol{B}^T)^{-1}$ is known. See [2, 6, 13], for example. Another formula for computing diagonals of the inverse $((\boldsymbol{B}\boldsymbol{B}^T)^2)^{-1}$ is presented by von Matt [6].

Finally in this section, for a fixed positive integer M, we consider computational complexity for the trace $J_M(\boldsymbol{B})$ with the formula in Theorem 4.1. The following corollary of Theorem 4.1 holds.

Corollary 4.8

The trace $J_M(\boldsymbol{B})$ for a fixed M can be obtained within $O(NM)$ operations through the formula in Theorem 4.1. □

Proof.

We estimate computational complexity for computing all the diagonals of $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$. Let us consider the case where all the quantities $v_i^{(q)}$, $w_i^{(q)}$ and $z_i^{(q)}$ for all i $(1 \le i \le N)$ and q $(0 \le q \le M-1)$ are obtained before obtaining the diagonals $v_i^{(M)}$ for $1 \le i \le N$. These quantities are sufficient to determine all the diagonals $v_i^{(M)}$ for $1 \le i \le N$. As is discussed in the previous subsection, $v_i^{(0)}$, $w_i^{(0)}$ and $z_i^{(0)}$ for $1 \le i \le N$ are given as $v_i^{(0)} = 1$, $w_i^{(0)} = 1$ and $z_i^{(0)} = 2$, respectively. Then, the number of the remaining quantities to be obtained is $N(3M-2)$. Each of these quantities can be obtained with within at most six times of the four basic operations of arithmetic according to the recurrence relations in Theorem. Then, all the diagonals of $((\boldsymbol{B}^T\boldsymbol{B})^M)^{-1}$ are obtained less than $18NM$ operations. □

5 Concluding remarks

In this paper, a new application of conserved quantities of discrete-time integrable systems to numerical algorithm is presented. Starting from the Lax form of the discrete finite Toda equation (6) of the qd form, we see that traces $J_M(\boldsymbol{B}^{(n)}) = \mathrm{Tr}((((\boldsymbol{B}^{(n)})^T\boldsymbol{B}^{(n)})^M)^{-1})$ $(M = 1, 2, \cdots)$ are conserved quantities of Eq. (6) for each n $(n = 0, 1, 2, \cdots)$. It is shown that the traces $J_M(\boldsymbol{B})$ $(M = 1, 2, \cdots)$ give a sequence of lower bounds of the minimal singular value $\sigma_N(\boldsymbol{B})$ of $\boldsymbol{B} = \boldsymbol{B}^{(0)}$ which monotonically goes to the minimal singular value as $M \to \infty$. These bounds are defined by applying the Newton method to the characteristic equation (8) as described in Section 3. Therefore we name these bounds the generalized Newton bounds in this paper.

Secondly, recurrence relations for computing higher order conserved quantities $J_M(\boldsymbol{B})$ of Eq. (6) are presented. Computational complexity for $J_M(\boldsymbol{B})$ is shown to be $O(NM)$.

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