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# Subtraction-free recurrence relations for lower bounds of the minimal singular value of an upper bidiagonal matrix

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**Abstract.** On an $N \times N$ upper bidiagonal matrix $B$, where all the diagonals and the upper subdiagonals are positive, and its transpose $B^T$, it is shown in the recent paper [4] that quantities $J_M(B) \equiv \mathrm{Tr}(((B^TB)^M)^{-1})$ $(M = 1, 2, \dots)$ gives a sequence of lower bounds $\theta_M(B)$ of the minimal singular value of $B$ through $\theta_M(B) \equiv (J_M(B))^{-1/(2M)}$. In [4], simple recurrence relations for computing all the diagonals of $((B^TB)^M)^{-1}$ and $((BB^T)^M)^{-1}$ are also presented. The square of $\theta_M(B)$ can be used as a shift of origin in numerical algorithms for computing all the singular values of $B$. In this paper, new recurrence relations which have advantages over the old ones in [4] are presented. The new recurrence relations consist of only addition, multiplication and division among positive quantities. Namely, they are subtraction-free. This property excludes any possibility of cancellation error in numerical computation of the traces $J_M(B)$. Computational cost for the trace $J_M(B)$ $(M = 1, 2, \dots)$ and efficient implementations for $J_2(B)$ and $J_3(B)$ are also discussed.

*Keywords.* lower bound of the minimal singular value, subtraction-free recurrence relations

## 1. Introduction

On numerical problem of matrix singular values, computation of a lower bound of the minimal singular value is important in both theory and applications. For example, in the dqds (differential quotient difference with shift) algorithm [1] and the mdLVs (modified discrete Lotka-Volterra with shift) algorithm [3] for computing all the singular values, the square of such a bound can be used as a shift of origin. Generally speaking, choice of larger lower bound brings larger acceleration effect on convergence of the algorithms. Therefore, it is desirable to obtain larger lower bound with less computational cost.

Let us consider an $N \times N$ $(N \geq 2)$ real upper bidiagonal matrix $B = (B_{i,j})$, where all the diagonals and the upper subdiagonals are positive. Let $B^T$ be the transpose of $B$. Let the singular values of $B$ be $\sigma_1(B), \dots, \sigma_N(B)$. Since all the upper subdiagonals of $B$ are positive, the singular values are simple [6, p. 124]. Thus, we can set $\sigma_1(B) > \cdots > \sigma_N(B) > 0$ without losing generality. In the recent paper [4], a sequence of lower bounds of the minimal singular value $\sigma_N(B)$ of $B$ obtained from conserved quantities

$$J_M(B) \equiv \mathrm{Tr}(((B^TB)^M)^{-1}) \qquad (M = 1, 2, \dots)$$

of the discrete finite Toda equation [2] are discussed. Such lower bounds are given as

$$\theta_M(B) \equiv (J_M(B))^{-\frac{1}{2M}} \qquad (M = 1, 2, \dots).$$

For a fixed $M$, the bound $\theta_M(B)$ is named the *generalized Newton bound of order $M$*. These lower bounds increase monotonically and converge to $\sigma_N(B)$ as $M$ goes to infinity [4, Theorem 3.1], that is,

$$\theta_1(B) < \theta_2(B) < \cdots < \sigma_N(B), \tag{1}$$

$$\lim_{M\to\infty} \theta_M(B) = \sigma_N(B). \tag{2}$$

For an arbitrary positive integer $M$, the lower bound $\theta_M(B)$ is obtained by applying one iteration of the well-known Newton method to the characteristic equation

$$\det((B^TB)^M - \lambda I) = 0, \tag{3}$$

where $I$ is the $N \times N$ unit matrix, starting from $\lambda = 0$. In singular value computation, a shift of origin in the dqds algorithm given as the square of the Newton bound $\theta_1(B)$ and a method for computing $\theta_1(B)$ by using recurrence relations are discussed by Fernando and Parlett [1]. Recurrence relations for computing diagonals of inverses $((B^TB)^M)^{-1}$ and $((BB^T)^M)^{-1}$, which can be used to compute the lower bound $\theta_M(B)$, are also presented in [4]. Note that for $M \geq 2$, subtraction is included in these recurrence relations.

Since $\theta_M(B) < \sigma_N(B)$, $(\theta_M(B))^2$ can be used as a shift of origin in the dqds and the mdLVs algorithms. Let us call $(\theta_M(B))^2$ the *generalized Newton shift of order $M$*.

In this paper, new recurrence relations are presented which have advantages compared to those in [4]. The new recurrence relations are shown to be subtraction-free though they are derived from those in [4]. Namely, these recurrence relations for diagonals of inverses $((B^TB)^M)^{-1}$ and $((BB^T)^M)^{-1}$ consist of only addition, multiplication and division among positive quantities. Therefore, cancellation error cannot occur in computation of the diagonals of $((B^TB)^M)^{-1}$ and $((BB^T)^M)^{-1}$ and the trace $J_M(B)$. Computational cost for computation of the trace $J_M(B)$ by the old and the new recurrence relations are shown to be $O(MN)$ and $O(M^2N)$, respectively. In the cases of $M = 2$ and 3, efficient implementations of algorithms for computing $J_M(B)$ are presented.

This paper is organized as follows. The old recurrence relations found in [4] are reviewed in Section 2. The new recurrence relations which are subtraction-free are described at the end of Section 2. In Section 3, as a preliminary of the proof, lemmas for derivation of the new recurrence relations are given. Proof of the new recurrence relations is given in Sections 4 and 5. In Section 6, computational costs for the traces $J_M(B)$ by the old and the new recurrence relations are shown to be $O(MN)$ and $O(M^2N)$, respectively. Efficient implementations of algorithms for computing the traces $J_2(B)$ and $J_3(B)$ are also performed. Section 7 is devoted for concluding remarks.

## 2. The old and new recurrence relations

In this section, we give a brief review on the old recurrence relations found in [4] and present an expression of the new ones. Let the diagonal and the upper subdiagonal in the $i$-th row of $B$ be denoted by $b_i$ and $c_i$, respectively, that is,

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

Let the superscript $T$ of a matrix denote its transpose. For a fixed positive integer $M$ and integers $m$ $(0 \le m \le M)$ and $q$ $(0 \le q \le M-1)$, let us set

$$\begin{cases} V^{(m)} = (V_{i,j}^{(m)}) \equiv ((B^TB)^m)^{-1}, \\ W^{(m)} = (W_{i,j}^{(m)}) \equiv ((BB^T)^m)^{-1}, \\ X^{(q)} = (X_{i,j}^{(q)}) \equiv (B(B^TB)^q)^{-1} = ((BB^T)^qB)^{-1}, \\ Y^{(q)} = (Y_{i,j}^{(q)}) \equiv (X^{(q)})^T. \end{cases} \tag{4}$$

For simplicity, we write the diagonals of these matrices as $v_i^{(m)} = V_{i,i}^{(m)}$, $w_i^{(m)} = W_{i,i}^{(m)}$, $x_i^{(q)} = X_{i,i}^{(q)}$ and $y_i^{(q)} = Y_{i,i}^{(q)}$ for $1 \le i \le N$. Let us introduce quantities $z_i^{(q)}$ for $1 \le i \le N$ and $0 \le q \le M-1$ defined as

$$z_i^{(q)} \equiv b_i(x_i^{(q)} + y_i^{(q)}). \tag{5}$$

### 2.1. The old recurrence relations

In this subsection, we describe old results in [4].

The following theorem holds.

**Theorem 2.1.1.** *Let $M$ be a fixed positive integer. Let $p$ and $q$ be integers such that $1 \le p \le M$ and $0 \le q \le M-1$, respectively. As a formula for computing diagonals of $((B^TB)^M)^{-1}$ and $((BB^T)^M)^{-1}$ through a finite number of arithmetics, the following simple recurrence relations hold.*

$$v_i^{(0)} = 1 \qquad (1 \le i \le N), \tag{6}$$

$$w_i^{(0)} = 1 \qquad (1 \le i \le N), \tag{7}$$

$$v_N^{(p)} = \frac{1}{b_N^2} w_N^{(p-1)}, \tag{8}$$

$$v_i^{(p)} = \frac{1}{b_i^2}(c_i^2 v_{i+1}^{(p)} + z_i^{(p-1)} - w_i^{(p-1)}) \qquad (1 \le i \le N-1), \tag{9}$$

$$w_1^{(p)} = \frac{1}{b_1^2} v_1^{(p-1)}, \tag{10}$$

$$w_i^{(p)} = \frac{1}{b_i^2}(c_{i-1}^2 w_{i-1}^{(p)} + z_i^{(p-1)} - v_i^{(p-1)}) \qquad (2 \le i \le N), \tag{11}$$

$$z_1^{(q)} = 2v_1^{(q)}, \tag{12}$$

$$z_i^{(q)} = z_{i-1}^{(q)} + 2(v_i^{(q)} - w_{i-1}^{(q)}) \qquad (2 \le i \le N). \tag{13}$$

*The following relations hold.*

$$z_N^{(q)} = 2w_N^{(q)}, \tag{14}$$

$$z_i^{(q)} = z_{i+1}^{(q)} + 2(w_i^{(q)} - v_{i+1}^{(q)}) \qquad (1 \le i \le N-1) \tag{15}$$

*Instead of Eqs. from (6) to (13), we can use Eqs. from (6) to (11), (14) and (15) as a formula for computing the diagonals of $((B^TB)^M)^{-1}$ and $((BB^T)^M)^{-1}$.*

We have the following remark.

**Remark 2.1.2.** For $p = 1$, the recurrence relations from (8) to (11) in Theorem 2.1.1 are simplified to the recurrence relations

$$v_N^{(1)} = \frac{1}{b_N^2}, \tag{16}$$

$$v_i^{(1)} = \frac{1}{b_i^2}(c_i^2 v_{i+1}^{(1)} + 1) \qquad (1 \le i \le N-1), \tag{17}$$

$$w_1^{(1)} = \frac{1}{b_1^2}, \tag{18}$$

$$w_i^{(1)} = \frac{1}{b_i^2}(c_{i-1}^2 w_{i-1}^{(1)} + 1) \qquad (2 \le i \le N). \tag{19}$$

In the case of $M = 1$, Theorem 2.1.1 is reduced to these recurrence relations.

On computation of diagonals of inverses $(BB^T)^{-1}$ and $((BB^T)^2)^{-1}$, there exist some preceding works in numerical analysis.

**Remark 2.1.3.** A formula related to Eqs. from (16) to (19) for computing diagonals of the inverse $(BB^T)^{-1}$ has been known. See [1, 5, 7], for example. On computation of diagonals of $((BB^T)^2)^{-1}$, von Matt [5] presented another formula.

### 2.2. New result: subtraction-free recurrence relations

Let us introduce quantities $\check{B}_i$ $(1 \le i \le N)$, $F_i$ $(1 \le i \le N-1)$ and $\tilde{F}_i$ $(2 \le i \le N)$ as follows.

**Definition 2.2.1.**

$$\check{B}_i = \frac{1}{b_i^2} \qquad (1 \le i \le N), \tag{20}$$

$$F_i = \frac{c_i^2}{b_i^2} = c_i^2 \check{B}_i \qquad (1 \le i \le N-1), \tag{21}$$

$$\tilde{F}_i = \frac{c_{i-1}^2}{b_i^2} = c_{i-1}^2 \check{B}_i \qquad (2 \le i \le N). \tag{22}$$

Note that all these quantities are positive.

Next, let us introduce quantities $g_i^{(r)}$ and $\tilde{g}_i^{(r)}$ defined for $1 \le i \le N$ and $r = 1, 2, \ldots$.

**Definition 2.2.2.** The quantities $g_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \ldots$ are defined as follows.

- For $i = N$ and arbitrary positive integer $r$, $g_N^{(r)}$ is given as $g_N^{(r)} = 0$.
- For $1 \le i \le N-1$ and $r = 1$, $g_i^{(1)}$ is given as $g_i^{(1)} = F_i v_{i+1}^{(1)}$.
- For $1 \le i \le N-1$ and $r = 2, 3, \ldots$, $g_i^{(r)}$ is given as

$$g_i^{(r)} = F_i g_{i+1}^{(r)} + \check{B}_{i+1} g_i^{(r-1)} + \sum_{k=1}^{r-1} g_{i+1}^{(k)} g_i^{(r-k)}. \tag{23}$$

**Definition 2.2.3.** The quantities $\tilde{g}_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \ldots$ are defined as follows.

- For $i = 1$ and arbitrary positive integer $r$, $\tilde{g}_1^{(r)}$ is given as $\tilde{g}_1^{(r)} = 0$.
- For $2 \le i \le N$ and $r = 1$, $\tilde{g}_i^{(1)}$ is given as $\tilde{g}_i^{(1)} = \tilde{F}_i w_{i-1}^{(1)}$.
- For $2 \le i \le N$ and $r = 2, 3, \ldots$, $\tilde{g}_i^{(r)}$ is given as

$$\tilde{g}_i^{(r)} = \tilde{F}_i \tilde{g}_{i-1}^{(r)} + \check{B}_{i-1} \tilde{g}_i^{(r-1)} + \sum_{k=1}^{r-1} \tilde{g}_{i-1}^{(k)} \tilde{g}_i^{(r-k)}. \tag{24}$$

**Remark 2.2.4.** The recurrence relations in Remark 2.1.2 can be rewritten with the quantities defined by Definitions from 2.2.1 to 2.2.3 as follows.

$$v_N^{(1)} = \check{B}_N, \tag{25}$$

$$v_i^{(1)} = F_i v_{i+1}^{(1)} + \check{B}_i = g_i^{(1)} + \check{B}_i \qquad (1 \le i \le N-1), \tag{26}$$

$$w_1^{(1)} = \check{B}_1, \tag{27}$$

$$w_i^{(1)} = \tilde{F}_i w_{i-1}^{(1)} + \check{B}_i = \tilde{g}_i^{(1)} + \check{B}_i \quad (2 \le i \le N). \tag{28}$$

Then, the main theorem of this paper is described.

**Theorem 2.2.5.** *For $M \ge 2$, the diagonals $v_i^{(s)}$ and $w_i^{(s)}$ of $((B^TB)^s)^{-1}$ and $((BB^T)^s)^{-1}$, respectively, for $1 \le i \le N$ and $2 \le s \le M$ are computed by the recurrence relations*

$$v_N^{(s)} = \check{B}_N w_N^{(s-1)}, \tag{29}$$

$$w_1^{(s)} = \check{B}_1 v_1^{(s-1)}, \tag{30}$$

$$v_i^{(s)} = F_i v_{i+1}^{(s)} + \check{B}_i w_i^{(s-1)} + 2 \sum_{k=1}^{s-1} g_i^{(k)} w_i^{(s-k)} \tag{31}$$

$$(1 \le i \le N-1),$$

$$w_i^{(s)} = \tilde{F}_i w_{i-1}^{(s)} + \check{B}_i v_i^{(s-1)} + 2 \sum_{k=1}^{s-1} \tilde{g}_i^{(k)} v_i^{(s-k)} \tag{32}$$

$$(2 \le i \le N),$$

*with the recurrence relations from (25) to (28).*

From Definitions from 2.2.1 to 2.2.3, Remark 2.2.4 and Theorem 2.2.5, all the diagonals $v_i^{(M)}$ of $((B^TB)^M)^{-1}$ and $w_i^{(M)}$ of $((BB^T)^M)^{-1}$ $(1 \le i \le N,\ M = 1, 2, \ldots)$ are computed through only addition, multiplication and division among positive quantities. Namely, the recurrence relations are *subtraction-free*. Let us call them the new recurrence relations. On the other hand, let us call the recurrence relations in Theorem 2.1.1 and Remark 2.1.2 the old recurrence relations. It is to be noted that both old and new give the traces $\mathrm{Tr}(((B^TB)^M)^{-1})$ through the diagonals of $((B^TB)^M)^{-1}$ or $((BB^T)^M)^{-1}$.

## 3. Preparation for the proof of the theorem

In this section, we show lemmas for derivation of the new recurrence relations in Section 2.2. For convenience, let us represent the inverse of $B$ with the notation

$$S = (S_{i,j}) \equiv B^{-1}.$$

$S$ is an upper triangle matrix, and the elements of $S$ have the following relations [4].

$$\begin{cases} S_{i,j} = 0 & (1 \le j < i \le N), \\ S_{i,j} = \dfrac{1}{b_i} & (1 \le i = j \le N), \\ S_{i+1,j} = -\dfrac{b_i}{c_i} S_{i,j} & (1 \le i < j \le N), \\ S_{i,j} = -\dfrac{c_{j-1}}{b_j} S_{i,j-1} & (1 \le i < j \le N). \end{cases} \tag{33}$$

In this section, $M$ is an arbitrary positive integer. The elements of $S$, $V^{(p)}$, $W^{(p)}$, $X^{(q)}$ and $Y^{(q)}$ for $1 \le p \le M$ and $0 \le q \le M-1$ satisfy the following relations.

**Lemma 3.0.1.** *The elements of $V^{(p)}$ and $W^{(p)}$ for $1 \le p \le M$ satisfy*

$$\begin{cases} V_{i,j}^{(p)} = \displaystyle\sum_{k=j}^{N} S_{j,k} X_{i,k}^{(p-1)} = \sum_{k=i}^{N} S_{i,k} Y_{k,j}^{(p-1)}, \\ W_{i,j}^{(p)} = \displaystyle\sum_{k=1}^{i} S_{k,i} X_{k,j}^{(p-1)} = \sum_{k=1}^{j} S_{k,j} Y_{i,k}^{(p-1)}, \end{cases} \tag{34}$$

*for $1 \le i \le N$ and $1 \le j \le N$. In particular, on the diagonals of $V^{(p)}$ and $W^{(p)}$ for $1 \le p \le M$, it holds*

$$\begin{cases} v_i^{(p)} = V_{i,i}^{(p)} = \sum_{k=i}^{N} S_{i,k} X_{i,k}^{(p-1)} = \sum_{k=i}^{N} S_{i,k} Y_{k,i}^{(p-1)}, \\ w_i^{(p)} = W_{i,i}^{(p)} = \sum_{k=1}^{i} S_{k,i} X_{k,i}^{(p-1)} = \sum_{k=1}^{i} S_{k,i} Y_{i,k}^{(p-1)} \end{cases} \quad (35)$$

*for $1 \le i \le N$.*

*Proof.* Since the relationships $V^{(p)} = X^{(p-1)}S^T = SY^{(p-1)}$ and $W^{(p)} = S^T X^{(p-1)} = Y^{(p-1)}S$ hold for $1 \le p \le M$ and $S$ is an upper triangle matrix, we have Eq. (34). Eq. (35) is directly obtained by substituting $j = i$ to Eq. (34). □

### 3.1. Lemmas—Part I

Proof of lemmas in this subsection is given in Appendix.

For $1 \le i \le N$ and $0 \le \rho \le \mu \le N - i$, let $\beta_{i,\mu,\rho}$ and $\gamma_{i,\mu,\rho}$ be defined as

$$\beta_{i,\mu,\rho} \equiv \begin{cases} \prod_{\nu=\rho+1}^{\mu} \left( -\frac{b_{i+\nu-1}}{c_{i+\nu-1}} \right) & (\rho < \mu), \\ 1 & (\rho = \mu), \end{cases} \quad (36)$$

$$\gamma_{i,\mu,\rho} \equiv \begin{cases} \prod_{\nu=\rho+1}^{\mu} \left( -\frac{c_{i+\nu-1}}{b_{i+\nu}} \right) & (\rho < \mu), \\ 1 & (\rho = \mu), \end{cases} \quad (37)$$

respectively. We have

**Lemma 3.1.1.** *For $1 \le i \le N$ and $0 \le \rho \le \mu \le N - i$, the following relationships among elements of $S$ hold.*

$$S_{i+\mu,j} = \beta_{i,\mu,\rho} S_{i+\rho,j} \qquad (i + \mu \le j \le N),$$
$$S_{j,i+\mu} = \gamma_{i,\mu,\rho} S_{j,i+\rho} \qquad (1 \le j \le i + \rho).$$

This lemma represents some relationships between two elements among the diagonal and the upper triangle part of $S$ which are in the same row or column. We also consider the case where these two elements are identical. This consideration is reflected to the definitions (36) and (37). These definitions help us to express equations in a simpler form. Note that

$$\gamma_{i,\mu,\rho}^2 = \begin{cases} \prod_{\nu=\rho+1}^{\mu} \tilde{F}_{i+\nu} & (\rho < \mu), \\ 1 & (\rho = \mu). \end{cases} \quad (38)$$

For the quantities $\gamma_{i,\mu,\rho}$, the following lemma holds.

**Lemma 3.1.2.** *For $1 \le i \le N-1$ and $1 \le \xi \le \mu \le N-i$, it holds*

$$\gamma_{i+1,\mu-1,\xi-1}^2 = \gamma_{i,\mu,\xi}^2.$$

Let us consider a set of quantities $\{\varphi_{i,\xi}\}$ defined for $1 \le i \le N - 1$ and $1 \le \xi \le N - i$. Let us introduce linear functions $h_{i,\lambda}(\varphi)$ defined for $1 \le i \le N$ and $1 \le \lambda \le N$ and computed from such quantities $\varphi_{i,\xi}$ $(1 \le i \le N-1,\ 1 \le \xi \le N - i)$. The definition of the function $h_{i,\lambda}(\varphi)$ is

$$h_{i,\lambda}(\varphi) \equiv \begin{cases} \sum_{\mu=\lambda}^{N-i} \sum_{\xi=1}^{\mu} \check{B}_{i+\xi} \gamma_{i,\mu,\xi}^2 \varphi_{i,\xi} & (\lambda \le N - i), \\ 0 & (\lambda > N - i). \end{cases} \quad (39)$$

These functions are linear with respect to the quantities $\varphi_{i,\xi}$. Suppose that the quantities $\varphi_{i,\xi}$ in Eq. (39) are given with another sets of quantities $\{\varphi_{i,\xi}^{(j)}\}$ $(j = 1, 2, \dots)$ defined for $1 \le i \le N - 1$ and $1 \le \xi \le N - i$ by $\varphi_{i,\xi} = \sum_j a^{(j)} \varphi_{i,\xi}^{(j)}$ where the coefficients $a^{(j)}$ $(j = 1, 2, \dots)$ are invariable for all of $\xi$ such that $1 \le \xi \le N - i$. Then, it holds

$$h_{i,\lambda}(\varphi) = h_{i,\lambda}(\textstyle\sum_j a^{(j)} \varphi^{(j)}) = \sum_j a^{(j)} h_{i,\lambda}(\varphi^{(j)}). \quad (40)$$

When $\lambda > N - i$, then the linearity (40) is obvious since $h_{i,\lambda}(\varphi)$ is identically zero. When $\lambda \le N - i$, then we can readily verify the linearity (40) from the definition (39).

Let us consider the case where all of $\varphi_{i,\xi}$ for $1 \le i \le N-1$ and $1 \le \xi \le N - i$ are zero. From the definition (39), we have

$$h_{i,\lambda}(0) = 0 \qquad (1 \le i \le N,\ 1 \le \lambda \le N). \quad (41)$$

Next, let $\{\phi_{i,\lambda}\}$ denote a set of quantities defined for $1 \le i \le N$ and $1 \le \lambda \le N$. We make an additional condition to $\phi_{i,\lambda}$ that they satisfy

$$\phi_{i,\lambda} = 0 \qquad (1 \le i \le N,\ N - i + 1 \le \lambda \le N). \quad (42)$$

Then, let us introduce quantities $H_{i,\lambda}^{(r)}(\phi)$ defined for $1 \le i \le N$, $1 \le \lambda \le N$ and $r = 0, 1, 2, \dots$. Through the function $h_{i,\lambda}$, the quantity $H_{i,\lambda}^{(r)}(\phi)$ is defined as

$$\begin{cases} H_{i,\lambda}^{(0)}(\phi) \equiv \phi_{i,\lambda} & (r = 0), \\ H_{i,\lambda}^{(r)}(\phi) \equiv h_{i,\lambda}(H^{(r-1)}(\phi)) & (r = 1, 2, \dots). \end{cases} \quad (43)$$

As is shown in Section 5, among these quantities, only $H_{i,1}^{(r)}$ $(r = 1, 2, \dots)$ are directly relevant to the computation of the conserved quantities. Note that the set $\{H_{i,\xi}^{(r)}(\phi)\}$ $(1 \le i \le N - 1,\ 1 \le \xi \le N - i)$ can be used as quantities $\varphi_{i,\xi}$ in Eq. (39) for each $r$ $(= 0, 1, 2, \dots)$. From the definitions (39) and (43) and the condition (42), when $\lambda > N - i$, it is obvious that

$$H_{i,\lambda}^{(r)}(\phi) = 0 \qquad (r = 0, 1, 2, \dots). \quad (44)$$

Let us consider the case where all of $\phi_{i,\xi}$ for $1 \le i \le N$ and $1 \le \xi \le N$ are zero. From the definition (43) and Eq. (41), we readily obtain

$$H_{i,\lambda}^{(r)}(0) = 0 \quad (45)$$

for $1 \le i \le N$, $1 \le \lambda \le N$ and $r = 0, 1, 2, \dots$.

Let us introduce constants $\chi_{i,\lambda}$ defined for $1 \le i \le N$ and $0 \le \lambda \le N$. Depending on $i$ and $\lambda$, these constants $\chi_{i,\lambda}$ are defined as

$$\chi_{i,\lambda} \equiv \begin{cases} \sum_{\mu=\lambda}^{N-i} \gamma_{i,\mu,0}^2 & (\lambda \le N - i), \\ 0 & (\lambda > N - i). \end{cases} \quad (46)$$

Note that the set $\{\chi_{i,\lambda}\}$ $(1 \leq i \leq N,\ 1 \leq \lambda \leq N)$ can be used as quantities $\phi_{i,\lambda}$ in Eq. (43). Therefore, note that the set $\{\chi_{i,\xi}\}$ $(1 \leq i \leq N-1,\ 1 \leq \xi \leq N-i)$ can be used as quantities $\varphi_{i,\xi}$ in Eq. (39).

The following three lemmas hold.

**Lemma 3.1.3.** *For $1 \leq i \leq N-1$, it holds*

$$H^{(0)}_{i,1}(\chi) = \chi_{i,1} = \sum_{\mu=1}^{N-i} \gamma^2_{i,\mu,0} = c_i^2 v^{(1)}_{i+1}.$$

**Lemma 3.1.4.** *For $1 \leq i \leq N-1$ and $1 \leq \lambda \leq N-i$, it holds*

$$\sum_{\mu=\lambda}^{N-i} \gamma^2_{i,\mu,1} = \tilde{F}^{-1}_{i+1}\chi_{i,\lambda}.$$

**Lemma 3.1.5.** *For $1 \leq i \leq N-1$ and $1 \leq \lambda \leq N$, it holds*

$$\chi_{i+1,\lambda-1} = \tilde{F}^{-1}_{i+1}\chi_{i,\lambda}.$$

### 3.2. Lemmas—Part II

In this subsection, we prepare Lemmas from 3.2.1 to 3.2.5 which correspond to Lemmas from 3.1.1 to 3.1.5 in the previous subsection. Proof of these lemmas is given in a similar way to that of Lemmas from 3.1.1 to 3.1.5.

For $1 \leq i \leq N$ and $0 \leq \rho \leq \mu \leq i-1$, let $\tilde{\beta}_{i,\mu,\rho}$ and $\tilde{\gamma}_{i,\mu,\rho}$ be defined as

$$\tilde{\beta}_{i,\mu,\rho} \equiv \begin{cases} \prod_{\nu=\rho+1}^{\mu} \left(-\dfrac{b_{i-\nu+1}}{c_{i-\nu}}\right) & (\rho < \mu), \\ 1 & (\rho = \mu), \end{cases}$$

$$\tilde{\gamma}_{i,\mu,\rho} \equiv \begin{cases} \prod_{\nu=\rho+1}^{\mu} \left(-\dfrac{c_{i-\nu}}{b_{i-\nu}}\right) & (\rho < \mu), \\ 1 & (\rho = \mu), \end{cases}$$

respectively. The following lemma holds.

**Lemma 3.2.1.** *For $1 \leq i \leq N$ and $0 \leq \rho \leq \mu \leq i-1$, the following relationships among elements of $S$ hold.*

$$S_{j,i-\mu} = \tilde{\beta}_{i,\mu,\rho} S_{j,i-\rho} \qquad (1 \leq j \leq i-\mu),$$
$$S_{i-\mu,j} = \tilde{\gamma}_{i,\mu,\rho} S_{i-\rho,j} \qquad (i-\rho \leq j \leq N).$$

Based on a reason similar to what we mentioned about Lemma 3.1.1, these definitions help us to express equations in simpler form. Note that

$$\tilde{\gamma}^2_{i,\mu,\rho} = \begin{cases} \prod_{\nu=\rho+1}^{\mu} F_{i-\nu} & (\rho < \mu), \\ 1 & (\rho = \mu). \end{cases}$$

For the quantities $\tilde{\gamma}_{i,\mu,\rho}$, the following lemma holds.

**Lemma 3.2.2.** *For $2 \leq i \leq N$ and $1 \leq \xi \leq \mu \leq i-1$, it holds*

$$\tilde{\gamma}^2_{i-1,\mu-1,\xi-1} = \tilde{\gamma}^2_{i,\mu,\xi}.$$

Let us consider a set of quantities $\{\tilde{\varphi}_{i,\xi}\}$ defined for $2 \leq i \leq N$ and $1 \leq \xi \leq i-1$. Let us introduce linear functions $\tilde{h}_{i,\lambda}(\tilde{\varphi})$ defined for $1 \leq i \leq N$ and $1 \leq \lambda \leq N$ and computed from such quantities $\tilde{\varphi}_{i,\xi}$ $(2 \leq i \leq N,\ 1 \leq \xi \leq i-1)$. The definition of the function $\tilde{h}_{i,\lambda}(\tilde{\varphi})$ is

$$\tilde{h}_{i,\lambda}(\tilde{\varphi}) \equiv \begin{cases} \sum_{\mu=\lambda}^{i-1} \sum_{\xi=1}^{\mu} \check{B}_{i-\xi} \tilde{\gamma}^2_{i,\mu,\xi} \tilde{\varphi}_{i,\xi} & (\lambda < i), \\ 0 & (\lambda \geq i). \end{cases} \tag{47}$$

Similar to $h_{i,\lambda}(\varphi)$, these functions are linear with respect to the quantities $\tilde{\varphi}_{i,\xi}$ and it holds

$$\tilde{h}_{i,\lambda}(0) = 0 \qquad (1 \leq i \leq N,\ 1 \leq \lambda \leq N).$$

Next, let $\{\tilde{\phi}_{i,\lambda}\}$ denote a set of quantities defined for $1 \leq i \leq N$ and $1 \leq \lambda \leq N$. We make an additional condition to $\tilde{\phi}_{i,\lambda}$ that they satisfy

$$\tilde{\phi}_{i,\lambda} = 0 \qquad (1 \leq i \leq N,\ i \leq \lambda \leq N).$$

Then, let us introduce quantities $\tilde{H}^{(r)}_{i,\lambda}(\tilde{\phi})$ defined for $1 \leq i \leq N$, $1 \leq \lambda \leq N$ and $r = 0, 1, 2, \ldots$. Through the function $\tilde{h}_{i,\lambda}$, the quantity $\tilde{H}^{(r)}_{i,\lambda}(\tilde{\phi})$ is defined as

$$\begin{cases} \tilde{H}^{(0)}_{i,\lambda}(\tilde{\phi}) \equiv \tilde{\phi}_{i,\lambda} & (r = 0), \\ \tilde{H}^{(r)}_{i,\lambda}(\tilde{\phi}) \equiv \tilde{h}_{i,\lambda}(\tilde{H}^{(r-1)}(\tilde{\phi})) & (r = 1, 2, \ldots). \end{cases} \tag{48}$$

Similarly to the quantities $H^{(r)}_{i,\lambda}$, among these quantities, only $\tilde{H}^{(r)}_{i,1}$ $(r = 1, 2, \ldots)$ are directly relevant to the computation of the conserved quantities. Note that the set $\{\tilde{H}^{(r)}_{i,\xi}(\tilde{\phi})\}$ $(2 \leq i \leq N,\ 1 \leq \xi \leq i-1)$ can be used as quantities $\tilde{\varphi}_{i,\xi}$ in Eq. (47) for each $r$ $(= 0, 1, 2, \ldots)$. Similarly to $H^{(r)}_{i,\lambda}(\phi)$, the following two relations hold. If $\lambda \geq i$, it holds

$$\tilde{H}^{(r)}_{i,\lambda}(\tilde{\phi}) = 0 \qquad (r = 0, 1, 2, \ldots).$$

It holds

$$\tilde{H}^{(r)}_{i,\lambda}(0) = 0$$

for $1 \leq i \leq N$, $1 \leq \lambda \leq N$ and $r = 0, 1, 2, \ldots$.

Let us introduce constants $\tilde{\chi}_{i,\lambda}$ defined for $1 \leq i \leq N$ and $0 \leq \lambda \leq N$. Depending on $i$ and $\lambda$, these constants $\tilde{\chi}_{i,\lambda}$ are defined as

$$\tilde{\chi}_{i,\lambda} \equiv \begin{cases} \sum_{\mu=\lambda}^{i-1} \tilde{\gamma}^2_{i,\mu,0} & (\lambda < i), \\ 0 & (\lambda \geq i). \end{cases}$$

Note that the set $\{\tilde{\chi}_{i,\lambda}\}$ $(1 \leq i \leq N,\ 1 \leq \lambda \leq N)$ can be used as quantities $\tilde{\phi}_{i,\lambda}$ in Eq. (48). Therefore, note that the set $\{\tilde{\chi}_{i,\xi}\}$ $(2 \leq i \leq N,\ 1 \leq \xi \leq i-1)$ can be used as quantities $\tilde{\varphi}_{i,\xi}$ in Eq. (47).

The remaining lemmas are as follows.

**Lemma 3.2.3.** *For $2 \leq i \leq N$, it holds*

$$\tilde{H}^{(0)}_{i,1}(\tilde{\chi}) = \tilde{\chi}_{i,1} = \sum_{\mu=1}^{i-1} \tilde{\gamma}^2_{i,\mu,0} = c^2_{i-1} w^{(1)}_{i-1}.$$

**Lemma 3.2.4.** *For $2 \le i \le N$ and $1 \le \lambda \le i-1$, it holds*

$$\sum_{\mu=\lambda}^{i-1} \tilde{\gamma}_{i,\mu,1}^2 = F_{i-1}^{-1} \tilde{\chi}_{i,\lambda}.$$

**Lemma 3.2.5.** *For $2 \le i \le N$ and $1 \le \lambda \le N$, it holds*

$$\tilde{\chi}_{i-1,\lambda-1} = F_{i-1}^{-1} \tilde{\chi}_{i,\lambda}.$$

# 4. Proof of the new recurrence relations—Step 1

The recurrence relations in Theorem 2.2.5 are obtained by rearranging the recurrence relations in Theorem 2.1.1 judiciously.

Hereafter, let $M \ge 2$ unless we specify the range of $M$ through this section.

Eqs. (8) and (10) in Theorem 2.1.1 correspond to Eqs. (29) and (30) in Theorem 2.2.5, respectively. Let us start from Eq. (13) in Theorem 2.1.1. Let us use symbol $k$ instead of the symbol $i$ used in Eq. (13). Namely, for $2 \le k \le N$ and $0 \le q \le M-1$, it holds

$$z_k^{(q)} = z_{k-1}^{(q)} + 2(v_k^{(q)} - w_{k-1}^{(q)}).$$

Summing both hand sides for $k$ from 2 to $i$ $(2 \le i \le N)$ and considering the recurrence relation (12) in Theorem 2.1.1, we have

$$\begin{aligned} z_i^{(q)} &= z_1^{(q)} + 2\left(\sum_{k=2}^{i} v_k^{(q)} - \sum_{k=1}^{i-1} w_k^{(q)}\right) \qquad (49)\\ &= 2v_1^{(q)} + 2\left(\sum_{k=2}^{i} v_k^{(q)} - \sum_{k=1}^{i-1} w_k^{(q)}\right) \\ &= 2\left(\sum_{k=1}^{i} v_k^{(q)} - \sum_{k=1}^{i-1} w_k^{(q)}\right) \end{aligned}$$

for $2 \le i \le N$ and $0 \le q \le M-1$.

## 4.1. Proof—Part I

The goal of this subsection is to show that it holds

$$v_i^{(s)} = F_i v_{i+1}^{(s)} + \check{B}_i w_i^{(s-1)} + 2\sum_{k=1}^{s-1} \check{B}_i H_{i,1}^{(k-1)}(\chi) w_i^{(s-k)} \qquad (50)$$

for $2 \le s \le M$ and $1 \le i \le N-1$.

Let us show that it holds

$$z_i^{(q)} - w_i^{(q)} = 2\sum_{k=1}^{i} (v_k^{(q)} - w_k^{(q)}) + w_i^{(q)} \qquad (51)$$

for $1 \le i \le N$ and $0 \le q \le M-1$. For $2 \le i \le N$ and $0 \le q \le M-1$, Eq. (51) is obtained from Eq. (49). For $i=1$ and $0 \le q \le M-1$, Eq. (51) holds since

$$z_1^{(q)} - w_1^{(q)} = 2v_1^{(q)} - w_1^{(q)} = 2(v_1^{(q)} - w_1^{(q)}) + w_1^{(q)}.$$

From Lemma 3.0.1, it holds

$$\begin{cases} \displaystyle\sum_{k=1}^{i} v_k^{(p)} = \sum_{k=1}^{i}\sum_{l=k}^{N} S_{k,l} Y_{l,k}^{(p-1)}, \\ \displaystyle\sum_{k=1}^{i} w_k^{(p)} = \sum_{k=1}^{i}\sum_{l=1}^{k} S_{l,k} Y_{k,l}^{(p-1)} = \sum_{l=1}^{i}\sum_{k=1}^{l} S_{k,l} Y_{l,k}^{(p-1)} \end{cases}$$

for $1 \le i \le N$ and $1 \le p \le M$. From these equations, we have

$$\begin{aligned} \sum_{k=1}^{i} (v_k^{(p)} - w_k^{(p)}) &= \sum_{k=1}^{i}\sum_{l=i+1}^{N} S_{k,l} Y_{l,k}^{(p-1)} \qquad (52)\\ &= \sum_{k=1}^{i}\sum_{\mu=1}^{N-i} S_{k,i+\mu} Y_{i+\mu,k}^{(p-1)} \end{aligned}$$

for $1 \le i \le N-1$ and $1 \le p \le M$. Let us introduce $\Delta_{i,\lambda}^{(t)}$ defined for $1 \le i \le N$, $1 \le \lambda \le N$ and $0 \le t \le M$. The definition of $\Delta_{i,\lambda}^{(t)}$ is

$$\Delta_{i,\lambda}^{(t)} \equiv \begin{cases} \displaystyle\sum_{k=1}^{i}\sum_{\mu=\lambda}^{N-i}\sum_{\xi=1}^{\mu} \frac{1}{b_{i+\xi}} \gamma_{i,\mu,\xi}^2 S_{k,i+\xi} V_{i+\xi,k}^{(t)} & (\lambda \le N-i), \\ 0 & (\lambda > N-i). \end{cases} \qquad (53)$$

Note that the set $\{\Delta_{i,\lambda}^{(t)}\}$ $(1 \le i \le N,\ 1 \le \lambda \le N)$ can be used as quantities $\phi_{i,\lambda}$ in Eq. (43) for each $t$ $(0 \le t \le M)$. Therefore, note that the set $\{\Delta_{i,\xi}^{(t)}\}$ $(1 \le i \le N-1,\ 1 \le \xi \le N-i)$ can be used as quantities $\varphi_{i,\xi}$ in Eq. (39) for each $t$ $(0 \le t \le M)$. Moreover, since $V^{(0)} = I$, it holds

$$\Delta_{i,\lambda}^{(0)} = 0 \qquad (1 \le i \le N,\ 1 \le \lambda \le N). \qquad (54)$$

The following lemma holds.

**Lemma 4.1.1.** *For $1 \le i \le N-1$, $1 \le \lambda \le N-i$ and $1 \le \alpha \le M$, it holds*

$$\sum_{k=1}^{i}\sum_{\mu=\lambda}^{N-i} S_{k,i+\mu} Y_{i+\mu,k}^{(\alpha-1)} = \chi_{i,\lambda} w_i^{(\alpha)} + \Delta_{i,\lambda}^{(\alpha-1)}.$$

*Proof.* Let $\mu$, $k$ and $q$ be integers such that $1 \le \mu \le N-i$, $1 \le k \le i$ and $0 \le q \le M-1$, respectively.

Since the relationship $Y^{(q)} = S^T V^{(q)}$ holds and $S$ is an upper triangular matrix, we have

$$Y_{i,j}^{(q)} = \sum_{l=1}^{N} S_{i,l}^T V_{l,j}^{(q)} = \sum_{l=1}^{N} S_{l,i} V_{l,j}^{(q)} = \sum_{l=1}^{i} S_{l,i} V_{l,j}^{(q)}$$

for $1 \le i \le N$ and $1 \le j \le N$. Considering this result, Lemma 3.1.1 and Eq. (33), it holds

$$\begin{aligned}
Y^{(q)}_{i+\mu,k} &= \sum_{l=1}^{i+\mu} S_{l,i+\mu} V^{(q)}_{l,k} \\
&= \sum_{l=1}^{i} S_{l,i+\mu} V^{(q)}_{l,k} + \sum_{l=i+1}^{i+\mu} S_{l,i+\mu} V^{(q)}_{l,k} \\
&= \sum_{l=1}^{i} \gamma_{i,\mu,0} S_{l,i} V^{(q)}_{l,k} + \sum_{\xi=1}^{\mu} S_{i+\xi,i+\mu} V^{(q)}_{i+\xi,k} \\
&= \gamma_{i,\mu,0} \sum_{l=1}^{i} S_{l,i} V^{(q)}_{l,k} + \sum_{\xi=1}^{\mu} \gamma_{i,\mu,\xi} S_{i+\xi,i+\xi} V^{(q)}_{i+\xi,k} \\
&= \gamma_{i,\mu,0} Y^{(q)}_{i,k} + \sum_{\xi=1}^{\mu} \frac{1}{b_{i+\xi}} \gamma_{i,\mu,\xi} V^{(q)}_{i+\xi,k}
\end{aligned}$$

for $1 \le i \le N-1$. Then, with consideration of Lemma 3.1.1, it holds

$$\begin{aligned}
&S_{k,i+\mu} Y^{(q)}_{i+\mu,k} \\
&= \gamma_{i,\mu,0} S_{k,i+\mu} Y^{(q)}_{i,k} + \sum_{\xi=1}^{\mu} \frac{1}{b_{i+\xi}} \gamma_{i,\mu,\xi} S_{k,i+\mu} V^{(q)}_{i+\xi,k} \\
&= \gamma^2_{i,\mu,0} S_{k,i} Y^{(q)}_{i,k} + \sum_{\xi=1}^{\mu} \frac{1}{b_{i+\xi}} \gamma^2_{i,\mu,\xi} S_{k,i+\xi} V^{(q)}_{i+\xi,k}
\end{aligned}$$

for $1 \le i \le N-1$. Therefore, with consideration of Lemma 3.0.1 and the definitions (46) and (53), we obtain

$$\begin{aligned}
&\sum_{k=1}^{i} \sum_{\mu=\lambda}^{N-i} S_{k,i+\mu} Y^{(\alpha-1)}_{i+\mu,k} \\
&= \sum_{k=1}^{i} \sum_{\mu=\lambda}^{N-i} \gamma^2_{i,\mu,0} S_{k,i} Y^{(\alpha-1)}_{i,k} + \Delta^{(\alpha-1)}_{i,\lambda} \\
&= \left( \sum_{\mu=\lambda}^{N-i} \gamma^2_{i,\mu,0} \right) \left( \sum_{k=1}^{i} S_{k,i} Y^{(\alpha-1)}_{i,k} \right) + \Delta^{(\alpha-1)}_{i,\lambda} \\
&= \chi_{i,\lambda} w^{(\alpha)}_i + \Delta^{(\alpha-1)}_{i,\lambda}
\end{aligned}$$

for $1 \le i \le N-1$, $1 \le \lambda \le N-i$ and $1 \le \alpha \le M$. □

From Eq. (52), Lemma 4.1.1 and the definition (43), for $1 \le i \le N-1$ and $1 \le u \le M-1$, we have

$$\begin{aligned}
\sum_{k=1}^{i} (v^{(u)}_k - w^{(u)}_k) &= \chi_{i,1} w^{(u)}_i + \Delta^{(u-1)}_{i,1} \qquad (55) \\
&= H^{(0)}_{i,1}(\chi) w^{(u)}_i + \Delta^{(u-1)}_{i,1}.
\end{aligned}$$

From Eqs. (51) and (55), for $1 \le i \le N-1$ and $1 \le u \le M-1$, we obtain

$$z^{(u)}_i - w^{(u)}_i = 2(H^{(0)}_{i,1}(\chi) w^{(u)}_i + \Delta^{(u-1)}_{i,1}) + w^{(u)}_i.$$

Therefore, from Eq. (9), for $2 \le s \le M$ and $1 \le i \le N-1$, it holds

$$\begin{aligned}
v^{(s)}_i =& F_i v^{(s)}_{i+1} + \check{B}_i w^{(s-1)}_i \qquad (56) \\
&+ 2\check{B}_i (H^{(0)}_{i,1}(\chi) w^{(s-1)}_i + \Delta^{(s-2)}_{i,1}).
\end{aligned}$$

For $s = 2$ and $1 \le i \le N-1$, we obtain Eq. (50) by substituting $s = 2$ into Eq. (56) and applying Eq. (54).

Before considering the cases of $M \ge 3$, we prepare the following two lemmas.

**Lemma 4.1.2.** *For $1 \le i \le N$, $1 \le \lambda \le N$ and $1 \le \alpha \le M$, it holds*

$$\Delta^{(\alpha)}_{i,\lambda} = h_{i,\lambda}(\chi) w^{(\alpha)}_i + h_{i,\lambda}(\Delta^{(\alpha-1)}).$$

*Proof.* For $1 \le i \le N$ and $N-i+1 \le \lambda \le N$, it is trivial since $\Delta^{(\alpha)}_{i,\lambda}$, $h_{i,\lambda}(\chi)$ and $h_{i,\lambda}(\Delta^{(\alpha-1)})$ are zero from their definitions. Then hereafter, in this proof, let $i$ and $\lambda$ be integers such that $1 \le i \le N-1$ and $1 \le \lambda \le N-i$, respectively.

Additionally, let $\xi$ be an integer such that $1 \le \xi \le N-i$ in this proof. We see that

$$\begin{aligned}
&\sum_{k=1}^{i} S_{k,i+\xi} V^{(\alpha)}_{i+\xi,k} \\
&= \sum_{k=1}^{i} \left( \gamma_{i,\xi,0} S_{k,i} \sum_{l=i+\xi}^{N} S_{i+\xi,l} Y^{(\alpha-1)}_{l,k} \right) \\
&= \gamma_{i,\xi,0} \sum_{k=1}^{i} \left( S_{k,i} \sum_{\rho=\xi}^{N-i} S_{i+\xi,i+\rho} Y^{(\alpha-1)}_{i+\rho,k} \right) \\
&= \gamma_{i,\xi,0} \sum_{k=1}^{i} \sum_{\rho=\xi}^{N-i} S_{k,i} \cdot \beta_{i,\xi,0} \gamma_{i,\rho,0} S_{i,i} \cdot Y^{(\alpha-1)}_{i+\rho,k} \\
&= \beta_{i,\xi,0} \gamma_{i,\xi,0} S_{i,i} \sum_{k=1}^{i} \sum_{\rho=\xi}^{N-i} S_{k,i+\rho} Y^{(\alpha-1)}_{i+\rho,k}
\end{aligned}$$

with help of Lemmas 3.0.1 and 3.1.1. We have

$$\begin{aligned}
&\beta_{i,\xi,0} \gamma_{i,\xi,0} S_{i,i} \\
&= \left( \prod_{\nu=1}^{\xi} \left( -\frac{b_{i+\nu-1}}{c_{i+\nu-1}} \right) \right) \left( \prod_{\nu'=1}^{\xi} \left( -\frac{c_{i+\nu'-1}}{b_{i+\nu'}} \right) \right) \cdot \frac{1}{b_i} \\
&= \frac{1}{b_{i+\xi}}
\end{aligned}$$

from Eq. (33) and the definitions (36) and (37). Therefore, we obtain

$$\sum_{k=1}^{i} S_{k,i+\xi} V^{(\alpha)}_{i+\xi,k} = \frac{1}{b_{i+\xi}} (\chi_{i,\xi} w^{(\alpha)}_i + \Delta^{(\alpha-1)}_{i,\xi})$$

with consideration of Lemma 4.1.1. From this equation and the definition of $\Delta^{(\alpha)}_{i,\lambda}$, we obtain

$$\begin{aligned}
\Delta^{(\alpha)}_{i,\lambda} &= \sum_{\mu=\lambda}^{N-i} \sum_{\xi=1}^{\mu} \left( \frac{1}{b_{i+\xi}} \gamma^2_{i,\mu,\xi} \cdot \frac{1}{b_{i+\xi}} (\chi_{i,\xi} w^{(\alpha)}_i + \Delta^{(\alpha-1)}_{i,\xi}) \right) \\
&= \left( \sum_{\mu=\lambda}^{N-i} \sum_{\xi=1}^{\mu} \check{B}_{i+\xi} \gamma^2_{i,\mu,\xi} \chi_{i,\xi} \right) w^{(\alpha)}_i \\
&\quad + \sum_{\mu=\lambda}^{N-i} \sum_{\xi=1}^{\mu} \check{B}_{i+\xi} \gamma^2_{i,\mu,\xi} \Delta^{(\alpha-1)}_{i,\xi} \\
&= h_{i,\lambda}(\chi) w^{(\alpha)}_i + h_{i,\lambda}(\Delta^{(\alpha-1)}).
\end{aligned}$$

□

**Lemma 4.1.3.** *For $1 \le i \le N$, $1 \le \lambda \le N$, $r = 0, 1, 2, \ldots$ and $1 \le \alpha \le M$, it holds*

$$H_{i,\lambda}^{(r)}(\Delta^{(\alpha)}) = H_{i,\lambda}^{(r+1)}(\chi) w_i^{(\alpha)} + H_{i,\lambda}^{(r+1)}(\Delta^{(\alpha-1)}). \quad (57)$$

*Proof.* For $1 \le i \le N$ and $N - i + 1 \le \lambda \le N$, it is trivial since $H_{i,\lambda}^{(r)}(\Delta^{(\alpha)})$, $H_{i,\lambda}^{(r+1)}(\chi)$ and $H_{i,\lambda}^{(r+1)}(\Delta^{(\alpha-1)})$ are zero from their definitions. Then hereafter, in this proof, let $i$ and $\lambda$ are integers such that $1 \le i \le N-1$ and $1 \le \lambda \le N - i$, respectively.

We here use mathematical induction. For $r = 0$, Eq. (57) holds since it holds

$$\begin{aligned} H_{i,\lambda}^{(0)}(\Delta^{(\alpha)}) &= \Delta_{i,\lambda}^{(\alpha)} \\ &= h_{i,\lambda}(\chi) w_i^{(\alpha)} + h_{i,\lambda}(\Delta^{(\alpha-1)}) \\ &= h_{i,\lambda}(H^{(0)}(\chi)) w_i^{(\alpha)} + h_{i,\lambda}(H^{(0)}(\Delta^{(\alpha-1)})) \\ &= H_{i,\lambda}^{(1)}(\chi) w_i^{(\alpha)} + H_{i,\lambda}^{(1)}(\Delta^{(\alpha-1)}) \end{aligned}$$

with consideration of Lemma 4.1.2. Let $k$ denote an integer such that $0 \le k$. If Eq. (57) holds for all $r$ such that $0 \le r \le k$, then, Eq. (57) holds for $r = k+1$ since it holds

$$\begin{aligned} & H_{i,\lambda}^{(k+1)}(\Delta^{(\alpha)}) \\ &= h_{i,\lambda}(H^{(k)}(\Delta^{(\alpha)})) \\ &= h_{i,\lambda}(H^{(k+1)}(\chi) w_i^{(\alpha)} + H^{(k+1)}(\Delta^{(\alpha-1)})) \\ &= h_{i,\lambda}(H^{(k+1)}(\chi)) w_i^{(\alpha)} + h_{i,\lambda}(H^{(k+1)}(\Delta^{(\alpha-1)})) \\ &= H_{i,\lambda}^{(k+2)}(\chi) w_i^{(\alpha)} + H_{i,\lambda}^{(k+2)}(\Delta^{(\alpha-1)}). \end{aligned}$$

□

Let us consider cases where $M \ge 3$. From Lemma 4.1.3, for $3 \le s \le M$, $1 \le i \le N-1$ and an integer $k$ such that $2 \le k \le s-1$, it holds

$$H_{i,1}^{(k-2)}(\Delta^{(s-k)}) = H_{i,1}^{(k-1)}(\chi) w_i^{(s-k)} + H_{i,1}^{(k-1)}(\Delta^{(s-k-1)}).$$

Summing the both hand sides of this equation from $k = 2$ to $k = s-1$, we have

$$H_{i,1}^{(0)}(\Delta^{(s-2)}) = \sum_{k=2}^{s-1} H_{i,1}^{(k-1)}(\chi) w_i^{(s-k)} + H_{i,1}^{(s-2)}(\Delta^{(0)})$$

for $3 \le s \le M$ and $1 \le i \le N-1$. Then, from the definition (43) and Eqs. (45) and (54), we obtain

$$\Delta_{i,1}^{(s-2)} = \sum_{k=2}^{s-1} H_{i,1}^{(k-1)}(\chi) w_i^{(s-k)}$$

for $3 \le s \le M$ and $1 \le i \le N-1$. Substituting this result into Eq. (56), we have Eq. (50) for $3 \le s \le M$ and $1 \le i \le N-1$.

Finally, we have shown that Eq. (50) holds for $M \ge 2$, $2 \le s \le M$ and $1 \le i \le N-1$.

## 4.2. Proof—Part II

The goal of this subsection is to show that it holds

$$w_i^{(s)} = \tilde{F}_i w_{i-1}^{(s)} + \check{B}_i v_i^{(s-1)} + 2 \sum_{k=1}^{s-1} \check{B}_i \tilde{H}_{i,1}^{(k-1)}(\tilde{\chi}) v_i^{(s-k)} \quad (58)$$

for $2 \le s \le M$ and $2 \le i \le N$.

From Eq. (49), it holds

$$z_i^{(q)} - v_i^{(q)} = 2 \sum_{k=1}^{i-1} (v_k^{(q)} - w_k^{(q)}) + v_i^{(q)} \quad (59)$$

for $2 \le i \le N$ and $0 \le q \le M-1$.

From Lemma 3.0.1, it holds

$$\begin{cases} \displaystyle\sum_{k=1}^{i-1} v_k^{(p)} = \sum_{k=1}^{i-1} \sum_{l=k}^{N} S_{k,l} X_{k,l}^{(p-1)}, \\ \displaystyle\sum_{k=1}^{i-1} w_k^{(p)} = \sum_{k=1}^{i-1} \sum_{l=1}^{k} S_{l,k} X_{l,k}^{(p-1)} = \sum_{l=1}^{i-1} \sum_{k=1}^{l} S_{k,l} X_{k,l}^{(p-1)} \end{cases}$$

for $2 \le i \le N$ and $1 \le p \le M$. From these equations, we have

$$\begin{aligned} \sum_{k=1}^{i-1} (v_k^{(p)} - w_k^{(p)}) &= \sum_{l=i}^{N} \sum_{k=1}^{i-1} S_{k,l} X_{k,l}^{(p-1)} \\ &= \sum_{l=i}^{N} \sum_{\mu=1}^{i-1} S_{i-\mu,l} X_{i-\mu,l}^{(p-1)} \end{aligned}$$

for $2 \le i \le N$ and $1 \le p \le M$. Let us introduce $\tilde{\Delta}_{i,\lambda}^{(t)}$ defined for $1 \le i \le N$, $1 \le \lambda \le N$ and $0 \le t \le M$. The definition of $\tilde{\Delta}_{i,\lambda}^{(t)}$ is

$$\tilde{\Delta}_{i,\lambda}^{(t)} \equiv \begin{cases} \displaystyle\sum_{l=i}^{N} \sum_{\mu=\lambda}^{i-1} \sum_{\xi=1}^{\mu} \frac{1}{b_{i-\xi}} \tilde{\gamma}_{i,\mu,\xi}^2 S_{i-\xi,l} W_{i-\xi,l}^{(t)} & (\lambda < i), \\ 0 & (\lambda \ge i) \end{cases}$$

Note that the set $\{\tilde{\Delta}_{i,\lambda}^{(t)}\}$ $(1 \le i \le N,\ 1 \le \lambda \le N)$ can be used as quantities $\tilde{\phi}_{i,\lambda}$ in Eq. (48) for each $t$ $(0 \le t \le M)$. Therefore, note that the set $\{\tilde{\Delta}_{i,\xi}^{(t)}\}$ $(2 \le i \le N,\ 1 \le \xi \le i-1)$ can be used as quantities $\tilde{\varphi}_{i,\xi}$ in Eq. (47) for each $t$ $(0 \le t \le M)$. Moreover, since $W^{(0)} = I$, it holds

$$\tilde{\Delta}_{i,\lambda}^{(0)} = 0 \qquad (1 \le i \le N,\ 1 \le \lambda \le N). \quad (60)$$

The following lemma holds.

**Lemma 4.2.1.** *For $2 \le i \le N$, $1 \le \lambda \le i-1$ and $1 \le \alpha \le M$, it holds*

$$\sum_{l=i}^{N} \sum_{\mu=\lambda}^{i-1} S_{i-\mu,l} X_{i-\mu,l}^{(\alpha-1)} = \tilde{\chi}_{i,\lambda} v_i^{(\alpha)} + \tilde{\Delta}_{i,\lambda}^{(\alpha-1)}.$$

Proof of this lemma is similar to that of Lemma 4.1.1.

Similarly to the derivation of Eq. (55), for $2 \le i \le N$ and $1 \le u \le M-1$, we have

$$\begin{aligned} \sum_{k=1}^{i-1} (v_k^{(u)} - w_k^{(u)}) &= \tilde{\chi}_{i,1} v_i^{(u)} + \tilde{\Delta}_{i,1}^{(u-1)} \quad (61) \\ &= \tilde{H}_{i,1}^{(0)}(\tilde{\chi}) v_i^{(u)} + \tilde{\Delta}_{i,1}^{(u-1)}. \end{aligned}$$

From Eqs. (59) and (61), for $2 \le i \le N$ and $1 \le u \le M-1$, we obtain

$$z_i^{(u)} - v_i^{(u)} = 2(\tilde{H}_{i,1}^{(0)}(\tilde{\chi})v_i^{(u)} + \tilde{\Delta}_{i,1}^{(u-1)}) + v_i^{(u)}.$$

Therefore, from Eq. (11), for $2 \le s \le M$ and $2 \le i \le N$, it holds

$$\begin{aligned} w_i^{(s)} =& \tilde{F}_i w_{i-1}^{(s)} + \check{B}_i v_i^{(s-1)} \\ &+ 2\check{B}_i(\tilde{H}_{i,1}^{(0)}(\tilde{\chi})v_i^{(s-1)} + \tilde{\Delta}_{i,1}^{(s-2)}). \end{aligned} \tag{62}$$

For $s = 2$ and $2 \le i \le N$, we obtain Eq. (58) by substituting $s = 2$ into Eq. (62) and applying Eq. (60).

Before considering the cases of $M \ge 3$, we prepare the following two lemmas.

**Lemma 4.2.2.** *For $1 \le i \le N$, $1 \le \lambda \le N$ and $1 \le \alpha \le M$, it holds*

$$\tilde{\Delta}_{i,\lambda}^{(\alpha)} = \tilde{h}_{i,\lambda}(\tilde{\chi})v_i^{(\alpha)} + \tilde{h}_{i,\lambda}(\tilde{\Delta}^{(\alpha-1)}).$$

**Lemma 4.2.3.** *For $1 \le i \le N$, $1 \le \lambda \le N$, $r = 0, 1, 2, \dots$ and $1 \le \alpha \le M$, it holds*

$$\tilde{H}_{i,\lambda}^{(r)}(\tilde{\Delta}^{(\alpha)}) = \tilde{H}_{i,\lambda}^{(r+1)}(\tilde{\chi})v_i^{(\alpha)} + \tilde{H}_{i,\lambda}^{(r+1)}(\tilde{\Delta}^{(\alpha-1)}).$$

Proof of these lemmas is similar to that of Lemmas 4.1.2 and 4.1.3.

Let us consider cases where $M \ge 3$. Similarly to Section 4.1, it holds

$$\tilde{\Delta}_{i,1}^{(s-2)} = \sum_{k=2}^{s-1} \tilde{H}_{i,1}^{(k-1)}(\tilde{\chi})v_i^{(s-k)}$$

for $3 \le s \le M$ and $2 \le i \le N$. Substituting this result into Eq. (62), we have Eq. (58) for $3 \le s \le M$ and $2 \le i \le N$.

Finally, we have shown that Eq. (58) holds for $M \ge 2$, $2 \le s \le M$ and $2 \le i \le N$.

## 5. Proof of the new recurrence relations—Step 2

In this section, we show that $\check{B}_i H_{i,1}^{(r-1)}(\chi)$ and $\check{B}_i \tilde{H}_{i,1}^{(r-1)}(\tilde{\chi})$ are equal to $g_i^{(r)}$ and $\tilde{g}_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \dots$, respectively. If this assertion is verified, then the new recurrence relations in Section 2.2 are finally proved by combining the proof of these correspondences in this section with the argument in Section 4.

For convenience, let $\check{C}_i$ $(1 \le i \le N-1)$ denote $\check{C}_i = 1/c_i^2$.

### 5.1. Proof—Part I

In this subsection, we show that $\check{B}_i H_{i,1}^{(r-1)}(\chi)$ correspond to $g_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \dots$.

We have the following three lemmas.

**Lemma 5.1.1.** *For $r = 1, 2, \dots$, it holds $\check{B}_N H_{N,1}^{(r-1)}(\chi) = g_N^{(r)}$.*

**Lemma 5.1.2.** *For $1 \le i \le N-1$, it holds $\check{B}_i H_{i,1}^{(0)}(\chi) = g_i^{(1)}$.*

**Lemma 5.1.3.** *For $r = 1, 2, \dots$, it holds $\check{B}_{N-1} H_{N-1,1}^{(r-1)}(\chi) = g_{N-1}^{(r)}$.*

Proof of these lemmas is given in Appendix.

For $N = 2$, the correspondences between $\check{B}_i H_{i,1}^{(r-1)}(\chi)$ and $g_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \dots$ are shown from Lemmas 5.1.1 and 5.1.3.

Let us consider the cases where $N \ge 3$. The following lemma holds.

**Lemma 5.1.4.** *Let $N$ be $N \ge 3$. Let us consider sets of quantities $\{\varphi_{i,\xi}\}$ and $\{\psi_{i,\xi}\}$ defined for $1 \le i \le N-1$ and $1 \le \xi \le N-i$. Assume that $\{\varphi_{i,\xi}\}$ and $\{\psi_{i,\xi}\}$ satisfy*

$$\varphi_{i+1,\xi-1} = \psi_{i,\xi} \qquad (1 \le i \le N-2,\ 2 \le \xi \le N-i).$$

*Then, for $1 \le i \le N-2$ and $2 \le \lambda \le N-i$, it holds*

$$\begin{aligned} h_{i+1,\lambda-1}(\varphi) &= h_{i,\lambda}(\psi) - \check{C}_i \psi_{i,1} \chi_{i,\lambda}, \\ h_{i+1,1}(\varphi) &= h_{i,1}(\psi) - \check{C}_i \psi_{i,1} \chi_{i,1}. \end{aligned}$$

*Proof.* Let $i$ and $\lambda$ be integers such that $1 \le i \le N-2$ and $2 \le \lambda \le N-i$, respectively.

With help of Lemma 3.1.4, we see that

$$\begin{aligned} &\sum_{\mu=\lambda}^{N-i} \sum_{\xi=2}^{\mu} \check{B}_{i+\xi} \gamma_{i,\mu,\xi}^2 \psi_{i,\xi} \\ &= \sum_{\mu=\lambda}^{N-i} \left( \sum_{\xi=1}^{\mu} \check{B}_{i+\xi} \gamma_{i,\mu,\xi}^2 \psi_{i,\xi} - \check{B}_{i+1} \gamma_{i,\mu,1}^2 \psi_{i,1} \right) \\ &= \sum_{\mu=\lambda}^{N-i} \sum_{\xi=1}^{\mu} \check{B}_{i+\xi} \gamma_{i,\mu,\xi}^2 \psi_{i,\xi} - \check{B}_{i+1} \psi_{i,1} \sum_{\mu=\lambda}^{N-i} \gamma_{i,\mu,1}^2 \\ &= h_{i,\lambda}(\psi) - \check{B}_{i+1} \psi_{i,1} \cdot \tilde{F}_{i+1}^{-1} \chi_{i,\lambda} \\ &= h_{i,\lambda}(\psi) - \check{C}_i \psi_{i,1} \chi_{i,\lambda}. \end{aligned}$$

Considering this result and Lemma 3.1.2, we have

$$\begin{aligned} &h_{i+1,\lambda-1}(\varphi) \\ &\quad = \sum_{\mu=\lambda-1}^{N-i-1} \sum_{\xi=1}^{\mu} \check{B}_{i+1+\xi} \gamma_{i+1,\mu,\xi}^2 \varphi_{i+1,\xi} \\ &\quad = \sum_{\mu=\lambda-1}^{N-i-1} \sum_{\xi'=2}^{\mu+1} \check{B}_{i+\xi'} \gamma_{i+1,\mu,\xi'-1}^2 \varphi_{i+1,\xi'-1} \\ &\quad = \sum_{\mu'=\lambda}^{N-i} \sum_{\xi'=2}^{\mu'} \check{B}_{i+\xi'} \gamma_{i+1,\mu'-1,\xi'-1}^2 \varphi_{i+1,\xi'-1} \\ &\quad = \sum_{\mu'=\lambda}^{N-i} \sum_{\xi'=2}^{\mu'} \check{B}_{i+\xi'} \gamma_{i,\mu',\xi'}^2 \psi_{i,\xi'} \\ &\quad = h_{i,\lambda}(\psi) - \check{C}_i \psi_{i,1} \chi_{i,\lambda}. \end{aligned}$$

From this result, we have

$$\begin{aligned}
&h_{i+1,1}(\varphi)\\
&= h_{i,2}(\psi) - \check{C}_i\psi_{i,1}\chi_{i,2}\\
&= \sum_{\mu=2}^{N-i}\sum_{\xi=1}^{\mu} \check{B}_{i+\xi}\gamma^2_{i,\mu,\xi}\psi_{i,\xi} - \check{C}_i\psi_{i,1}\cdot\tilde{F}_{i+1}\chi_{i+1,1}\\
&= \sum_{\mu=1}^{N-i}\sum_{\xi=1}^{\mu} \check{B}_{i+\xi}\gamma^2_{i,\mu,\xi}\psi_{i,\xi} - \check{B}_{i+1}\gamma^2_{i,1,1}\psi_{i,1}\\
&\quad - \check{B}_{i+1}\psi_{i,1}\cdot c^2_{i+1}v^{(1)}_{i+2}\\
&= h_{i,1}(\psi) - (\check{B}_{i+1} + F_{i+1}v^{(1)}_{i+2})\psi_{i,1}\\
&= h_{i,1}(\psi) - v^{(1)}_{i+1}\psi_{i,1}\\
&= h_{i,1}(\psi) - \check{C}_i\psi_{i,1}\chi_{i,1}
\end{aligned}$$

with consideration of Remark 2.2.4 and Lemmas 3.1.3 and 3.1.5. □

For convenience, we introduce new quantities. The new quantities $K^{(r)}_{i,\lambda}$ defined for $N \geq 2$, $1 \leq i \leq N-1$, $1 \leq \lambda \leq N$ and $r = 1, 2, \ldots$ are given as follows:

$$\begin{aligned}
K^{(r)}_{i,\lambda} \equiv &\tilde{F}^{-1}_{i+1}H^{(r)}_{i,\lambda}(\chi) - \check{C}_iH^{(r-1)}_{i,\lambda}(\chi)\\
&- \check{C}_i\sum_{k=1}^{r} H^{(k-1)}_{i+1,1}(\chi)H^{(r-k)}_{i,\lambda}(\chi).
\end{aligned} \tag{63}$$

We show the following three lemmas.

**Lemma 5.1.5.** *Only in this lemma, let $N$ be $N \geq 2$. For $1 \leq i \leq N-1$, $1 \leq \lambda \leq N$ and $r = 1, 2, \ldots,$ it holds*

$$h_{i,\lambda}(K^{(r)}) = K^{(r+1)}_{i,\lambda} + \check{C}_iH^{(r)}_{i+1,1}(\chi)H^{(0)}_{i,\lambda}(\chi).$$

Proof of this lemma is given in Appendix.

**Lemma 5.1.6.** *Let $N$ be $N \geq 3$. For $1 \leq i \leq N-2$, $2 \leq \lambda \leq N-i$ and $r = 1, 2, \ldots,$ it holds*

$$\begin{cases} H^{(r)}_{i+1,\lambda-1}(\chi) = K^{(r)}_{i,\lambda},\\ H^{(r)}_{i+1,1}(\chi) = K^{(r)}_{i,1}. \end{cases} \tag{64}$$

*Proof.* Firstly, note that we have

$$\begin{aligned}
\tilde{F}^{-1}_{i+1}H^{(0)}_{i,1}(\chi) &= \tilde{F}^{-1}_{i+1}\cdot c^2_iv^{(1)}_{i+1} = b^2_{i+1}(F_{i+1}v^{(1)}_{i+2} + \check{B}_{i+1})\\
&= c^2_{i+1}v^{(1)}_{i+2} + 1 = H^{(0)}_{i+1,1}(\chi) + 1
\end{aligned}$$

with help of Remark 2.2.4 and Lemma 3.1.3. Secondly, note that

$$H^{(0)}_{i+1,\xi-1}(\chi) = \chi_{i+1,\xi-1} = \tilde{F}^{-1}_{i+1}\chi_{i,\xi} = \tilde{F}^{-1}_{i+1}H^{(0)}_{i,\xi}(\chi)$$

holds for $N \geq 3$, $1 \leq i \leq N-2$ and $2 \leq \xi \leq N-1$ from Lemma 3.1.5. Considering these results and Lemma 5.1.4, we obtain

$$\begin{aligned}
&H^{(1)}_{i+1,\lambda-1}(\chi)\\
&= h_{i+1,\lambda-1}(H^{(0)}(\chi))\\
&= h_{i,\lambda}(\tilde{F}^{-1}_{i+1}H^{(0)}(\chi)) - \check{C}_i\cdot\tilde{F}^{-1}_{i+1}H^{(0)}_{i,1}(\chi)\cdot\chi_{i,\lambda}\\
&= \tilde{F}^{-1}_{i+1}H^{(1)}_{i,\lambda}(\chi) - \check{C}_iH^{(0)}_{i,\lambda}(\chi) - \check{C}_iH^{(0)}_{i+1,1}(\chi)H^{(0)}_{i,\lambda}(\chi)\\
&= K^{(1)}_{i,\lambda}
\end{aligned}$$

and

$$\begin{aligned}
&H^{(1)}_{i+1,1}(\chi)\\
&= h_{i+1,1}(H^{(0)}(\chi))\\
&= h_{i,1}(\tilde{F}^{-1}_{i+1}H^{(0)}(\chi)) - \check{C}_i\cdot\tilde{F}^{-1}_{i+1}H^{(0)}_{i,1}(\chi)\cdot\chi_{i,1}\\
&= \tilde{F}^{-1}_{i+1}H^{(1)}_{i,1}(\chi) - \check{C}_iH^{(0)}_{i,1}(\chi) - \check{C}_iH^{(0)}_{i+1,1}(\chi)H^{(0)}_{i,1}(\chi)\\
&= K^{(1)}_{i,1}.
\end{aligned}$$

Assume that it holds

$$\begin{cases} H^{(l)}_{i+1,\lambda-1}(\chi) = K^{(l)}_{i,\lambda},\\ H^{(l)}_{i+1,1}(\chi) = K^{(l)}_{i,1} \end{cases}$$

for all $l$ such that $1 \leq l \leq s$. Then, we have

$$\begin{aligned}
&H^{(s+1)}_{i+1,\lambda-1}(\chi)\\
&= h_{i+1,\lambda-1}(H^{(s)}(\chi))\\
&= h_{i,\lambda}(K^{(s)}) - \check{C}_iK^{(s)}_{i,1}\chi_{i,\lambda}\\
&= K^{(s+1)}_{i,\lambda} + \check{C}_iH^{(s)}_{i+1,1}(\chi)H^{(0)}_{i,\lambda}(\chi) - \check{C}_iH^{(s)}_{i+1,1}(\chi)H^{(0)}_{i,\lambda}(\chi)\\
&= K^{(s+1)}_{i,\lambda}
\end{aligned}$$

and

$$\begin{aligned}
&H^{(s+1)}_{i+1,1}(\chi)\\
&= h_{i+1,1}(H^{(s)}(\chi))\\
&= h_{i,1}(K^{(s)}) - \check{C}_iK^{(s)}_{i,1}\chi_{i,1}\\
&= K^{(s+1)}_{i,1} + \check{C}_iH^{(s)}_{i+1,1}(\chi)H^{(0)}_{i,1}(\chi) - \check{C}_iH^{(s)}_{i+1,1}(\chi)H^{(0)}_{i,1}(\chi)\\
&= K^{(s+1)}_{i,1}
\end{aligned}$$

with consideration of Lemmas 5.1.4 and 5.1.5. Therefore, it is shown that Eq. (64) holds for $1 \leq i \leq N-2$, $2 \leq \lambda \leq N-i$, and $r = 1, 2, \cdots$ by mathematical induction. □

**Lemma 5.1.7.** *Let $N$ be $N \geq 3$. For $1 \leq i \leq N-2$ and $s = 2, 3, \ldots,$ it holds $\check{B}_iH^{(s-1)}_{i,1}(\chi) = g^{(s)}_i$.*

*Proof.* For $r = 1, 2, \ldots,$ from Lemma 5.1.6 and the definition (63), it holds

$$\begin{aligned}
H^{(r)}_{i+1,1}(\chi) = &\tilde{F}^{-1}_{i+1}H^{(r)}_{i,1}(\chi) - \check{C}_iH^{(r-1)}_{i,1}(\chi)\\
&- \check{C}_i\sum_{k=1}^{r} H^{(k-1)}_{i+1,1}(\chi)H^{(r-k)}_{i,1}(\chi).
\end{aligned}$$

Multiplying the both hand sides by $\check{B}_i\tilde{F}_{i+1}(= \check{B}_{i+1}F_i)$ and rearranging, we have

$$\begin{aligned}
\check{B}_iH^{(r)}_{i,1}(\chi) = &F_i\cdot\check{B}_{i+1}H^{(r)}_{i+1,1}(\chi) + \check{B}_{i+1}\cdot\check{B}_iH^{(r-1)}_{i,1}(\chi)\\
&+ \sum_{k=1}^{r}\check{B}_{i+1}H^{(k-1)}_{i+1,1}(\chi)\cdot\check{B}_iH^{(r-k)}_{i,1}(\chi).
\end{aligned}$$

From this result, Definition 2.2.2 and Lemmas 5.1.2 and 5.1.3, $\check{B}_iH^{(s-1)}_{i,1}(\chi) = g^{(s)}_i$ holds for $1 \leq i \leq N-2$ and $s = 2, 3, \ldots.$ □

From Lemmas 5.1.1, 5.1.2, 5.1.3 and 5.1.7, the correspondence

$$\check{B}_i H_{i,1}^{(r-1)}(\chi) = g_i^{(r)} \qquad (1 \le i \le N,\ r = 1, 2, \dots)$$

is shown.

### 5.2. Proof—Part II

In this subsection, we show that $\check{B}_i \tilde{H}_{i,1}^{(r-1)}(\tilde{\chi})$ correspond to $\tilde{g}_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \dots$.

We have the following three lemmas.

**Lemma 5.2.1.** *For $r = 1, 2, \dots$, it holds $\check{B}_1 \tilde{H}_{1,1}^{(r-1)}(\tilde{\chi}) = \tilde{g}_1^{(r)}$.*

**Lemma 5.2.2.** *For $2 \le i \le N$, it holds $\check{B}_i \tilde{H}_{i,1}^{(0)}(\tilde{\chi}) = \tilde{g}_i^{(1)}$.*

**Lemma 5.2.3.** *For $r = 1, 2, \dots$, it holds $\check{B}_2 \tilde{H}_{2,1}^{(r-1)}(\tilde{\chi}) = \tilde{g}_2^{(r)}$.*

Proof of these lemmas is similar to that of Lemmas from 5.1.1 to 5.1.3. We omit them.

For $N = 2$, the correspondences between $\check{B}_i \tilde{H}_{i,1}^{(r-1)}(\tilde{\chi})$ and $\tilde{g}_i^{(r)}$ for $1 \le i \le N$ and $r = 1, 2, \dots$ are shown from Lemmas 5.2.1 and 5.2.3.

Let us consider the cases where $N \ge 3$. The following lemma holds.

**Lemma 5.2.4.** *Let $N$ be $N \ge 3$. Let us consider sets of quantities $\{\tilde{\varphi}_{i,\xi}\}$ and $\{\tilde{\psi}_{i,\xi}\}$ defined for $2 \le i \le N$ and $1 \le \xi \le i-1$. Assume that $\{\tilde{\varphi}_{i,\xi}\}$ and $\{\tilde{\psi}_{i,\xi}\}$ satisfy*

$$\tilde{\varphi}_{i-1,\xi-1} = \tilde{\psi}_{i,\xi} \qquad (3 \le i \le N,\ 2 \le \xi \le i-1).$$

*Then, for $3 \le i \le N$ and $2 \le \lambda \le i-1$, it holds*

$$\begin{aligned} \tilde{h}_{i-1,\lambda-1}(\tilde{\varphi}) &= \tilde{h}_{i,\lambda}(\tilde{\psi}) - \check{C}_{i-1} \tilde{\psi}_{i,1} \tilde{\chi}_{i,\lambda}, \\ \tilde{h}_{i-1,1}(\tilde{\varphi}) &= \tilde{h}_{i,1}(\tilde{\psi}) - \check{C}_{i-1} \tilde{\psi}_{i,1} \tilde{\chi}_{i,1}. \end{aligned}$$

Proof of this lemma is similar to that of Lemma 5.1.4.

For convenience, we introduce new quantities. The new quantities $\tilde{K}_{i,\lambda}^{(r)}$ defined for $N \ge 2$, $2 \le i \le N$, $1 \le \lambda \le N$ and $r = 1, 2, \dots$ are given as follows:

$$\begin{aligned} \tilde{K}_{i,\lambda}^{(r)} \equiv & F_{i-1}^{-1} \tilde{H}_{i,\lambda}^{(r)}(\tilde{\chi}) - \check{C}_{i-1} \tilde{H}_{i,\lambda}^{(r-1)}(\tilde{\chi}) \\ & - \check{C}_{i-1} \sum_{k=1}^{r} \tilde{H}_{i-1,1}^{(k-1)}(\tilde{\chi}) \tilde{H}_{i,\lambda}^{(r-k)}(\tilde{\chi}). \end{aligned}$$

Similarly to Section 5.1, we have the following three lemmas.

**Lemma 5.2.5.** *Only in this lemma, let $N$ be $N \ge 2$. For $2 \le i \le N$, $1 \le \lambda \le N$ and $r = 1, 2, \dots$, it holds*

$$\tilde{h}_{i,\lambda}(\tilde{K}^{(r)}) = \tilde{K}_{i,\lambda}^{(r+1)} + \check{C}_{i-1} \tilde{H}_{i-1,1}^{(r)}(\tilde{\chi}) \tilde{H}_{i,\lambda}^{(0)}(\tilde{\chi}).$$

**Lemma 5.2.6.** *Let $N$ be $N \ge 3$. For $3 \le i \le N$, $2 \le \lambda \le i-1$ and $r = 1, 2, \dots$, it holds*

$$\begin{cases} \tilde{H}_{i-1,\lambda-1}^{(r)}(\tilde{\chi}) = \tilde{K}_{i,\lambda}^{(r)}, \\ \tilde{H}_{i-1,1}^{(r)}(\tilde{\chi}) = \tilde{K}_{i,1}^{(r)}. \end{cases}$$

**Lemma 5.2.7.** *Let $N$ be $N \ge 3$. For $3 \le i \le N$ and $s = 2, 3, \dots$, it holds $\check{B}_i \tilde{H}_{i,1}^{(s-1)}(\tilde{\chi}) = \tilde{g}_i^{(s)}$.*

Proof of these lemmas is similar to that of Lemmas from 5.1.5 to 5.1.7.

From Lemmas 5.2.1, 5.2.2, 5.2.3 and 5.2.7, the correspondence

$$\check{B}_i \tilde{H}_{i,1}^{(r-1)}(\tilde{\chi}) = \tilde{g}_i^{(r)} \qquad (1 \le i \le N,\ r = 1, 2, \dots)$$

is shown.

Thus, derivation of the new recurrence relations in Section 2.2 is completed. □

## 6. Computational cost for computing the trace $J_M(B)$

In this section, computational cost of the trace $J_M(B)$ for a fixed $M$ is considered. In Section 6.1, the computational cost with the old recurrence relations [4] in Theorem 2.1.1 is discussed. In Section 6.2, the computational cost with the new recurrence relations in Section 2.2 is discussed. In Section 6.3, a reduction of the number of operations of the recurrence relations in Section 2.2 is discussed. In Section 6.4, implementations of algorithms for computing the traces $J_M(B)$ $(M = 2,\ 3)$ are performed. The numbers of operations of these implementations are also discussed.

### 6.1. Computational cost with the old recurrence relations

In this subsection, computational cost for the trace $J_M(B)$ for a fixed $M$ with the recurrence relations in Theorem 2.1.1 is estimated. The following corollary of Theorem 2.1.1 holds.

**Corollary 6.1.1.** *Let $M$ be a fixed positive integer. The trace $J_M(B)$ can be obtained $O(MN)$ operations through the old recurrence relations in Theorem 2.1.1.*

*Proof.* We estimate computational cost for computing all the diagonals of $((BB^T)^M)^{-1}$. 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 $w_i^{(M)}$ for $1 \le i \le N$. These quantities are sufficient to determine all the diagonals $w_i^{(M)}$ for $1 \le i \le N$. As is shown in [4], $v_i^{(0)}$, $w_i^{(0)}$ 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 remaining quantities to be obtained is $(3M-2)N$. They are not given directly. Each of these quantities can be obtained within at most six times of the four basic operations of arithmetic according to the recurrence relations in Theorem 2.1.1. Then, all the diagonals of $((BB^T)^M)^{-1}$ are obtained less than $18MN$ operations. The trace $J_M(B)$ is computed with $N-1$ times addition after all the diagonals of $((BB^T)^M)^{-1}$ are computed. □

Note that the generalized Newton bound $\theta_M(B)$ and the generalized Newton shift $(\theta_M(B))^2$ can be obtained by once division from $(J_M(B))^{\frac{1}{2M}}$ and $(J_M(B))^{\frac{1}{M}}$, respectively.

**Remark 6.1.2.** For some integer $m$ $(\geq 2)$ and positive real number $\zeta$, assume that computational cost for computing $\zeta^{\frac{1}{m}}$ from $\zeta$ is negligible. Then, the computational costs for the generalized Newton bound $\theta_M(B)$ and the generalized Newton shift $(\theta_M(B))^2$ with the old recurrence relations in Theorem 2.2.1 are both $O(MN)$.

### 6.2. Computational cost with the new recurrence relations

In this subsection, computational cost for the trace $J_M(B)$ with the new recurrence relations is discussed. Note that computational cost should be considered for sufficiently large $M$ and $N$.

In the case of $M = 1$, the trace $J_1(B)$ can be computed with the recurrence relations in Remark 2.2.4. An algorithm for computing $J_1(B)$ by these recurrence relations is shown in Algorithm 1. In the case of $M \geq 2$, an algorithm for computing diagonals of the inverse $(BB^T)^{-1}$ is shown in Algorithm 2. In the case of $M \geq 3$, algorithms for computing diagonals of the inverse $(B^TB)^{-1}$ and $\tilde{g}_i^{(r)}$ $(1 \leq i \leq N,\ 2 \leq r \leq M-1)$ are shown in Algorithms 3 and 4, respectively. In the case of $M \geq 4$, an algorithm for computing $g_i^{(r)}$ $(1 \leq i \leq N,\ 2 \leq r \leq M-2)$ is shown in Algorithm 5. Moreover, in the case of $M \geq 2$, Algorithm 6 is utilized. Algorithms for computing the traces $J_2(B)$, $J_3(B)$ and $J_M(B)$ $(M \geq 4)$ are shown in Algorithms 7, 8 and 9, respectively. Note that Algorithms 3, 4 and 6 are called after Algorithm 2 is called. Moreover, note that Algorithm 5 is called after Algorithm 3 is called.

From Algorithm 9, the following Remark 6.2.1 follows.

**Remark 6.2.1.** The computational cost for the trace $J_M(B)$ with the new recurrence relations is $O(M^2N)$.

**Remark 6.2.2.** Under the same assumption in Remark 6.1.2, the computational costs for the generalized Newton bound $\theta_M(B)$ and the generalized Newton shift $(\theta_M(B))^2$ with the new recurrence relations in Section 2.2 are both $O(M^2N)$.

**Algorithm 1** computation of the trace $J_1(B)$

$\check{B}_1 \leftarrow 1.0/(b_1 * b_1)$
$w_1^{(1)} \leftarrow \check{B}_1$
$J \leftarrow w_1^{(1)}$
**for** $i = 2$ **to** $N$ **by** $+1$ **do**
    $\check{B}_i \leftarrow 1.0/(b_i * b_i)$
    $\tilde{F}_i \leftarrow c_{i-1} * c_{i-1} * \check{B}_i$
    $w_i^{(1)} \leftarrow \tilde{F}_i * w_{i-1}^{(1)} + \check{B}_i$
    $J \leftarrow J + w_i^{(1)}$
**end for**
**return** $J$

**Algorithm 2** computation of diagonals of $(BB^T)^{-1}$

$\check{B}_1 \leftarrow 1.0/(b_1 * b_1)$
$w_1^{(1)} \leftarrow \check{B}_1$
**for** $i = 2$ **to** $N$ **by** $+1$ **do**
    $\check{B}_i \leftarrow 1.0/(b_i * b_i)$
    $\hat{C}_{i-1} \leftarrow c_{i-1} * c_{i-1}$
    $\tilde{F}_i \leftarrow \hat{C}_{i-1} * \check{B}_i$
    $\tilde{g}_i^{(1)} \leftarrow \tilde{F}_i * w_{i-1}^{(1)}$
    $w_i^{(1)} \leftarrow \tilde{g}_i^{(1)} + \check{B}_i$
**end for**

**Algorithm 3** computation of diagonals of $(B^TB)^{-1}$

$v_N^{(1)} \leftarrow \check{B}_N$
**for** $i = N-1$ **to** $1$ **by** $-1$ **do**
    $F_i \leftarrow \hat{C}_i * \check{B}_i$
    $g_i^{(1)} \leftarrow F_i * v_{i+1}^{(1)}$
    $v_i^{(1)} \leftarrow g_i^{(1)} + \check{B}_i$
**end for**

**Algorithm 4** computation of $\tilde{g}_i^{(r)}$ $(1 \leq i \leq N,\ 2 \leq r \leq M-1)$ in the case of $M \geq 3$

$\tilde{g}_1^{(1)} \leftarrow 0$
**for** $r = 2$ **to** $M-1$ **by** $+1$ **do**
    $\tilde{g}_1^{(r)} \leftarrow 0$
    **for** $i = 2$ **to** $N$ **by** $+1$ **do**
        $tmp \leftarrow 0$
        **for** $k = 1$ **to** $r-1$ **by** $+1$ **do**
            $tmp \leftarrow tmp + \tilde{g}_{i-1}^{(k)} * \tilde{g}_i^{(r-k)}$
        **end for**
        $\tilde{g}_i^{(r)} \leftarrow \tilde{F}_i * \tilde{g}_{i-1}^{(r)} + \check{B}_{i-1} * \tilde{g}_i^{(r-1)} + tmp$
    **end for**
**end for**

**Algorithm 5** computation of $g_i^{(r)}$ $(1 \leq i \leq N,\ 2 \leq r \leq M-2)$ in the case of $M \geq 4$

$g_N^{(1)} \leftarrow 0$
**for** $r = 2$ **to** $M-2$ **by** $+1$ **do**
    $g_N^{(r)} \leftarrow 0$
    **for** $i = N-1$ **to** $1$ **by** $-1$ **do**
        $tmp \leftarrow 0$
        **for** $k = 1$ **to** $r-1$ **by** $+1$ **do**
            $tmp \leftarrow tmp + g_{i+1}^{(k)} * g_i^{(r-k)}$
        **end for**
        $g_i^{(r)} \leftarrow F_i * g_{i+1}^{(r)} + \check{B}_{i+1} * g_i^{(r-1)} + tmp$
    **end for**
**end for**

**Algorithm 6** common part for computation of the trace $J_M(B)$ with the new recurrence relations in the case of $M \geq 2$

```
for s = 2 to M by +1 do
  if s < M then
    v_N^(s) ← B̌_N * w_N^(s-1)
    for i = N - 1 to 1 by -1 do
      tmp ← 0
      for k = 1 to s - 1 by +1 do
        tmp ← tmp + g_i^(k) * w_i^(s-k)
      end for
      v_i^(s) ← F_i * v_{i+1}^(s) + B̌_i * w_i^(s-1) + 2 * tmp
    end for
  end if
  if s ≠ M - 1 then
    w_1^(s) ← B̌_1 * v_1^(s-1)
    if s = M then
      J ← w_1^(s)
    end if
    for i = 2 to N by +1 do
      tmp ← 0
      for k = 1 to s - 1 by +1 do
        tmp ← tmp + g̃_i^(k) * v_i^(s-k)
      end for
      w_i^(s) ← F̃_i * w_{i-1}^(s) + B̌_i * v_i^(s-1) + 2 * tmp
      if s = M then
        J ← J + w_i^(s)
      end if
    end for
  end if
end for
```

**Algorithm 7** computation of the trace $J_2(B)$ with the new recurrence relations

```
call Algorithm 2
v_N^(1) ← B̌_N
for i = N - 1 to 1 by -1 do
  F_i ← Ĉ_i * B̌_i
  v_i^(1) ← F_i * v_{i+1}^(1) + B̌_i
end for
call Algorithm 6
return J
```

**Algorithm 8** computation of the trace $J_3(B)$ with the new recurrence relations

```
call Algorithm 2
call Algorithm 3
call Algorithm 4
call Algorithm 6
return J
```

**Algorithm 9** computation of the trace $J_M(B)$ with the new recurrence relations in the case of $M \geq 4$

```
call Algorithm 2
call Algorithm 3
call Algorithm 4
call Algorithm 5
call Algorithm 6
return J
```

### 6.3. A reduction of the number of operations

The recurrence relations for computing $g_i^{(2)}$ $(1 \leq i \leq N-1)$ in Definition 2.2.2 can be rearranged as follows.

$$\begin{aligned} g_i^{(2)} &= F_i g_{i+1}^{(2)} + \check{B}_{i+1} g_i^{(1)} + g_{i+1}^{(1)} g_i^{(1)} \\ &= F_i g_{i+1}^{(2)} + (\check{B}_{i+1} + g_{i+1}^{(1)}) g_i^{(1)} \\ &= F_i g_{i+1}^{(2)} + v_{i+1}^{(1)} g_i^{(1)} \qquad (1 \leq i \leq N-1). \end{aligned}$$

Similarly, the recurrence relations for computing $\tilde{g}_i^{(2)}$ $(2 \leq i \leq N)$ in Definition 2.2.3 can be rearranged as follows.

$$\tilde{g}_i^{(2)} = \tilde{F}_i \tilde{g}_{i-1}^{(2)} + w_{i-1}^{(1)} \tilde{g}_i^{(1)} \qquad (2 \leq i \leq N).$$

By these rearrangements, the number of multiplication and addition are reduced from three times to twice and from twice to once, respectively. Moreover, for $r = 3, 4, \ldots,$ the recurrence relations (23) in Definition 2.2.2 and (24) in Definition 2.2.3 can be rewritten as follows,

$$\begin{aligned} g_i^{(r)} &= F_i g_{i+1}^{(r)} + v_{i+1}^{(1)} g_i^{(r-1)} + \sum_{k=2}^{r-1} g_{i+1}^{(k)} g_i^{(r-k)} \\ &\qquad (1 \leq i \leq N-1), \\ \tilde{g}_i^{(r)} &= \tilde{F}_i \tilde{g}_{i-1}^{(r)} + w_{i-1}^{(1)} \tilde{g}_i^{(r-1)} + \sum_{k=2}^{r-1} \tilde{g}_{i-1}^{(k)} \tilde{g}_i^{(r-k)} \\ &\qquad (2 \leq i \leq N). \end{aligned}$$

These modified recurrence relations require less number of multiplication and addition by once compared with the original recurrence relation (23) or (24).

Let us consider the following relationships.

$$\begin{aligned} \check{B}_i + 2 g_i^{(1)} &= v_i^{(1)} + g_i^{(1)} \qquad (1 \leq i \leq N-1), \\ \check{B}_i + 2 \tilde{g}_i^{(1)} &= w_i^{(1)} + \tilde{g}_i^{(1)} \qquad (2 \leq i \leq N). \end{aligned}$$

See Remark 2.2.4. For $M \geq 2$, the modified recurrence relations for computing $v_i^{(2)}$ $(1 \leq i \leq N-1)$ and $w_i^{(2)}$ $(2 \leq i \leq N)$ in Theorem 2.2.5 can be written as follows,

$$\begin{aligned} v_i^{(2)} &= F_i v_{i+1}^{(2)} + \check{B}_i w_i^{(1)} + 2 g_i^{(1)} w_i^{(1)} \\ &= F_i v_{i+1}^{(2)} + (v_i^{(1)} + g_i^{(1)}) w_i^{(1)} \qquad (1 \leq i \leq N-1), \\ w_i^{(2)} &= \tilde{F}_i w_{i-1}^{(2)} + \check{B}_i v_i^{(1)} + 2 \tilde{g}_i^{(1)} v_i^{(1)} \\ &= \tilde{F}_i w_{i-1}^{(2)} + (w_i^{(1)} + \tilde{g}_i^{(1)}) v_i^{(1)} \qquad (2 \leq i \leq N). \end{aligned}$$

By these rearrangements, the number of multiplication is reduced from four times to twice. For $M \geq 3$ and $3 \leq s \leq$

$M$, modified relations for computing $v_i^{(s)}$ $(1 \le i \le N-1)$ and $w_i^{(s)}$ $(2 \le i \le N)$ in Theorem 2.2.5 can be written as follows,

$$v_i^{(s)} = F_i v_{i+1}^{(s)} + (v_i^{(1)} + g_i^{(1)}) w_i^{(s-1)} + 2 \sum_{k=2}^{s-1} g_i^{(k)} w_i^{(s-k)} \quad (1 \le i \le N-1),$$

$$w_i^{(s)} = \tilde{F}_i w_{i-1}^{(s)} + (w_i^{(1)} + \tilde{g}_i^{(1)}) v_i^{(s-1)} + 2 \sum_{k=2}^{s-1} \tilde{g}_i^{(k)} v_i^{(s-k)} \quad (2 \le i \le N).$$

By these rearrangements, the number of multiplication is reduced form $s+2$ to $s+1$.

On the other hand, on the old recurrence relations, we have not found such rearrangement.

### 6.4. Efficient implementations of algorithms for the cases of $M = 2$ and 3

In this subsection, we consider cases of $M = 2$ and 3. On the new recurrence relations in Section 2.2, to reduce the number of operations, we consider modified new recurrence relations in Section 6.3. As well as the new recurrence relations in Section 2.2, these modified new recurrence relations are subtraction-free. We perform implementations of algorithms for computing the traces $J_M(B)$. For each $M$, one implementation is based on the old recurrence relations in Section 2.1 and another implementation is based on the modified new recurrence relations. The numbers of operations of these implementations are compared.

For $i = 1, \ldots, N$, let $b_i$ be recorded in "array" B[$i$]. For $i = 1, \ldots, N-1$, let $c_i$ be recorded in "array" C[$i$]. In this discussion, we consider the case where these "arrays" are not destroyed by "overwriting". Moreover, we consider the following devises for numerical computation in information processing.

- We try to reduce the number of "loops" by the technique of "loop fusion".
- We try to raise "register hit rate" or "cash hit rate" by trial to reduce "working memories". We avoid use of an "array" if it is not necessary.
- We try to raise "cash hit rate" by trial to use the same "variable" or an "element" in an "array" continuously.
- We try to reduce the number of divisions which takes a longer time than multiplications.

Algorithms for computing the trace $J_2(B)$ based on the old and the modified new recurrence relations are shown in Algorithms 10 and 11, respectively. The numbers of operations are shown in Table 1. Algorithms for computing the trace $J_3(B)$ based on the old and the modified new recurrence relations are shown in Algorithms 12 and 13, respectively. The numbers of operations are shown in Table 2. Among these implementations, the traces $J_2(B)$ and $J_3(B)$ are computed by the implementations based on the modified new recurrence relations in less number of operations than by those based on the old recurrence relations. We see Algorithms 11 and 13 are better than Algorithms 10 and 12, respectively.

Table 1: Comparison of the number of operations in computation of $J_2(B)$

| | Algo. 10 (old) | Algo. 11 (new) |
|---|---|---|
| addition | $5N-5$ | $5N-5$ |
| subtraction | $2N-2$ | 0 |
| multiplication | $9N-6$ | $8N-6$ |
| division | $N$ | $N$ |

Table 2: Comparison of the number of operations in computation of $J_3(B)$

| | Algo. 12 (old) | Algo. 13 (new) |
|---|---|---|
| addition | $8N-8$ | $9N-8$ |
| subtraction | $5N-4$ | 0 |
| multiplication | $14N-8$ | $14N-8$ |
| division | $N$ | $N$ |

**Algorithm 10** An implementation of an algorithm for computing the trace $J_2(B)$ with a method based on the old recurrence relations

```
IB[N] ← 1.0/(B[N] ∗ B[N])   : B̌_N
D[N] ← IB[N]                : v_N^(1)
for i = N − 1 to 1 by −1 do
    SC[i] ← C[i] ∗ C[i]                        : c_i^2
    IB[i] ← 1.0/(B[i] ∗ B[i])                  : B̌_i
    D[i] ← IB[i] ∗ (SC[i] ∗ D[i + 1] + 1.0)    : v_i^(1)
end for
W2 ← IB[1] ∗ D[1]   : w_1^(2)
W1 ← IB[1]          : w_1^(1)
Z1 ← 2.0 ∗ D[1]     : z_1^(1)
J ← W2
for i = 2 to N by +1 do
    Z1 ← Z1 + 2.0 ∗ (D[i] − W1)                 : z_i^(1)
    W2 ← IB[i] ∗ (SC[i − 1] ∗ W2 + Z1 − D[i])   : w_i^(2)
    W1 ← IB[i] ∗ (SC[i − 1] ∗ W1 + 1.0)         : w_i^(1)
    J ← J + W2
end for
return J
```

## 7. Concluding remarks

In this paper, new recurrence relations for computing diagonals of $((B^T B)^M)^{-1}$ and $((BB^T)^M)^{-1}$ are derived starting from the old ones in [4]. From these diagonals, the trace $J_M(B)$ can be obtained. Moreover, the generalized Newton bound $\theta_M(B)$ of order $M$, which is a lower bound

**Algorithm 11** An implementation of an algorithm for computing the trace $J_2(B)$ with a method based on the new recurrence relations

IB[$N$] ← 1.0/(B[$N$] ∗ B[$N$]) : $\check{B}_N$
D[$N$] ← IB[$N$] : $v_N^{(1)}$
**for** $i = N-1$ **to** 1 **by** −1 **do**
  SC[$i$] ← C[$i$] ∗ C[$i$] : $c_i^2$
  IB[$i$] ← 1.0/(B[$i$] ∗ B[$i$]) : $\check{B}_i$
  D[$i$] ← IB[$i$] ∗ (SC[$i$] ∗ D[$i+1$] + 1.0) : $v_i^{(1)}$
**end for**
W1 ← IB[1] : $w_1^{(1)}$
W2 ← W1 ∗ D[1] : $w_1^{(2)}$
J ← W2
**for** $i = 2$ **to** $N$ **by** +1 **do**
  FW ← SC[$i-1$] ∗ IB[$i$] : $\tilde{F}_i$
  H1 ← FW ∗ W1 : $\tilde{g}_i^{(1)}$
  W1 ← H1 + IB[$i$] : $w_i^{(1)}$
  W2 ← FW ∗ W2 + (W1 + H1) ∗ D[$i$] : $w_i^{(2)}$
  J ← J + W2
**end for**
**return** J

**Algorithm 12** An implementation of an algorithm for computing the trace $J_3(B)$ with a method based on the old recurrence relations

IB[1] ← 1.0/(B[1] ∗ B[1]) : $\check{B}_1$
D[1] ← IB[1] : $w_1^{(1)}$
**for** $i = 2$ **to** $N$ **by** +1 **do**
  SC[$i-1$] ← C[$i-1$] ∗ C[$i-1$] : $c_{i-1}^2$
  IB[$i$] ← 1.0/(B[$i$] ∗ B[$i$]) : $\check{B}_i$
  D[$i$] ← IB[$i$] ∗ (SC[$i-1$] ∗ D[$i-1$] + 1.0) : $w_i^{(1)}$
**end for**
Z ← 2.0 ∗ D[$N$] : $z_N^{(1)}$
D[$N$] ← IB[$N$] ∗ D[$N$] : $v_N^{(2)}$
R ← IB[$N$] : $v_N^{(1)}$
A[$N$] ← Z − R
**for** $i = N-1$ **to** 1 **by** −1 **do**
  Z ← Z + 2.0 ∗ (D[$i$] − R) : $z_i^{(1)}$
  D[$i$] ← IB[$i$] ∗ (SC[$i$] ∗ D[$i+1$] + Z − D[$i$]) : $v_i^{(2)}$
  R ← IB[$i$] ∗ (SC[$i$] ∗ R + 1.0) : $v_i^{(1)}$
  A[$i$] ← Z − R
**end for**
W ← IB[1] ∗ D[1] : $w_1^{(3)}$
R ← IB[1] ∗ R : $w_1^{(2)}$
Z ← 2.0 ∗ D[1] : $z_1^{(2)}$
J ← W
**for** $i = 2$ **to** $N$ **by** +1 **do**
  Z ← Z + 2.0 ∗ (D[$i$] − R) : $z_i^{(2)}$
  W ← IB[$i$] ∗ (SC[$i-1$] ∗ W + Z − D[$i$]) : $w_i^{(3)}$
  R ← IB[$i$] ∗ (SC[$i-1$] ∗ R + A[$i$]) : $w_i^{(2)}$
  J ← J + W
**end for**
**return** J

**Algorithm 13** An implementation of an algorithm for computing the trace $J_3(B)$ with a method based on the new recurrence relations

H2[1] ← 0.0 : $\tilde{g}_1^{(2)}$
IB[1] ← 1.0/(B[1] ∗ B[1]) : $\check{B}_1$
A[1] ← IB[1] : $\check{B}_1 + 2\tilde{g}_1^{(1)}$
W1[1] ← A[1] : $w_1^{(1)}$
**for** $i = 2$ **to** $N$ **by** +1 **do**
  SC[$i-1$] ← C[$i-1$] ∗ C[$i-1$] : $c_{i-1}^2$
  IB[$i$] ← 1.0/(B[$i$] ∗ B[$i$]) : $\check{B}_i$
  FW[$i$] ← SC[$i-1$] ∗ IB[$i$] : $\tilde{F}_i$
  A[$i$] ← FW[$i$] ∗ W1[$i-1$] : $\tilde{g}_i^{(1)}$
  H2[$i$] ← FW[$i$] ∗ H2[$i-1$] + W1[$i-1$] ∗ A[$i$] : $\tilde{g}_i^{(2)}$
  W1[$i$] ← A[$i$] + IB[$i$] : $w_i^{(1)}$
  A[$i$] ← A[$i$] + W1[$i$] : $\check{B}_i + 2\tilde{g}_i^{(1)}$
**end for**
J ← IB[$N$] : $v_N^{(1)}$
K ← W1[$N$] ∗ J : $v_N^{(2)}$
A[$N$] ← A[$N$] ∗ K + 2.0 ∗ H2[$N$] ∗ J
**for** $i = N-1$ **to** 1 **by** −1 **do**
  FV ← SC[$i$] ∗ IB[$i$] : $F_i$
  G1 ← FV ∗ J : $g_i^{(1)}$
  J ← G1 + IB[$i$] : $v_i^{(1)}$
  K ← FV ∗ K + (J + G1) ∗ W1[$i$] : $v_i^{(2)}$
  A[$i$] ← A[$i$] ∗ K + 2.0 ∗ H2[$i$] ∗ J
**end for**
K ← IB[1] ∗ K : $w_1^{(3)}$
J ← K
**for** $i = 2$ **to** $N$ **by** +1 **do**
  K ← FW[$i$] ∗ K + A[$i$] : $w_i^{(3)}$
  J ← J + K
**end for**
**return** J

of the minimal singular value $\sigma_{\min}(B)$ of $B$, is computed from the trace $J_M(B)$. As is shown in [4], the generalized Newton bounds increase monotonically with increase of $M$, namely, $\theta_M(B)$ of larger $M$ gives a better lower bound of $\sigma_{\min}(B)$. Different from the old recurrence relations in [4], the new recurrence relations are subtraction-free. Namely, they consist only addition, multiplication and division among positive quantities. Therefore, any possibility of cancellation error is clearly excluded.

Computational cost for the trace $J_M(B)$ with the old and the new recurrence relations are shown to be $O(MN)$ and $O(M^2N)$, respectively. In the cases of $M = 2$ and 3, efficient implementations of the algorithms for computing the traces $J_M(B)$ are also performed. Though the order of computational cost for the trace $J_M(B)$ with the new recurrence relations is higher than that with the old recurrence relations, the implementations for $M = 2$ and 3 based on the modified new recurrence relations require less number of operations than those based on the old recurrence relations.

The square of the generalized Newton bound $\theta_M(B)$ of order $M$ can be used as a shift of origin in the dqds algorithm and the mdLVs algorithm which are singular value computation algorithms. Therefore, a shift in terms of $(\theta_M(B))^2$ is named the generalized Newton shift of order $M$. Since $\theta_M(B)$ increases monotonically with increase of $M$, the dqds and the mdLVs algorithms with the generalized Newton shift of higher order $M$ are expected to converge faster. However, such shift itself needs more computational cost than that of lower order $M$. There has to be a trade-off between convergence speed and computational cost.

A shift strategy for the mdLVs algorithm, which utilizes the traces $J_1(B)$ and $J_2(B)$, is discussed in [8]. Another shift strategy for the dqds algorithm, which is advanced from the one in [8] and utilizes the traces $J_1(B)$ and $J_2(B)$, will be discussed in [9]. Asymptotic convergence analysis of the dqds algorithms with the generalized Newton shift and another approach for computing the traces $J_M(B)$ will be discussed in the subsequent papers.

## Appendix

*Proof of Lemma 3.1.1.* First, we discuss in the case of $1 \le i \le N$, $0 \le \rho \le \mu$ and $i + \mu \le j \le N$. When $\rho = \mu$, it is obvious that $S_{i+\mu,j} = 1 \cdot S_{i+\mu,j} = \beta_{i,\mu,\rho} S_{i+\rho,j}$. When $\rho < \mu$, by applying

$$S_{i+1,j} = -\frac{b_i}{c_i} S_{i,j} \qquad (1 \le i < j \le N)$$

in Eq. (33) to $S_{i+\mu,j}$ once or repeatedly, we have the equation $S_{i+\mu,j} = \beta_{i,\mu,\rho} S_{i+\rho,j}$.

Secondly, we discuss the case of $1 \le i \le N$, $0 \le \rho \le \mu \le N - i$ and $1 \le j \le i + \rho$. When $\rho = \mu$, it is obvious that $S_{j,i+\mu} = 1 \cdot S_{j,i+\mu} = \gamma_{i,\mu,\rho} S_{j,i+\rho}$. When $\rho < \mu$, by applying

$$S_{j,i+1} = -\frac{c_i}{b_{i+1}} S_{j,i} \qquad (1 \le j \le i \le N - 1)$$

obtained from Eq. (33) to $S_{j,i+\mu}$ once or repeatedly, we have the equation $S_{j,i+\mu} = \gamma_{i,\mu,\rho} S_{j,i+\rho}$. □

*Proof of Lemma 3.1.2.* When $\xi = \mu$, then it is obvious that $\gamma^2_{i+1,\mu-1,\xi-1} = 1 = \gamma^2_{i,\mu,\xi}$. When $\xi < \mu$, then we have

$$\gamma^2_{i+1,\mu-1,\xi-1} = \prod_{\nu=\xi}^{\mu-1} \tilde{F}_{i+\nu+1} = \prod_{\nu'=\xi+1}^{\mu} \tilde{F}_{i+\nu'} = \gamma^2_{i,\mu,\xi}$$

from Eq. (38). □

*Proof of Lemma 3.1.3.* It holds

$$H^{(0)}_{i,1}(\chi) = \chi_{i,1} = \sum_{\mu=1}^{N-i} \gamma^2_{i,\mu,0}$$

from the definitions (43) and (46).

Eq. (33) and Lemma 3.1.1 lead

$$\begin{aligned} c_i^2 S^2_{i+1,i+\mu} &= c_i^2 \left( -\frac{b_i}{c_i} S_{i,i+\mu} \right)^2 \\ &= b_i^2 (\gamma_{i,\mu,0} S_{i,i})^2 = \gamma^2_{i,\mu,0} \quad (1 \le \mu \le N - i). \end{aligned}$$

Therefore, since $S$ is an upper triangle matrix and $SS^T = V^{(1)}$, we have

$$\begin{aligned} \sum_{\mu=1}^{N-i} \gamma^2_{i,\mu,0} &= \sum_{\mu=1}^{N-i} c_i^2 S^2_{i+1,i+\mu} = c_i^2 \sum_{\mu=1}^{N-i} S_{i+1,i+\mu} S^T_{i+\mu,i+1} \\ &= c_i^2 \sum_{\rho=i+1}^{N} S_{i+1,\rho} S^T_{\rho,i+1} = c_i^2 \sum_{\rho=1}^{N} S_{i+1,\rho} S^T_{\rho,i+1} \\ &= c_i^2 V^{(1)}_{i+1,i+1} = c_i^2 v^{(1)}_{i+1}. \end{aligned}$$ □

*Proof of Lemma 3.1.4.* From Eq. (38), it can be readily verified that

$$\tilde{F}_{i+1} \gamma^2_{i,\mu,1} = \prod_{\nu=1}^{\mu} \tilde{F}_{i+\nu} = \gamma^2_{i,\mu,0}$$

for $1 \le i \le N - 1$ and $1 \le \mu \le N - i$. From this relation and the definition of $\chi_{i,\lambda}$, we have

$$\sum_{\mu=\lambda}^{N-i} \gamma^2_{i,\mu,1} = \tilde{F}^{-1}_{i+1} \sum_{\mu=\lambda}^{N-i} \gamma^2_{i,\mu,0} = \tilde{F}^{-1}_{i+1} \chi_{i,\lambda}$$

for $1 \le i \le N - 1$ and $1 \le \lambda \le N - i$. □

*Proof of Lemma 3.1.5.* For $N - i + 1 \le \lambda \le N$, it is trivial that

$$\chi_{i+1,\lambda-1} = \chi_{i,\lambda} = 0$$

from the definition (46).

For $1 \le \lambda \le N - i$, we have

$$\begin{aligned} \chi_{i+1,\lambda-1} &= \sum_{\mu=\lambda-1}^{N-i-1} \gamma^2_{i+1,\mu,0} = \sum_{\mu=\lambda-1}^{N-i-1} \gamma^2_{i,\mu+1,1} \\ &= \sum_{\mu'=\lambda}^{N-i} \gamma^2_{i,\mu',1} = \tilde{F}^{-1}_{i+1} \chi_{i,\lambda} \end{aligned}$$

with consideration of Lemmas 3.1.2 and 3.1.4. □

*Proof of Lemma 5.1.1.* From Eq. (44) and Definition 2.2.2, it is obvious that

$$\check{B}_N H^{(r-1)}_{N,1}(\chi) = 0 = g^{(r)}_N \qquad (r = 1, 2, \dots). \qquad \square$$

*Proof of Lemma 5.1.2.* For $1 \le i \le N-1$, considering Lemma 3.1.3 and Definition 2.2.2, it holds

$$\check{B}_i H^{(0)}_{i,1}(\chi) = \check{B}_i \cdot c_i^2 v^{(1)}_{i+1} = F_i v^{(1)}_{i+1} = g^{(1)}_i. \qquad \square$$

*Proof of Lemma 5.1.3.* From Definition 2.2.2, we see

$$g^{(r)}_{N-1} = \check{B}_N g^{(r-1)}_{N-1} \qquad (r = 2, 3, \dots). \qquad (65)$$

For $r = 1, 2, \dots$, since it holds

$$\begin{aligned} H^{(r)}_{N-1,1}(\chi) &= h_{N-1,1}(H^{(r-1)}(\chi)) \\ &= \sum_{\mu=1}^{1} \sum_{\xi=1}^{\mu} \check{B}_{N-1+\xi} \gamma^2_{N-1,\mu,\xi} H^{(r-1)}_{N-1,\xi}(\chi) \\ &= \check{B}_N \gamma^2_{N-1,1,1} H^{(r-1)}_{N-1,1}(\chi) \\ &= \check{B}_N H^{(r-1)}_{N-1,1}(\chi), \end{aligned}$$

we have

$$\check{B}_{N-1} H^{(r)}_{N-1,1}(\chi) = \check{B}_N \cdot \check{B}_{N-1} H^{(r-1)}_{N-1,1}(\chi). \qquad (66)$$

It holds $\check{B}_{N-1} H^{(r-1)}_{N-1,1}(\chi) = g^{(r)}_{N-1}$ for $r = 1, 2, \dots$ from Lemma 5.1.2 and Eqs. (65) and (66). $\square$

*Proof of Lemma 5.1.5.* For $r = 1, 2, \dots$, it holds

$$\begin{aligned} h_{i,\lambda}(K^{(r)}) &= h_{i,\lambda}\Bigg( \tilde{F}^{-1}_{i+1} H^{(r)}(\chi) - \check{C}_i H^{(r-1)}(\chi) \\ &\qquad - \check{C}_i \sum_{k=1}^{r} H^{(k-1)}_{i+1,1}(\chi) H^{(r-k)}(\chi) \Bigg) \\ &= \tilde{F}^{-1}_{i+1} H^{(r+1)}_{i,\lambda}(\chi) - \check{C}_i H^{(r)}_{i,\lambda}(\chi) \\ &\quad - \check{C}_i \sum_{k=1}^{r} H^{(k-1)}_{i+1,1}(\chi) H^{(r+1-k)}_{i,\lambda}(\chi) \\ &= K^{(r+1)}_{i,\lambda} + \check{C}_i H^{(r)}_{i+1,1}(\chi) H^{(0)}_{i,\lambda}(\chi). \qquad \square \end{aligned}$$

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