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Abstract

This is a survey on convergence theorems for the differential quotient difference with shifts (dqds) algorithm, which is one of the most efficient methods for computing matrix singular values. Emphasis is laid on the relationship and comparison between the global convergence theorem obtained recently by the present authors and Rutishauser's convergence theorem for the Cholesky LR method with shifts for the positive-definite eigenvalue problem. Theorems on convergence rate of the dqds algorithm with different shift strategies are also reviewed.

1 Introduction

Matrix singular values play important roles in many applications such as the method of least squares, and accordingly numerical methods for computing them are of great practical importance. The singular values of a matrix A are equal to the square roots of the eigenvalues of $A^{\mathrm{T}}A$ and hence an iterative computation is inevitable. Usually, in order to reduce the overall computational cost, the given matrix A is first transformed to a bidiagonal matrix with suitable orthogonal transformations, and then a certain iterative method is applied to the bidiagonal matrix.

Most of the standard methods for bidiagonal matrices had been based on the QR algorithm [7], until in 1994 Fernando–Parlett discovered a beautiful algorithm, which is now called the differential quotient difference with shifts (dqds) algorithm [8]. The dqds algorithm has then drawn strong interest of researchers due to its high accuracy, speed, and numerical stability often observed in actual computations. The algorithm is now available and widely used as DLASQ routine in LAPACK [12, 14].

In spite of this practical success, it is rather recently that the theoretical aspects of the dqds algorithm have been revealed in rigorous manners. To the authors' best knowledge, the global convergence theorem, i.e., a theoretical guarantee of convergence from arbitrary initial matrices, due to the present authors [3, 4] is the first result given in an explicit form.

In this context, however, we may recall two known facts:

(i) the dqds algorithm is mathematically equivalent to the Cholesky LR method with shifts, applied to tridiagonal symmetric matrices, and

(ii) as a classical result in eigenvalue computation we have the global convergence theorem of the Cholesky LR method by Rutishauser in 1960 [16].

One may be tempted to conclude that the above two facts immediately imply the global convergence property of the dqds algorithm. But this is not the case. The situation is not simple but very subtle. Rutishauser's theorem refers to a kind of regularity condition or assumption that a pathological phenomenon called "disorder of latent roots" does not occur. It is one of the major objectives of this paper[1] to give a detailed explanation to this subtle point in convergence argument. Furthermore we show that a complete global convergence result for the dqds algorithm can be obtained from the above two facts if we take in account another classical result on irreducible tridiagonal matrices.

In these two proofs—one by the present authors [3, 4] and the other by combining the known classical results—the former has several desirable features: it is simpler, direct, self-contained, and most importantly, it gives explicit estimates for *all* the elements of the matrices in iteration. This enables us to precisely investigate the asymptotic convergence rates, once a concrete shift strategy is specified. Taking advantage of this feature, the authors have considered the case of the Johnson bound [9], which is a Gershgorin type bound, to find the asymptotic convergence rate of 1.5 [3, 4]. Soon after this, several other authors have considered a variety of shift strategies [1, 2, 6, 22, 23]. These results are reviewed in Section 4 of this paper.

[1] This is an augmented English version of [5] included in a workshop proceedings in Japanese.

2 The dqds algorithm

We assume that the given real matrix A has already been transformed to a bidiagonal matrix

$$B = \begin{pmatrix} b_1 & b_2 & & \\ & b_3 & \ddots & \\ & & \ddots & b_{2m-2} \\ & & & b_{2m-1} \end{pmatrix},$$

to which the dqds algorithm is applied. Furthermore, following [8], we assume without loss of generality that the matrix has been normalized so that it satisfies the following assumption:

> **Assumption (A)** The bidiagonal elements of B are positive: $b_k > 0$ for $k = 1, 2, \dots, 2m-1$.

This assumption guarantees that the singular values of B are all distinct: $\sigma_1 > \cdots > \sigma_m > 0$ (see [13]).

The dqds algorithm in computer program form reads as follows.

Algorithm 1 The dqds algorithm

Require: $q_k^{(0)} := (b_{2k-1})^2$ $(k = 1, 2, \dots, m)$; $e_k^{(0)} := (b_{2k})^2$ $(k = 1, 2, \dots, m-1)$; $t^{(0)} := 0$

```
for n := 0, 1, ··· do
    choose shift s^(n) (≥ 0)
    d_1^(n+1) := q_1^(n) − s^(n)
    for k := 1, ··· , m − 1 do
        q_k^(n+1) := d_k^(n+1) + e_k^(n)
        e_k^(n+1) := e_k^(n) q_{k+1}^(n) / q_k^(n+1)
        d_{k+1}^(n+1) := d_k^(n+1) q_{k+1}^(n) / q_k^(n+1) − s^(n)
    end for
    q_m^(n+1) := d_m^(n+1)
    t^(n+1) := t^(n) + s^(n)
end for
```

The outer loop is terminated when some suitable convergence criterion, say $|e_{m-1}^{(n)}| \leq \epsilon$ for some prescribed constant $\epsilon > 0$, is satisfied. At the termination we have

$$\sigma_m{}^2 \approx q_m^{(n)} + t^{(n)} \left(= q_m^{(n)} + \sum_{l=0}^{n-1} s^{(l)} \right)$$

and hence σ_m can be approximated by $\sqrt{q_m^{(n)} + t^{(n)}}$. Then by the deflation process the problem is shrunk to an $(m-1) \times (m-1)$ problem, and the same procedure is repeated until $\sigma_{m-1}, \dots, \sigma_1$ are obtained in turn.

It is convenient to define a bidiagonal matrix

$$B^{(n)} = \begin{pmatrix} \sqrt{q_1^{(n)}} & \sqrt{e_1^{(n)}} & & \\ & \sqrt{q_2^{(n)}} & \ddots & \\ & & \ddots & \sqrt{e_{m-1}^{(n)}} \\ & & & \sqrt{q_m^{(n)}} \end{pmatrix} \tag{1}$$

to simplify the description of Algorithm 1. With this notation, Algorithm 1 can be rewritten in terms of the Cholesky decomposition (with shifts):

$$(B^{(n+1)})^{\mathrm{T}} B^{(n+1)} = B^{(n)} (B^{(n)})^{\mathrm{T}} - s^{(n)} I. \tag{2}$$

It is also convenient to introduce additional notations:

$$e_0^{(n)} = 0, \quad e_m^{(n)} = 0 \quad (n = 0, 1, \ldots). \tag{3}$$

3 Global convergence theorems of the dqds algorithm

In this section we review the global convergence theorems of the dqds algorithm for arbitrary initial matrices satisfying Assumption (A). We also discuss the relation of the theorem of the present authors [3, 4] and Rutishauser's theorem [16] for the global convergence of the shifted Cholesky LR method for symmetric positive definite matrices.

3.1 Global convergence theorem of the dqds algorithm by Aishima et al.

Here the global convergence theorem of the dqds algorithm recently established by the present authors is shown. The theorem states that, if $0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2$ in each iteration step n, where $\sigma_{\min}^{(n)}$ denotes the smallest singular value of $B^{(n)}$, then the variables in the dqds algorithm converge for any initial matrix B that satisfies Assumption (A). The proof [3, 4], consisting of a sequence of elementary calculations, is reproduced in Appendix A.

Theorem 1 (Global convergence of the dqds algorithm (Aishima *et al.* [3, 4]))**.** *Suppose the initial matrix B satisfies Assumption* (A)*, and the shifts in the dqds algorithm satisfy*

$$0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2 \qquad (n = 0, 1, 2, \ldots). \tag{4}$$

Then

$$\lim_{n\to\infty} e_k^{(n)} = 0 \quad (k = 1, 2, \ldots, m-1),$$
$$\lim_{n\to\infty} q_k^{(n)} + t^{(n)} = {\sigma_k}^2 \quad (k = 1, 2, \ldots, m).$$

The condition (4) is necessary for the Cholesky decomposition of $B^{(n)}(B^{(n)})^{\mathrm{T}} - s^{(n)}I$ in (2) to be well-defined. Conversely, this condition guarantees that the dqds algorithm does not break down, as is seen from (2). Hence Theorem 1 above states that the convergence is always guaranteed as far as the dqds algorithm runs without breakdown.

3.2 Relation to Rutishauser's classical result

The dqds algorithm is mathematically equivalent to the shifted Cholesky LR method applied to symmetric positive-definite irreducible tridiagonal matrices, where a tridiagonal matrix is said to be irreducible if all the subdiagonal elements are nonzero. This might ring a bell of some readers, since for general symmetric positive-definite matrices, we know Rutishauser's global convergence theorem on the shifted Cholesky LR method [16]. In what follows, however, we point out that Theorem 1 cannot be derived directly from Rutishauser's theorem. Furthermore, we point out that Rutishauser's theorem does imply a global convergence result, though weaker than Theorem 1, for the dqds algorithm, when it is combined with another observation about tridiagonal matrices. To the best of the authors' knowledge, there is no reference in the literature where this point is explicitly noted. The proof of Rutishauser's theorem, written in German, can be found in [16]; for readers' convenience, we give a brief English summary in Appendix B.

3.2.1 The shifted Cholesky LR method

The shifted Cholesky LR method for an $m \times m$ positive definite symmetric matrix A reads as follows.

Algorithm 2 The shifted Cholesky LR method

Require: $A^{(0)} := A, \quad t^{(0)} := 0$

for $n := 0, 1, \cdots$ **do**
- choose shift $s^{(n)} (\geq 0)$
- Cholesky decomposition:
  $(R^{(n+1)})^{\mathrm{T}} R^{(n+1)} = A^{(n)} - s^{(n)} I$
  ($R^{(n+1)}$ is upper triangular)
- $A^{(n+1)} := R^{(n+1)} (R^{(n+1)})^{\mathrm{T}}$
- $t^{(n+1)} := t^{(n)} + s^{(n)}$

end for

Let us write the matrix $A^{(n)}$ as

$$A^{(n)} = \left(\begin{array}{c|c} U^{(n)} & \boldsymbol{v}^{(n)} \\ \hline (\boldsymbol{v}^{(n)})^{\mathrm{T}} & w^{(n)} \end{array} \right), \tag{5}$$

where $U^{(n)}$ is the leading principal $(m-1)\times(m-1)$ submatrix of $A^{(n)}$, $\boldsymbol{v}^{(n)}$ is a vector of length $(m-1)$ and $w^{(n)}$ is the diagonal element at the position $(m,\ m)$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$ denote the eigenvalues of A and $\lambda_{\min}^{(n)}$ the smallest eigenvalue of $A^{(n)}$.

Suppose the Cholesky LR method is applied with suitable shifts. Then practically for almost all initial matrices A, $\|\boldsymbol{v}^{(n)}\|$ in (5) tends to 0, and $w^{(n)} + t^{(n)}$ converges to λ_m. Hence an approximation of one eigenvalue can be obtained by setting $\lambda_m \approx w^{(n)} + t^{(n)}$, when $\|\boldsymbol{v}^{(n)}\|$ becomes sufficiently small. Deflation is then carried out to obtain $\lambda_{m-1}, \lambda_{m-2}, \ldots, \lambda_1$ in turn.

3.2.2 Reformulation of Theorem 1 for the shifted Cholesky LR

Comparing the matrix form of the dqds algorithm (2) and the algorithm of the shifted Cholesky LR method, we easily see that "the dqds algorithm for the bidiagonal matrices satisfying Assumption (A)" is mathematically equivalent to "the shifted Cholesky LR method for symmetric positive-definite irreducible tridiagonal matrices." In order to discuss the relationship between the convergence theorem of the dqds algorithm (Theorem 1) and that of the shifted Cholesky LR method for general positive-definite matrices, it is convenient to reformulate Theorem 1 for the shifted Cholesky LR method.

Theorem 2 (Global convergence of the shifted Cholesky LR method for irreducible tridiagonal matrices (Aishima *et al.* [5]))**.** *Suppose A is an irreducible symmetric positive-definite tridiagonal matrix, and the shifts in the Cholesky LR method satisfy*

$$0 \leq s^{(n)} < \lambda_{\min}^{(n)} \qquad (n = 0, 1, 2, \ldots).$$

Then

$$\lim_{n\to\infty} (A^{(n)} + t^{(n)} I) = \mathrm{diag}(\lambda_1, \ldots, \lambda_m).$$

3.2.3 Rutishauser's theorems

This section gives an overview of the global convergence theorems by Rutishauser on the unshifted and shifted Cholesky LR methods. We begin with the unshifted case [15]. The proof is simple and elementary, where the key is to fully utilize the positive-definiteness (see [15, 17, 18]).

Theorem 3 (Global convergence of the *unshifted* Cholesky LR method (Rutishauser [15]))**.** *If the unshifted Cholesky LR method is applied to a symmetric positive-definite matrix A, $A^{(n)}$ converges to a diagonal matrix whose diagonal elements are the eigenvalues of A.*

In most cases the eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$ appear in descending order on the diagonal of $A^{(n)}$, but there exist exceptional cases. Rutishauser called this exceptional phenomenon "disorder of latent roots," and gave a concrete example as follows.

Example 1 ("disorder of latent roots" [15])**.** *Let A be the positive-definite matrix:*

$$A = \begin{pmatrix} 5 & 4 & 1 & 1 \\ 4 & 5 & 1 & 1 \\ 1 & 1 & 4 & 2 \\ 1 & 1 & 2 & 4 \end{pmatrix}$$

whose eigenvalues are 10*,* 5*,* 2*,* 1*. If the unshifted Cholesky LR method is applied to A, $A^{(n)}$ converges to*

$$\begin{pmatrix} 10 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}.$$

Next we proceed to the shifted case. In this case the proof is no longer elementary and many technical tools are involved. The proof of [16], in German, is outlined in Appendix B.

Theorem 4 (Global convergence of the *shifted* Cholesky LR method (Rutishauser [16]))**.** *Suppose A is a symmetric positive-definite matrix for which "disorder of latent roots" does not occur, and whose smallest eigenvalue λ_m is simple: $\lambda_m < \lambda_k$ $(k = 1, \dots, m-1)$. Suppose also that the shifts in the Cholesky LR method satisfy*

$$0 \le s^{(n)} < \lambda^{(n)}_{\min}.$$

For the variables in (5) *we have*

$$\lim_{n\to\infty} (w^{(n)} + t^{(n)}) = \lambda_m,$$
$$\lim_{n\to\infty} \|\boldsymbol{v}^{(n)}\| = 0.$$

Obviously, Theorem 2, which is the Cholesky LR counterpart of the dqds global convergence theorem, cannot be derived immediately from Theorem 4 above. Theorem 4 states the convergence only for the case where "disorder of latent roots" is absent. We would like to find a missing link that connects these two theorems.

Actually the link is provided by the following known result: if the unshifted Cholesky LR method is applied to an irreducible symmetric positive-definite tridiagonal matrix, $A^{(n)}$ converges to a diagonal matrix, and eigenvalues appear properly in descending order (i.e., "disorder" does not occur). This seems to be a classical known fact, but as far as the authors know, there is no explicit statement in the literature. There seems to have been no explicit proof either, although it is not difficult to deduce it from the known result for the dqd algorithm [8] or for the qd algorithm [17, 18]. Thus we see the following fact.

Lemma 1. *The "disorder of latent roots" does not occur in irreducible symmetric positive-definite tridiagonal matrices.*

Combining this and another known fact: "eigenvalues of irreducible tridiagonal matrix are distinct," we finally obtain from Theorem 4 the global convergence theorem below.

Theorem 5 (Global convergence of the *shifted* Cholesky LR method (Rutishauser))**.** *Suppose A is an irreducible symmetric positive-definite tridiagonal matrix, and the shifts in the Cholesky LR method satisfy*

$$0 \leq s^{(n)} < \lambda_{\min}^{(n)} \qquad (n = 0, 1, 2, \ldots).$$

For the variables in (5) *we have*

$$\lim_{n\to\infty} (w^{(n)} + t^{(n)}) = \lambda_m,$$
$$\lim_{n\to\infty} \|\boldsymbol{v}^{(n)}\| = 0.$$

Translated for the dqds algorithm, the theorem reads as follows.

Theorem 6 (Global convergence of the dqds algorithm (Rutishauser))**.** *Suppose the initial matrix B satisfies Assumption* (A)*, and the shifts in the dqds algorithm satisfy*

$$0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2 \qquad (n = 0, 1, 2, \ldots).$$

Then

$$\lim_{n\to\infty} e_{m-1}^{(n)} = 0,$$
$$\lim_{n\to\infty} (q_m^{(n)} + t^{(n)}) = {\sigma_m}^2.$$

Thus a global convergence theorem of the dqds algorithm is obtained through the complicated discussion presented above, which is based on Rutishauser's convergence analysis of the shifted Cholesky LR method. Some experts in this area might have been aware of this proof scenario but, to the best of the authors' knowledge, it has not been explicitly given in the literature. One of the contributions of this paper is, as the authors believe, to give a complete description of this proof scenario for the first time in the literature.

Before concluding this section, we would like to emphasize the differences between Theorem 1 by the present authors and Theorem 6 based on Rutishauser's theorem. First, while the derivation of Theorem 6 is rather complicated, the proof of Theorem 1 is simple and direct. Second and more importantly, Theorem 6 considers the convergence of lower right elements $e_{m-1}^{(n)}$, $q_m^{(n)}$ only. Although this is enough in actual computation which incorporates deflation, we will need to know the behaviors of *all* of the diagonal and subdiagonal elements in order to reveal the theoretical asymptotic convergence rates. To this end, the proof of Theorem 1 is indispensable, where concrete estimates of *all* the elements are given.

4 Shift strategies and their convergence rates

In the previous section, we have seen that the condition (4) is essential for the global convergence (Theorem 1). This condition can be satisfied by various shift strategies. For some shift strategies, precise theoretical asymptotic convergence rates have been revealed in recent years, which we review in this section. In what follows, by "convergence rate of the dqds algorithm" we mean that of the bottom subdiagonal element $e_{m-1}^{(n)}$; this motivated by the stopping criterion $|e_{m-1}^{(n)}| \approx 0$.

4.1 Johnson shift

In order to find a shift satisfying the condition (4): $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$ in Theorem 1, let us look for a lower bound of $(\sigma_{\min}^{(n)})^2$. A possible choice would be the Johnson bound [9], which gives a lower bound of the smallest singular value of a given matrix. The Johnson bound reads

$$\tau_{\mathrm{J}}^{(n)} = \min_{k=1,\ldots,m} \left\{ \sqrt{q_k^{(n)}} - \frac{1}{2}\left(\sqrt{e_{k-1}^{(n)}} + \sqrt{e_k^{(n)}} \right) \right\}. \tag{6}$$

This satisfies $\tau_{\mathrm{J}}^{(n)} < \sigma_{\min}^{(n)}$, but since it can be negative as well, the shift should be chosen as

$$s^{(n)} = \left(\max\{\tau_{\mathrm{J}}^{(n)},\ 0\} \right)^2, \tag{7}$$

which we call the Johnson shift. With this shift, the global convergence of the dqds algorithm is guaranteed by Theorem 1. Furthermore, the convergence rate turns out to be 1.5 as follows.

Theorem 7 (Convergence rate with the Johnson shift (Aishima *et al.* [3, 4])). *For the dqds algorithm with the Johnson shift* (7) *we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}} = \frac{1}{\sqrt{{\sigma_{m-1}}^2 - {\sigma_m}^2}}.$$

Therefore the asymptotic convergence rate is 1.5.

4.2 Ostrowski shift

Yamamoto *et al.* proposes to use an Ostrowski-type lower bound [10], which is tighter [21] than the Johnson bound. The Ostrowski-type lower bound is given by

$$\tau_{\mathrm{O}}^{(n)} = \min_{k=1,\ldots,m} (X_k^{(n)} - Y_k^{(n)}), \tag{8}$$

where

$$X_k^{(n)} = \sqrt{q_k^{(n)} + \frac{1}{4}\left(\sqrt{e_{k-1}^{(n)}} - \sqrt{e_k^{(n)}}\right)^2},$$
$$Y_k^{(n)} = \frac{1}{2}\left(\sqrt{e_{k-1}^{(n)}} + \sqrt{e_k^{(n)}}\right).$$

This bound satisfies[2] $\tau_{\mathrm{O}}^{(n)} < \sigma_{\min}^{(n)}$, but it can be negative. Hence, the shift is determined by

$$s^{(n)} = \left(\max\{\tau_{\mathrm{O}}^{(n)},\ 0\}\right)^2 \tag{9}$$

to assure $0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2$. Then the global convergence of the dqds algorithm is guaranteed by Theorem 1. Furthermore, the convergence rate turns out to be 1.5 as follows.

Theorem 8 (Convergence rate with the Ostrowski shift (Yamamoto *et al.* [23]))**.** *For the dqds algorithm with the Ostrowski shift* (9) *we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}} = \frac{1}{\sqrt{\sigma_{m-1}{}^2 - \sigma_m{}^2}}.$$

Therefore the asymptotic convergence rate is 1.5.

4.3 Brauer shift

In Yamamoto *et al.* [21], it is also proposed to utilize a Brauer-type lower bound [10]. The bound is given by

$$\tau_{\mathrm{B}}^{(n)} = \min_{1\le j\le k\le m} \frac{1}{2}\left(X_{jk}^{(n)} - \sqrt{Y_{jk}^{(n)} + Z_{jk}^{(n)}}\right), \tag{10}$$

where

$$X_{jk}^{(n)} = \sqrt{q_j^{(n)}} + \sqrt{q_k^{(n)}},$$
$$Y_{jk}^{(n)} = (q_j^{(n)} - q_k^{(n)})^2,$$
$$Z_{jk}^{(n)} = (\sqrt{e_{j-1}^{(n)}} + \sqrt{e_j^{(n)}})(\sqrt{e_{k-1}^{(n)}} + \sqrt{e_k^{(n)}}).$$

This bound satisfies $\tau_{\mathrm{B}}^{(n)} < \sigma_{\min}^{(n)}$, but since it can be negative as before, the shift is determined by

$$s^{(n)} = \left(\max\{\tau_{\mathrm{B}}^{(n)},\ 0\}\right)^2 \tag{11}$$

[2]Strictly speaking, we should say $\sigma_{\min}^{(n)} \le \tau_{\mathrm{O}}^{(n)}$. The equality, however, holds rarely in practice (the exceptional cases are discussed in detail in [21, 23]). Furthermore, when the equality holds, the exact singular value is readily obtained. For these reasons we assume $\tau_{\mathrm{O}}^{(n)} < \sigma_{\min}^{(n)}$ here.

to meet the condition $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$. Then the dqds algorithm is convergent by Theorem 1. Furthermore, it can be shown that the convergence rate is "super-1.5" as follows.

Theorem 9 (Convergence rate with the Brauer shift (Yamamoto *et al.* [23]))**.** *For the dqds algorithm with the Brauer shift* (11) *we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}} = 0.$$

Therefore the asymptotic convergence rate is "super-1.5".

4.4 A shift strategy for superquadratic convergence

A shift strategy for superquadratic convergence has been proposed in [2]. Set

$$\tau_{\mathrm{Q}}^{(n)} = \frac{1}{2}\left(X^{(n)} - \sqrt{(X^{(n)})^2 - Y^{(n)}}\right),$$

where

$$\begin{aligned} X^{(n)} &= q_{m-1}^{(n)} + q_m^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)}, \\ Y^{(n)} &= 4q_m^{(n)}(q_{m-1}^{(n)} - e_{m-2}^{(n)}). \end{aligned}$$

Then the shift is determined as follows.

Shift strategy (Q)

$$s^{(n)} = \begin{cases} \tau_{\mathrm{Q}}^{(n)} & (0 < \tau_{\mathrm{Q}}^{(n)} < (\sigma_{\min}^{(n)})^2), \\ 0 & (\text{otherwise}). \end{cases}$$

In view of Theorem 1, we immediately see that the dqds algorithm with the shift strategy (Q) is convergent. It might seem difficult to check whether the condition $\tau_{\mathrm{Q}}^{(n)} < (\sigma_{\min}^{(n)})^2$ is satisfied or not, since $\sigma_{\min}^{(n)}$ is the unknown value to be determined. However, it can be done in the following way: suppose we are at the beginning of the n-th step. Then we execute tentatively one iteration of the dqds algorithm with $s^{(n)} = \tau_{\mathrm{Q}}^{(n)}$, and check if $q_k^{(n+1)} > 0$ $(k = 1, \dots, m)$ or not. The last condition is mathematically equivalent to $\tau_{\mathrm{Q}}^{(n)} < (\sigma_{\min}^{(n)})^2$ [8]. Hence the shift strategy (Q) can be implemented as follows.

1. Execute one iteration of the dqds algorithm with the tentative shift $s^{(n)} = \tau_{\mathrm{Q}}^{(n)}$.

2. If $q_k^{(n+1)} > 0$ $(k = 1, \dots, m)$, then accept this iteration and proceed to the next iteration. Otherwise reject this one iteration, and execute it again with $s^{(n)} = 0$.

In [2], it has been shown that in the dqds algorithm with the shift strategy (Q), $\tau_{\mathrm{Q}}^{(n)}$ is accepted as $s^{(n)}$ for all sufficiently large n. Then, by scrutinizing the asymptotic behaviour of the algorithm with $s^{(n)} = \tau_{\mathrm{Q}}^{(n)} < (\sigma_{\min}^{(n)})^2$, we see the next superquadratic convergence theorem.

Theorem 10 (Superquadratic convergence by the shift strategy (Q) (Aishima *et al.* [2]))**.** *For the dqds algorithm with the shift strategy* (Q)*, we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^2} = 0.$$

Therefore the convergence is asymptotically superquadratic.

4.5 Cubic convergence shift strategy based on Rutishauser's shift

Rutishauser proposed to use the following shift strategy at "the final stage of iterations" [16] in the second step of Algorithm 1 (strictly speaking, he proposed it in the context of the shifted Cholesky LR method).

Shift strategy (R)

1: $e_0^{(n)} := 0$, $\hat{d}_0^{(n)} := 1$
2: **for** $k := 1, \ldots, m-1$ **do**
3: $\quad \hat{d}_k^{(n+1)} := \hat{d}_{k-1}^{(n+1)} q_k^{(n)} / (\hat{d}_{k-1}^{(n+1)} + e_{k-1}^{(n)}) - q_m^{(n)}$
4: **end for**
5: choose shift $s^{(n)} := \hat{d}_{m-1}^{(n+1)} q_m^{(n)} (\hat{d}_{m-1}^{(n+1)} + e_{m-1}^{(n)})$
6: **return**

Furthermore, he showed that if "a certain condition" regarding a constant ϵ with $0 < \epsilon < \sigma_{m-1}{}^2 - \sigma_m{}^2$ (which is a condition that is likely to be satisfied in "the final stage of iterations") is fulfilled at n, then after one iteration of the dqds with the above shift, the subdiagonal element of $B^{(n)}(B^{(n)})^{\mathrm{T}}$ evolves in such a way that

$$|e_{m-1}^{(n+1)} q_m^{(n+1)}| \leq \frac{1}{(\sigma_{m-1}{}^2 - \sigma_m{}^2 - \epsilon)^4} |e_{m-1}^{(n)} q_m^{(n)}|^3. \tag{12}$$

In this sense, the convergence is locally cubic.

Although the study is quite inspiring, the analysis is unfortunately not rigorous enough to justify the "asymptotic" cubic convergence in the strict sense of the word. It is needed to prove that the above condition on ϵ is satisfied consecutively for all sufficiently large n. It must be also made clear when "the final stage of iterations" is reached before the strategy can actually be implemented.

As an answer to these questions, the present authors have designed a concrete shift strategy that guarantees asymptotic cubic convergence based on the shift strategy (R) of Rutishauser.

Shift strategy (C)

$e_0^{(n)} := 0$, $\hat{d}_0^{(n)} := 1$
for $k := 1, \ldots, m-1$ **do**
  $\hat{d}_k^{(n+1)} := \hat{d}_{k-1}^{(n+1)} q_k^{(n)} (\hat{d}_{k-1}^{(n+1)} + e_{k-1}^{(n)}) - q_m^{(n)}$
  if $\hat{d}_k^{(n+1)} \leq 0$ **then**
    choose shift $s^{(n)} := 0$
    return
  end if
end for
choose shift $s^{(n)} := \hat{d}_{m-1}^{(n+1)} q_m^{(n)} (\hat{d}_{m-1}^{(n+1)} + e_{m-1}^{(n)})$
return

The shift strategy (C) satisfies the condition (4) in the global convergence theorem (Theorem 1). Moreover, it is possible to prove that Rutishauser's shift is chosen for all sufficiently large n, and as a consequence, we arrive at the following result.

Theorem 11 (Cubic convergence with shift strategy (C) (Aishima *et al.* [1])). *For the dqds algorithm with the shift strategy* (C), *we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^3} = \frac{1}{({\sigma_{m-1}}^2 - {\sigma_m}^2)^2}.$$

Therefore the convergence is asymptotically cubic.

4.6 Generalized Newton shifts

Recently, Kimura *et al.* have generalized the Newton shift for symmetric tridiagonal matrices [13, 19] and proposed to use it in the dqds algorithm [11].

The original Newton shift, in the context of the dqds algorithm of matrix form (2), is defined by $\tau_{\mathrm{N}}^{(n)} = -\varphi(0)/\varphi'(0)$, where $\varphi(\lambda) = \det(B^{(n)}(B^{(n)})^{\mathrm{T}} - \lambda I)$ is the characteristic polynomial of $B^{(n)}(B^{(n)})^{\mathrm{T}}$. Clearly $-\varphi(0)/\varphi'(0) = [\mathrm{Tr}\,(B^{(n)}(B^{(n)})^{\mathrm{T}})^{-1}]^{-1}$ holds, and thus we immediately see that the Newton shift satisfies the convergence condition (4). The computational cost for $\tau_{\mathrm{N}}^{(n)}$ is $\mathrm{O}(m)$ [19].

Kimura *et al.* have generalized the Newton shift to

$$\tau_{p,\mathrm{N}}^{(n)} = [\mathrm{Tr}\,(B^{(n)}(B^{(n)})^{\mathrm{T}})^{-p}]^{-1/p},$$

where p is any positive integer. This is called the generalized Newton shift of order p.

Obviously

$$0 < \tau_{\mathrm{N}}^{(n)} = \tau_{1,\mathrm{N}}^{(n)} < \tau_{2,\mathrm{N}}^{(n)} < \cdots < (\sigma_{\min}^{(n)})^2,$$

$$\lim_{p\to\infty} \tau_{p,\mathrm{N}}^{(n)} = (\sigma_{\min}^{(n)})^2.$$

Thus the generalized Newton shifts satisfy the convergence condition (4), and are expected to be effective. Although at a first glance it seems expensive, an algorithm of complexity $\mathrm{O}(p\,m)$ has been found to compute $\tau_{p,\mathrm{N}}^{(n)}$ [24].

The next theorem reveals the convergence rate of the dqds algorithm with the generalized Newton shifts $\tau_{p,\mathrm{N}}^{(n)}$.

Theorem 12 (Convergence rate with the generalized Newton shifts (Yamamoto *et al.* [22]))**.** *For the dqds algorithm with the generalized Newton shifts $\tau_{p,\mathrm{N}}^{(n)}$, we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{p+1-\epsilon}} = 0,$$

where ϵ is an arbitrary positive number.

4.7 Superquadratic convergence of the DLASQ routine

The dqds algorithm is now implemented as the DLASQ routine in LAPACK. DLASQ incorporates an extremely sophisticated shift strategy for the best efficiency [14]. In spite of the apparent complications it is possible to show that the shifts always satisfy (4) (hence DLASQ is convergent), and the ultimate convergence rate is superquadratic.

Theorem 13 (Superquadratic convergence of the DLASQ routine (Aishima *et al.* [6]))**.** *For the DLASQ, we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{2}} = 0.$$

Therefore the convergence is asymptotically superquadratic.

5 Conclusion

In this paper, we surveyed known theoretical results on global convergence and convergence rate of the dqds algorithm for computing singular values. Despite their mathematical importance, the theorems have a practical drawback that they deal only with the asymptotic behavior in $n \to \infty$, and do not provide any information about how things go for finite n. Quantitative estimates for finite n, like the Kantorovich theorem for the Newton method [20], remain to be investigated.

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Appendix

A. Proof of Theorem 1 by Aishima et al. [3, 4]

First, we show the following lemma that states that, if $s^{(n)} < (\sigma_{\min}^{(n)})^2$ in each iteration n, then the variables remain positive. Recall that $\sigma_{\min}^{(n)}$ denotes the smallest singular value of $B^{(n)}$.

Lemma 2. *Suppose the dqds algorithm is applied to the matrix B satisfying Assumption* (A). *If $s^{(n)} < (\sigma_{\min}^{(n)})^2$ $(n = 0, 1, 2, \ldots)$, then $(B^{(n)})^{\mathrm{T}} B^{(n)}$ are positive definite, and hence $q_k^{(n)} > 0$ $(k = 1, \ldots, m)$ and $e_k^{(n)} > 0$ $(k = 1, \ldots, m-1)$ for $n = 0, 1, 2, \ldots$.*

Proof. We prove by induction on n. Under Assumption (A), we have $q_k^{(0)} > 0$, $e_k^{(0)} > 0$, and $(B^{(0)})^{\mathrm{T}} B^{(0)}$ is positive definite. Suppose that $(B^{(n)})^{\mathrm{T}} B^{(n)}$ is positive definite and $q_k^{(n)} > 0$, $e_k^{(n)} > 0$. By (2), if $s^{(n)} < (\sigma_{\min}^{(n)})^2$, then $(B^{(n+1)})^{\mathrm{T}} B^{(n+1)}$ is positive definite, because $B^{(n)}(B^{(n)})^{\mathrm{T}} - s^{(n)} I$ is positive definite. Therefore all the diagonal elements of $B^{(n+1)}$ are nonzero ($b_{2k-1}^{(n+1)} \neq 0$) and hence $q_k^{(n+1)} > 0$ due to (2). By line 6 of Algorithm 1, we have $e_k^{(n+1)} > 0$. $\square$

Now, we prove $\lim_{n\to\infty} e_k^{(n)} = 0$. By Lemma 2, we have $e_k^{(n)} > 0$. Therefore it is sufficient to prove $\sum_{n=0}^{\infty} e_k^{(n)} < +\infty$. From Algorithm 1, we see

$$\begin{aligned} q_k^{(n+1)} &= d_{k-1}^{(n+1)} \frac{q_k^{(n)}}{q_{k-1}^{(n+1)}} - s^{(n)} + e_k^{(n)} \\ &= (q_{k-1}^{(n+1)} - e_{k-1}^{(n)}) \frac{q_k^{(n)}}{q_{k-1}^{(n+1)}} - s^{(n)} + e_k^{(n)} \\ &= q_k^{(n)} - e_{k-1}^{(n+1)} + e_k^{(n)} - s^{(n)}, \end{aligned}$$

where the first equality is due to line 5 and line 7, the second equality to line 5, and the last equality to line 6. The equality

$$q_k^{(n+1)} = q_k^{(n)} - e_{k-1}^{(n+1)} + e_k^{(n)} - s^{(n)} \tag{13}$$

appearing above is crucial for the proof of the convergence. Adding both sides of (13) for n, we obtain

$$q_k^{(n+1)} = q_k^{(0)} + \sum_{l=0}^{n} e_k^{(l)} - \sum_{l=0}^{n} e_{k-1}^{(l+1)} - \sum_{l=0}^{n} s^{(l)} \tag{14}$$

for $k = 1, 2, \ldots, m$. Since $q_k^{(n+1)} > 0$ by Lemma 2, it follows that

$$\sum_{l=0}^{n} e_{k-1}^{(l+1)} < q_k^{(0)} + \sum_{l=0}^{n} e_k^{(l)} - \sum_{l=0}^{n} s^{(l)} \le q_k^{(0)} + \sum_{l=0}^{n} e_k^{(l)} \tag{15}$$

for $k = 1, 2, \ldots, m$. Setting $k = m$ in (15), we obtain $\sum_{l=0}^{\infty} e_{m-1}^{(l+1)} \le q_m^{(0)}$, with the aid of (3). Similarly, setting $k = m-1,\ m-2,\ \ldots,\ 2$ in (15), we obtain

$$\sum_{l=0}^{\infty} e_k^{(l+1)} < +\infty \qquad (k = m-1, m-2, \ldots, 1),$$

which completes the proof for $e_k^{(n)}$.

Next, we prove $\lim_{n\to\infty} q_k^{(n)} + t^{(n)} = {\sigma_k}^2$. From (2) and line 10 of Algorithm 1 we see

$$\begin{aligned} &(B^{(n)})^{\mathrm{T}} B^{(n)} \\ &= W^{(n)} \left((B^{(0)})^{\mathrm{T}} B^{(0)} - t^{(n)} I \right) (W^{(n)})^{-1}, \end{aligned} \tag{16}$$

where $W^{(n)} = (B^{(n-1)} \cdots B^{(0)})^{-\mathrm{T}}$ is a nonsingular matrix by Lemma 2. Therefore the eigenvalues of $(B^{(n)})^{\mathrm{T}} B^{(n)}$ are the same as those of $(B^{(0)})^{\mathrm{T}} B^{(0)} - t^{(n)} I$. By the assumption and Lemma 2, $(B^{(n)})^{\mathrm{T}} B^{(n)}$ is a symmetric positive-definite matrix. It then follows from (16) that

$$t^{(n)} < {\sigma_m}^2 \tag{17}$$

holds for any n. From line 10 of Algorithm 1, we see $\{t^{(n)}\}$ is a monotonically increasing sequence, and thus there exists $t^{(\infty)}$ such that

$$t^{(\infty)} \le {\sigma_m}^2. \tag{18}$$

Hence, the right-hand side of (14) converges as $n \to \infty$, and we see $q_k^{(\infty)} = \lim_{n\to\infty} q_k^{(n)}$ exists and satisfies

$$q_k^{(\infty)} = q_k^{(0)} + \sum_{n=0}^{\infty} e_k^{(n)} - \sum_{n=0}^{\infty} e_{k-1}^{(n+1)} - t^{(\infty)}.$$

Because $\lim_{n\to\infty} e_k^{(n)} = 0$, from (16) we have

$$\lim_{n\to\infty} W^{(n)} \left((B^{(0)})^{\mathrm{T}} B^{(0)} - t^{(n)} I \right) (W^{(n)})^{-1}$$
$$= \lim_{n\to\infty} (B^{(n)})^{\mathrm{T}} B^{(n)} = \mathrm{diag}(q_1^{(\infty)}, \cdots, q_m^{(\infty)}),$$

which shows the convergence of the form

$$q_k^{(\infty)} = {\sigma_{p(k)}}^2 - t^{(\infty)} \qquad (k = 1, \ldots, m),$$

where $p(k)$ denotes a permutation of indices k ($k = 1, \ldots, m$). It remains to show that $q_k^{(\infty)} + t^{(\infty)}$ line up in descending order. From line 6 of Algorithm 1, we have

$$e_k^{(n)} = e_k^{(0)} \prod_{l=0}^{n-1} \frac{q_{k+1}^{(l)}}{q_k^{(l+1)}} \qquad (k = 1, \ldots, m-1).$$

Because by assumption all the singular values are distinct, i.e., $\sigma_1 > \cdots > \sigma_m$, the limits $q_1^{(\infty)}, \ldots, q_m^{(\infty)}$ are also distinct. Since $\lim_{n\to\infty} e_k^{(n)} = 0$, we have

$$q_k^{(\infty)} > q_{k+1}^{(\infty)} \qquad (k = 1, 2, \ldots, m-1).$$

This completes the proof of Theorem 1.

B. Proof of Theorem 4 by Rutishauser [16]

From Algorithm 2 we see

$$\begin{aligned} A^{(n)} &= R^{(n)} (R^{(n)})^{\mathrm{T}} R^{(n)} (R^{(n)})^{-1} \\ &= R^{(n)} (A^{(n-1)} - s^{(n-1)} I) (R^{(n)})^{-1}, \end{aligned}$$

where the first equality is due to line 4 and the second equality to line 3. Combining this with line 5 of Algorithm 2, we have[3]

$$A^{(n)} = \Gamma^{(n)} (A - t^{(n)} I) (\Gamma^{(n)})^{-1} \qquad (n = 0, 1, \ldots), \tag{19}$$

where $\Gamma^{(n)} = R^{(n)} R^{(n-1)} \cdots R^{(1)}$. Since $A^{(n)}$ is a symmetric positive-definite matrix and $t^{(n)}$ is nonnegative from Algorithm 2, we have

$$0 \leq t^{(n)} < \lambda_m \qquad (n = 0, 1, \ldots). \tag{20}$$

Recall that $\lambda_1 \geq \cdots \geq \lambda_m$ denote the eigenvalues of A. Let $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_m$ denote the corresponding normalized eigenvectors (${\boldsymbol{z}_i}^{\mathrm{T}} \boldsymbol{z}_i = 1$), and c_i denote the mth element of $\boldsymbol{z}_i$ ($i = 1, \ldots, m$). $Z = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_m]$ is an orthogonal matrix, whose mth row is $(c_1, \ldots, c_m)$. Here we also utilize the expression of $A^{(n)}$ given in (5).

We first prepare the following lemmas.

[3] We define $\Gamma^{(0)} = I$ for convenience.

Lemma 3. *For $n \geq 1$,*

$$(A - t^{(1)}I) \cdots (A - t^{(n)}I) = (\Gamma^{(n)})^{\mathrm{T}} \Gamma^{(n)}. \tag{21}$$

Proof. We see

$$\begin{aligned}
&(R^{(n)})^{\mathrm{T}} R^{(n)} \\
&= A^{(n-1)} - s^{(n-1)} I \\
&= \Gamma^{(n-1)} (A - t^{(n-1)} I)(\Gamma^{(n-1)})^{-1} - s^{(n-1)} I \\
&= \Gamma^{(n-1)} (A - t^{(n)} I)(\Gamma^{(n-1)})^{-1},
\end{aligned}$$

where the first equality is due to line 3 of Algorithm 2, the second to (19), and the last to line 5 of Algorithm 2. Since $R^{(n)} = \Gamma^{(n)}(\Gamma^{(n-1)})^{-1}$ we have

$$A - t^{(n)} I = ((\Gamma^{(n-1)})^{\mathrm{T}} \Gamma^{(n-1)})^{-1} ((\Gamma^{(n)})^{\mathrm{T}} \Gamma^{(n)}),$$

which implies (21). □

Lemma 4. *For $n \geq 1$,*

$$\frac{1}{w^{(1)} \cdots w^{(n)}} = \sum_{k=1}^{m} {c_k}^2 \frac{1}{(\lambda_k - t^{(1)}) \cdots (\lambda_k - t^{(n)})}. \tag{22}$$

Proof. From Lemma 3 we have

$$(\Gamma^{(n)})^{-1} (\Gamma^{(n)})^{-\mathrm{T}} = [(A - t^{(1)} I) \cdots (A - t^{(n)} I)]^{-1}. \tag{23}$$

We will compute the (m, m) elements of both sides.

First we consider the left-hand side. From line 4 of Algorithm 2 we see $w^{(n)} = (r^{(n)}_{mm})^2$, where $r^{(n)}_{mm}$ is the (m, m) element of $R^{(n)}$. On the other hand $(R^{(n)})^{-1}$ is an upper triangular matrix and its (m, m) element is $1/r^{(n)}_{mm}$. Hence, $(\Gamma^{(n)})^{-1}$ is an upper triangular matrix whose (m, m) element is $1/\prod_{l=1}^{n} r^{(l)}_{mm}$. Therefore, the (m, m) element of the left-hand side of (23) is

$$\frac{1}{\prod_{l=1}^{n} (r^{(l)}_{mm})^2} = \frac{1}{\prod_{l=1}^{n} w^{(l)}}. \tag{24}$$

Next, we consider the right-hand side of (23). Let us introduce a diagonal matrix

$$D^{(n)} = \mathrm{diag}(1/(\lambda_1 - t^{(n)}), \ldots, 1/(\lambda_m - t^{(n)})).$$

Then we see $(A - t^{(n)} I)^{-1} = Z D^{(n)} Z^{\mathrm{T}}$. Recall that $Z = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_m]$ is orthogonal, and the mth row of Z is $(c_1, \ldots, c_m)$. Therefore, the right-hand side of (23) is expressed as a matrix product

$$[(A - t^{(1)} I) \cdots (A - t^{(n)} I)]^{-1} = Z (D^{(n)} \cdots D^{(1)}) Z^{\mathrm{T}},$$

the (m,m) element of which is equal to

$$\sum_{k=1}^{m} {c_k}^2 \frac{1}{(\lambda_k - t^{(1)}) \cdots (\lambda_k - t^{(n)})}.$$

This completes the proof. $\square$

We are now in the position to prove Theorem 4. From Lemma 4 we see

$$w^{(n)} = \frac{\displaystyle\sum_{k=1}^{m} {c_k}^2 \frac{1}{(\lambda_k - t^{(1)})(\lambda_k - t^{(2)}) \cdots (\lambda_k - t^{(n-1)})}}{\displaystyle\sum_{k=1}^{m} {c_k}^2 \frac{1}{(\lambda_k - t^{(1)})(\lambda_k - t^{(2)}) \cdots (\lambda_k - t^{(n)})}}.$$

It then follows that

$$\begin{aligned}
& w^{(n)} + t^{(n)} - \lambda_m \\
&= \frac{\displaystyle\sum_{k=1}^{m} {c_k}^2 \frac{\lambda_k - \lambda_m}{(\lambda_k - t^{(1)})(\lambda_k - t^{(2)}) \cdots (\lambda_k - t^{(n)})}}{\displaystyle\sum_{k=1}^{m} {c_k}^2 \frac{1}{(\lambda_k - t^{(1)})(\lambda_k - t^{(2)}) \cdots (\lambda_k - t^{(n)})}} \\
&= \frac{\displaystyle\sum_{k=1}^{m-1} {c_k}^2 (\lambda_k - \lambda_m) \frac{(\lambda_m - t^{(1)}) \cdots (\lambda_m - t^{(n)})}{(\lambda_k - t^{(1)}) \cdots (\lambda_k - t^{(n)})}}{\displaystyle {c_m}^2 + \sum_{k=1}^{m-1} {c_k}^2 \frac{(\lambda_m - t^{(1)}) \cdots (\lambda_m - t^{(n)})}{(\lambda_k - t^{(1)}) \cdots (\lambda_k - t^{(n)})}}. \qquad (25)
\end{aligned}$$

Since the smallest eigenvalue is simple by assumption, there exists a constant $\epsilon > 0$ such that $\lambda_k > \lambda_m + \epsilon$ $(k = 1, \ldots, m-1)$. This implies, in view of (20), that

$$\frac{(\lambda_m - t^{(1)})(\lambda_m - t^{(2)}) \cdots (\lambda_m - t^{(n)})}{(\lambda_k - t^{(1)})(\lambda_k - t^{(2)}) \cdots (\lambda_k - t^{(n)})} < \left(\frac{\lambda_m}{\lambda_m + \epsilon} \right)^n$$

for $k = 1, 2, \ldots, m-1$, which then yields

$$\lim_{n \to \infty} \frac{(\lambda_m - t^{(1)})(\lambda_m - t^{(2)}) \cdots (\lambda_m - t^{(n)})}{(\lambda_k - t^{(1)})(\lambda_k - t^{(2)}) \cdots (\lambda_k - t^{(n)})} = 0.$$

It then follows from (25) that $\lim_{n\to\infty} w^{(n)} + t^{(n)} = \lambda_m$, provided that $c_m \neq 0$.

The condition $c_m \neq 0$ is in fact true under the assumption that "disorder of latent root" does not occur. We show this by contradiction[4], i.e., that if $c_m = 0$ then "disorder of latent root" occurs. Put

$$\hat{m} = \max\{k \mid c_k \neq 0\}.$$

[4]The proof of $c_m \neq 0$ is not given in [16]. The proof here is by the present authors.

If $c_m = 0$, then necessarily $\hat{m} < m$ with $c_{\hat{m}+j} = 0$ $(j = 1, \ldots, m - \hat{m})$. Similarly to (25) we have

$$w^{(n)} + t^{(n)} - \lambda_{\hat{m}} = \frac{\displaystyle\sum_{k=1}^{\hat{m}-1} {c_k}^2 (\lambda_k - \lambda_{\hat{m}}) \frac{(\lambda_{\hat{m}} - t^{(1)}) \cdots (\lambda_{\hat{m}} - t^{(n)})}{(\lambda_k - t^{(1)}) \cdots (\lambda_k - t^{(n)})}}{\displaystyle {c_{\hat{m}}}^2 + \sum_{k=1}^{\hat{m}-1} {c_k}^2 \frac{(\lambda_{\hat{m}} - t^{(1)}) \cdots (\lambda_{\hat{m}} - t^{(n)})}{(\lambda_k - t^{(1)}) \cdots (\lambda_k - t^{(n)})}}.$$

Let us consider in particular the unshifted case with $t^{(n)} = 0$ $(n = 0, 1, \ldots)$. Then the (m, m) element of $A^{(n)}$ converges to $\lambda_{\hat{m}}$ by the same argument as for (25). Since $\lambda_{\hat{m}}$ is not the smallest eigenvalue, this means the "disorder of latent root" does occur in the unshifted Cholesky LR method. This completes the proof of $\lim_{n\to\infty} w^{(n)} + t^{(n)} = \lambda_m$.

Next, we prove $\lim_{n\to\infty} \|\boldsymbol{v}^{(n)}\| = 0$. Let $\mu_1^{(n)} \geq \cdots \geq \mu_{m-1}^{(n)}$ denote the eigenvalues of $U^{(n)} + t^{(n)} I$, which is the $(m-1) \times (m-1)$ leading principal submatrix of $A^{(n)} + t^{(n)} I$. Obviously,

$$\mu_k^{(n)} \leq \lambda_k \qquad (k = 1, \ldots, m-1). \tag{26}$$

Moreover, we see

$$\mathrm{Tr}(A^{(n)} + t^{(n)} I) = \sum_{k=1}^{m} \lambda_k = \sum_{k=1}^{m-1} \mu_k^{(n)} + w^{(n)} + t^{(n)}.$$

It follows that

$$\sum_{k=1}^{m-1} (\lambda_k - \mu_k^{(n)}) = w^{(n)} + t^{(n)} - \lambda_m. \tag{27}$$

From the convergence of the diagonal element:

$$\lim_{n\to\infty} w^{(n)} + t^{(n)} = \lambda_m,$$

we have

$$\lim_{n\to\infty} (\lambda_k - \mu_k^{(n)}) = 0 \quad (k = 1, \ldots, m-1). \tag{28}$$

Hence, there exist two constants $f < g$ such that

$$w^{(n)} + t^{(n)} \;<\; f, \tag{29}$$

$$\mu_k^{(n)} \;>\; g \quad (k = 1, \ldots, m-1) \tag{30}$$

for all sufficiently large n.

Let us write $R^{(n)}$ as

$$R^{(n)} = \left(\begin{array}{c|c} P^{(n)} & \boldsymbol{q}^{(n)} \\ \hline 0 & r^{(n)} \end{array}\right), \tag{31}$$

similarly to (5). From line 3 of Algorithm 2, we see

$$\begin{aligned} (P^{(n+1)})^{\mathrm{T}} P^{(n+1)} &= U^{(n)} - s^{(n)} I, \\ \boldsymbol{q}^{(n+1)} &= (P^{(n+1)})^{-\mathrm{T}} \boldsymbol{v}^{(n)}, \\ (r^{(n+1)})^2 &= w^{(n)} - s^{(n)} - (\boldsymbol{q}^{(n+1)})^{\mathrm{T}} \boldsymbol{q}^{(n+1)}, \end{aligned}$$

and from line 4 we see

$$\begin{aligned} \boldsymbol{v}^{(n+1)} &= r^{(n+1)} \boldsymbol{q}^{(n+1)}, \\ w^{(n+1)} &= (r^{(n+1)})^2. \end{aligned}$$

Therefore, we see

$$\begin{aligned} &\|\boldsymbol{v}^{(n+1)}\|^2 \\ &= (r^{(n+1)})^2 (\boldsymbol{q}^{(n+1)})^{\mathrm{T}} \boldsymbol{q}^{(n+1)} \\ &= w^{(n+1)} (\boldsymbol{v}^{(n)})^{\mathrm{T}} (P^{(n+1)})^{-1} (P^{(n+1)})^{-\mathrm{T}} \boldsymbol{v}^{(n)} \\ &= w^{(n+1)} (\boldsymbol{v}^{(n)})^{\mathrm{T}} (U^{(n)} - s^{(n)} I)^{-1} \boldsymbol{v}^{(n)}. \end{aligned}$$

The eigenvalues of $U^{(n)} - s^{(n)} I$ are $\mu_k^{(n)} - t^{(n+1)}$ $(k = 1, \ldots, m-1)$ because those of $U^{(n)} + t^{(n)} I$ are $\mu_k^{(n)}$ $(k = 1, \ldots, m-1)$. Hence, by using (29), (30), together with the equality above, we see

$$\|\boldsymbol{v}^{(n+1)}\|^2 < \frac{f - t^{(n+1)}}{g - t^{(n+1)}} \|\boldsymbol{v}^{(n)}\|^2.$$

From the condition (20), we finally obtain

$$\|\boldsymbol{v}^{(n+1)}\|^2 < \frac{f - t^{(n+1)}}{g - t^{(n+1)}} \|\boldsymbol{v}^{(n)}\|^2 \leq \frac{f}{g} \|\boldsymbol{v}^{(n)}\|^2. \tag{32}$$

This means that $\|\boldsymbol{v}^{(n)}\|$ converges to 0. This completes the proof of Theorem 4.

Remark 1. *In the original article [16], the accumulated shift is assumed to satisfy*

$$-M < t^{(n)} < \lambda_m \qquad (n = 0, 1, \ldots) \tag{33}$$

for some prescribed constant $M > 0$. The condition (33) *is weaker than* (20) *employed in the proof presented above. We employed the latter condition* *since we see no practical advantage in choosing negative shifts (which necessarily slows down the convergence). It is noted, however, that the proof goes almost the same way for* (33). *We also note that the inequality (15) in [16]:*

$$|v_{s+1}|^2 < \frac{f - z_{s+1}}{g - z_{s+1}}|v_s|^2 < \frac{M + \lambda_n}{M + \lambda_n + g - f}|v_s|^2$$

is incorrect. The correct inequality is

$$|v_{s+1}|^2 < \frac{f - z_{s+1}}{g - z_{s+1}}|v_s|^2 < \frac{f + M}{g + M}|v_s|^2.$$

The inequality (32) *above is rectified along this line.* ■

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