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Abstract

Convergence theorems are established with mathematical rigour for the differential quotient difference with shift (dqds) algorithm for the computation of singular values of bidiagonal matrices. Global convergence is guaranteed under a fairly general assumption on the shift, and the asymptotic rate of convergence is 1.5 for the Johnson bound shift. Numerical examples support these theoretical results.

1 Introduction

Every $n \times m$ real matrix A with $\mathrm{rank}(A) = r$ can be decomposed into

$$A = U\Sigma V^{\mathrm{T}}$$

with suitable orthogonal matrices $U \in \mathbf{R}^{n\times n}$ and $V \in \mathbf{R}^{m\times m}$, where

$$\Sigma = \begin{pmatrix} D & O_{r,m-r} \\ O_{n-r,r} & O_{n-r,m-r} \end{pmatrix}, \qquad D = \mathrm{diag}(\sigma_1, \ldots, \sigma_r),$$

and $\sigma_1 \geq \cdots \geq \sigma_r > 0$. The notation $O_{k,l}$ means a $k \times l$ zero matrix. The nonzero diagonal elements $\sigma_1, \ldots, \sigma_r$ are the singular values of A, which play important roles in application areas. Accordingly, numerical methods for computing singular values are of great importance in practice.

The singular values of A are equal to the square roots of the eigenvalues of $A^{\mathrm{T}}A$ and hence an iterative computation is inevitable for singular values. Usually, the given matrix A is first transformed to a bidiagonal matrix to reduce the overall computational cost. In the case of $n \geq m$, for example, the matrix A can be transformed, with appropriate orthogonal matrices $\tilde{U} \in \mathbf{R}^{n\times n}$ and $\tilde{V} \in \mathbf{R}^{m\times m}$, as

$$\tilde{U}^{\mathrm{T}} A \tilde{V} = \begin{pmatrix} B \\ O_{n-m,m} \end{pmatrix},$$

where $B \in \mathbf{R}^{m\times m}$ is an upper bidiagonal matrix. The singular values of B coincide with those of A.

Most of the current methods for computing singular values of diagonal matrices are based on the QR algorithm [2]. In 1990 Demmel and Kahan were awarded the second SIAM prize in numerical linear algebra for their improvement on the QR algorithm [3]. Their algorithm is open to the public as DBDSQR in LAPACK [1, 10].

In relation to the study of this algorithm, the differential quotient difference (dqd) algorithm was proposed by Fernando–Parlett [7] in 1994, with subsequent introduction of shifts to accelerate the convergence. This algorithm is now called the differential quotient difference with shift (dqds) algorithm. The dqds algorithm has received majority support due to its accuracy, speed and numerical stability, and is implemented as DLASQ in LAPACK. The dqds is integrated into Multiple Relatively Robust Representations (MR^3) algorithm [4, 5, 6].

In contrast to remarkable practical success, a number of fundamental theoretical questions still remain unanswered with the dqds algorithm. First, no convergence theorem has been established with full mathematical rigour when shifts are incorporated, although the dqd algorithm, a version of the dqds *without* employing shifts, has been analyzed successfully in [7]. Second, no satisfactory analysis of the convergence rate is available. It is certainly true that locally quadratic or cubic convergence has been discussed in [7] under certain assumptions, but the assumptions are not plausible and it is not clear (at least to the present authors) how the assumptions are to be satisfied.

The objective of this paper is to establish two convergence results for the dqds algorithm with mathematical rigour. The first result (Theorem 4.1) shows that the dqds always converges as far as the shift satisfies a certain natural condition. The second result (Theorem 5.1) shows that, if the shift is determined by the Johnson bound [9], the asymptotic rate of convergence is 1.5.

2 Notation

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

$$B = \begin{pmatrix} b_1 & b_2 & & \\ & b_3 & \ddots & \\ & & \ddots & b_{2m-2} \\ & & & b_{2m-1} \end{pmatrix}. \qquad (1)$$

Following [7], we assume

> **Assumption (A)** The bidiagonal elements of B are nonzero, i.e., $b_k \neq 0$ for $k = 1, \ldots, 2m-1$.

This assumption guarantees (see [12]) that the singular values of B are all distinct: $\sigma_1 > \cdots > \sigma_m > 0$.

Assumption (A) is not restrictive, in theory or in practice. In fact, if a subdiagonal element is zero, i.e., $b_{2k} = 0$ for some k, then the problem reduces to two independent problems on matrices of smaller sizes, $k \times k$ and $(m-k) \times (m-k)$. If there is a zero element in the diagonal, several iterations of the dqd algorithm (i.e., the dqds algorithm without shifts) suffice to remove the diagonal zero, and the problem is again separated into a set of smaller problems (see [7] for details).

In our problem setting we have assumed real matrices, whereas the singular value decomposition is also defined for complex matrices. Our restriction to real matrices is justified by the fact that any complex matrix can be transformed to a real bidiagonal matrix by, say, (complex) Householder transformations, while keeping its singular values [7].

3 The dqds algorithm

In this section, the dqds and related algorithms are summarized. Before describing the dqds algorithm, we review the pqds algorithm, which is mathematically equivalent to the dqds and serves as the main target in the subsequent theoretical analysis. The pqds algorithm is the pqd algorithm where shifts are incorporated to accelerate the convergence [8, 14]. The pqd algorithm consists of the so-called *rhombus rules* (Figure 1).

Algorithm 3.1 The pqds algorithm

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

for $n := 0, 1, \cdots$ **do**
  choose shift $s^{(n)} (\geq 0)$
  $e_0^{(n+1)} := 0$
  for $k := 1, \cdots, m-1$ **do**
    $q_k^{(n+1)} := q_k^{(n)} - e_{k-1}^{(n+1)} + e_k^{(n)} - s^{(n)}$
    $e_k^{(n+1)} := e_k^{(n)} q_{k+1}^{(n)} / q_k^{(n+1)}$
  end for
  $q_m^{(n+1)} := q_m^{(n)} - e_{m-1}^{(n+1)} - s^{(n)}$
end for

The pqds algorithm, in computer program form, is shown in Algorithm 3.1. The outermost 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

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

and hence σ_m can be approximated by $\sqrt{q_m^{(n)} + \sum_{l=0}^{n-1} s^{(l)}}$. Then by the deflation process the problem is shrunk to an $(m-1) \times (m-1)$ problem, and the same procedure is repeated until $\sigma_{m-1}, \ldots, \sigma_1$ are obtained in turn.

It turns out to be convenient to introduce additional notations $e_0^{(n)}$ and $e_m^{(n)}$ with "boundary conditions":

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

to simplify the expression of the algorithm.

Put

$$B^{(n)} = \begin{pmatrix} b_1^{(n)} & b_2^{(n)} & & \\ & b_3^{(n)} & \ddots & \\ & & \ddots & b_{2m-2}^{(n)} \\ & & & b_{2m-1}^{(n)} \end{pmatrix}, \tag{4}$$

$b_k^{(0)} = b_k$ $(k = 1, 2, \ldots, 2m-1)$, and

$$q_k^{(n)} = (b_{2k-1}^{(n)})^2 \quad (k = 1, 2, \ldots, m;\ n = 0, 1, \ldots), \tag{5}$$

$$e_k^{(n)} = (b_{2k}^{(n)})^2 \quad (k = 1, 2, \ldots, m-1;\ n = 0, 1, \ldots). \tag{6}$$

Then Algorithm 3.1 can be rewritten in terms of the Cholesky decomposition (with shifts):

$$(B^{(n+1)})^{\mathrm{T}} B^{(n+1)} = B^{(n)} (B^{(n)})^{\mathrm{T}} - s^{(n)} I, \tag{7}$$

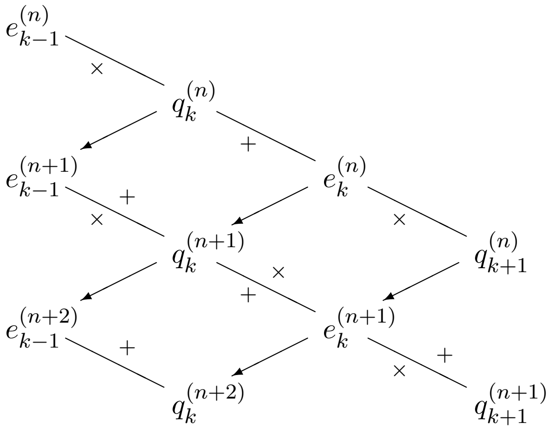

Figure 1: The rhombus rules

where $B^{(0)} = B$. It follows that

$$(B^{(n)})^{\mathrm{T}} B^{(n)} = W^{(n)} \left((B^{(0)})^{\mathrm{T}} B^{(0)} - \sum_{l=0}^{n-1} s^{(l)} I \right) (W^{(n)})^{-1}, \tag{8}$$

where $W^{(n)} = (B^{(n-1)} \cdots B^{(0)})^{-\mathrm{T}}$ is a nonsingular matrix (see Lemma 3.1). Therefore the eigenvalues of $(B^{(n)})^{\mathrm{T}} B^{(n)}$ are the same as those of $(B^{(0)})^{\mathrm{T}} B^{(0)} - \sum_{l=0}^{n-1} s^{(l)} I$. In actual computation it is often observed that $B^{(n)}$ converges to a diagonal matrix as $n \to \infty$, and then, by (8), the singular values of B can be obtained from the diagonal elements of $B^{(n)}$ with sufficiently large n. We give a theoretical proof for the global convergence in the next section.

The following lemma states that, if $s^{(n)} < (\sigma_{\min}^{(n)})^2$ in each iteration n, where $\sigma_{\min}^{(n)}$ is the smallest singular value of $B^{(n)}$, then the variables in the pqds algorithm are always positive so that the algorithm does not break down.

Lemma 3.1 (Positivity of the variables in the pqds algorithm)**.** *Suppose the pqds algorithm is applied to the matrix B satisfying Assumption* (A)*. If $s^{(n)} < (\sigma_{\min}^{(n)})^2$ $(n = 0, 1, 2, \ldots)$, then $(B^{(n)})^{\mathrm{T}} B^{(n)}$ $(n = 1, 2, \ldots)$ are positive definite, and hence $q_k^{(n)} > 0$ $(k = 1, \ldots, m)$ and $e_k^{(n)} > 0$ $(k = 1, \ldots, m-1)$.*

Proof. We prove by induction. Uuder Assumption (A), we have $q_k^{(0)} > 0$, $e_k^{(0)} > 0$ and that $(B^{(0)})^{\mathrm{T}} B^{(0)}$ is positive definite. Suppose that $(B^{(n)})^{\mathrm{T}} B^{(n)}$ is positive definite and $q_k^{(n)} > 0$, $e_k^{(n)} > 0$. By (7), 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 are nonzero ($b_{2k-1}^{(n+1)} \neq 0$) and hence $q_k^{(n+1)} > 0$ because of (5). By the 6th line of Algorithm 3.1, we have $e_k^{(n+1)} > 0$. $\square$

The dqds algorithm is obtained from the pqds algorithm by introducing the auxiliary quantities $d_k^{(n+1)}$ defined as follows [7]:

$$d_1^{(n+1)} = q_1^{(n)} - s^{(n)}; \quad d_k^{(n+1)} = q_k^{(n)} - e_{k-1}^{(n+1)} - s^{(n)} \quad (k = 2, \ldots, m). \quad (9)$$

The resulting algorithm is presented as Algorithm 3.2. Generally, the dqds algorithm outperforms the pqds algorithm. Since the variables of the dqds algorithm are positive (see Lemma 3.2) and no subtractions are used in the algorithm except for computing the shifts, the numerical instability due to loss of significant digits is less likely to happen in the dqds algorithm.

Algorithm 3.2 The dqds algorithm

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

1: **for** $n := 0, 1, \cdots$ **do**
2: choose shift $s^{(n)}(\geq 0)$
3: $d_1^{(n+1)} := q_1^{(n)} - s^{(n)}$
4: **for** $k := 1, \cdots, m-1$ **do**
5: $q_k^{(n+1)} := d_k^{(n+1)} + e_k^{(n)}$
6: $e_k^{(n+1)} := e_k^{(n)} q_{k+1}^{(n)} / q_k^{(n+1)}$
7: $d_{k+1}^{(n+1)} := d_k^{(n+1)} q_{k+1}^{(n)} / q_k^{(n+1)} - s^{(n)}$
8: **end for**
9: $q_m^{(n+1)} := d_m^{(n+1)}$
10: **end for**

Lemma 3.2 (Positivity of the variables in the dqds algorithm)**.** *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 $(B^{(n)})^{\mathrm{T}} B^{(n)}$ $(n = 1, 2, \ldots)$ are positive definite, and hence $q_k^{(n)} > 0$ $(k = 1, \ldots, m)$, $e_k^{(n)} > 0$ $(k = 1, \ldots, m-1)$, and $d_k^{(n)} > 0$ $(k = 1, \ldots, m)$.*

Proof. By Lemma 3.1, we have $e_k^{(n)} > 0$ and $q_k^{(n)} > 0$. The inequality $d_k^{(n)} > 0$ is proved by contradiction as follows. If we had $d_k^{(n)} \leq 0$ for some k, we would have $d_{k+1}^{(n)} \leq 0$ by the 7th line of Algorithm 3.2 and then $q_m^{(n)} = d_m^{(n)} \leq 0$. This contradicts $q_m^{(n)} > 0$. □

4 Convergence of the dqds

In this section, we prove that, for any matrix B that satisfies Assumption (A), the variables $q_k^{(n)}$ and $e_k^{(n)}$ in the dqds algorithm converge as far as the shift is chosen such that $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$, where $\sigma_{\min}^{(n)}$ is the smallest singular value of $B^{(n)}$. Since the dqds and pqds algorithms are equivalent, we will work with the pqds in place of the dqds in the proofs.

The next theorem establishes the convergence of the dqds. Moreover, the theorem states that the variables $q_k^{(n)}$ converge to the square of the singular values minus the sum of the shifts, and that they are placed in the descending order.

Theorem 4.1 (Convergence of the dqds algorithm)**.** *Suppose the matrix B satisfies Assumption* (A)*, and the shift in the dqds algorithm is taken so that* $0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2$ *holds. Then*

$$\sum_{n=0}^{\infty} s^{(n)} \le {\sigma_m}^2. \tag{10}$$

Moreover,

$$\lim_{n\to\infty} e_k^{(n)} = 0 \quad (k = 1, 2, \ldots, m-1), \tag{11}$$

$$\lim_{n\to\infty} q_k^{(n)} = {\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)} \quad (k = 1, 2, \ldots, m). \tag{12}$$

In matrix form, we have

$$\lim_{n\to\infty} (B^{(n)})^{\mathrm{T}} B^{(n)} = \mathrm{diag}\left({\sigma_1}^2 - \sum_{n=0}^{\infty} s^{(n)}, \ldots, {\sigma_m}^2 - \sum_{n=0}^{\infty} s^{(n)} \right).$$

Proof. On the basis of the equivalence between the dqds algorithm and the pqds algorithm, we show the convergence of the pqds to prove this theorem.

By the assumption and Lemma 3.1, $(B^{(n)})^{\mathrm{T}} B^{(n)}$ is a positive symmetric matrix. It then follows from (8) that

$$\sum_{n=0}^{N} s^{(n)} < {\sigma_m}^2 \tag{13}$$

holds for any $N \ge 1$. In the limit of $N \to \infty$, we obtain (10).

Next we prove $\lim_{n\to\infty} e_k^{(n)} = 0$. By Lemma 3.1, we have $e_k^{(n)} > 0$. Therefore it is sufficient to prove $\sum_{n=0}^{\infty} e_k^{(n)} < +\infty$. Adding both sides of the 5th line of Algorithm 3.1 for over n with k fixed, we obtain

$$q_k^{(n+1)} = q_k^{(0)} + \sum_{l=0}^{n} e_k^{(l)} - \sum_{l=0}^{n} e_{k-1}^{(l+1)} - \sum_{l=0}^{n} s^{(l)} \quad (k = 1, 2, \ldots, m). \tag{14}$$

Since $q_k^{(n+1)} > 0$ by Lemma 3.1, it follows that

$$\sum_{l=0}^{n} e_{k-1}^{(l+1)} < q_k^{(0)} + \sum_{l=0}^{n} e_k^{(l)} - \sum_{l=0}^{n} s^{(l)} \le q_k^{(0)} + \sum_{l=0}^{n} e_k^{(l)} \quad (k = 1, 2, \ldots, m). \tag{15}$$

Setting $k = m$ in (15), we obtain $\sum_{l=0}^{\infty} e_{m-1}^{(l+1)} \leq q_k^{(0)}$, with the aid of the boundary conditions (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 (12). By (14) with $n \to \infty$, we see

$$\lim_{n\to\infty} q_k^{(n)} = q_k^{(0)} + \lim_{n\to\infty} \sum_{l=0}^{n} e_k^{(l)} - \lim_{n\to\infty} \sum_{l=0}^{n} e_{k-1}^{(l+1)} - \lim_{n\to\infty} \sum_{l=0}^{n} s^{(l)}. \tag{16}$$

Since the right-hand side of the equation (16) converges, $q_k^{(\infty)} = \lim_{n\to\infty} q_k^{(n)}$ exists. Because $\lim_{n\to\infty} e_k^{(n)} = 0$, (8) reads

$$\begin{aligned} &\lim_{n\to\infty} W^{(n)} \left((B^{(0)})^{\mathrm{T}} B^{(0)} - \sum_{l=0}^{n-1} s^{(l)} I \right) (W^{(n)})^{-1} \\ &= \lim_{n\to\infty} (B^{(n)})^{\mathrm{T}} B^{(n)} = \mathrm{diag}(q_1^{(\infty)}, \cdots, q_m^{(\infty)}), \end{aligned}$$

which shows the convergence as a set, i.e.,

$$\{q_1^{(\infty)}, \ldots, q_m^{(\infty)}\} = \{{\sigma_1}^2 - \sum_{n=0}^{\infty} s^{(n)}, \ldots, {\sigma_m}^2 - \sum_{n=0}^{\infty} s^{(n)}\},$$

where it is not claimed here that $q_k^{(\infty)} = {\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)}$ for each k. It remains to show that $q_k^{(\infty)}$ are in the descending order. From the 6th line of Algorithm 3.1, we have

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

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

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

□

The next theorem states the asymptotic rate of convergence of the dqds algorithm.

Theorem 4.2 (Rate of convergence of the dqds algorithm)**.** *Under the same assumption as in Theorem* 4.1*, we have*

$$\lim_{n\to\infty} \frac{e_k^{(n+1)}}{e_k^{(n)}} = \frac{{\sigma_{k+1}}^2 - \sum_{n=0}^{\infty} s^{(n)}}{{\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)}} \qquad (k = 1, \ldots, m-1). \tag{17}$$

Therefore, for each $k = 1, \ldots, m-2$, $e_k^{(n)}$ is always of linear convergence as $n \to \infty$. If ${\sigma_m}^2 - \sum_{n=0}^{\infty} s^{(n)} > 0$, then $e_{m-1}^{(n)}$ is also of linear convergence, and it is of superlinear convergence if ${\sigma_m}^2 - \sum_{n=0}^{\infty} s^{(n)} = 0$.

Proof. From the 6th line of Algorithm 3.1, we have

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

Then the claim is obvious from Theorem 4.1. □

5 Convergence rate of the dqds with the Johnson bound

In this section, we prove that the asymptotic rate of convergence of the dqds algorithm is 1.5 if the shift is determined by the Johnson bound [9]. In the proofs we will work with the pqds in place of the dqds, as we did in the previous section.

Though the Johnson bound is valid for a general matrix, we present here its version for a bidiagonal matrix B.

Lemma 5.1 (Johnson bound [9])**.** *For a matrix B of the form* (1)*, define*

$$\lambda = \min_{k=1,\ldots,m} \left\{ \mid b_{2k-1} \mid - \frac{\mid b_{2k-2} \mid + \mid b_{2k} \mid}{2} \right\},$$

where $b_0 = b_{2m} = 0$ and let σ_m denote the smallest singular value of B. Then $\sigma_m \geq \lambda$. Moreover, if the subdiagonal elements $(b_2, b_4, \ldots, b_{2m-2})$ are nonzero, then $\sigma_m > \lambda$.

With reference to (4), (5) and (6) we define the shift by the Johnson bound as follows:

$$\lambda^{(n)} = \min_{k=1,\ldots,m} \left\{ \sqrt{q_k^{(n)}} - \frac{1}{2}\left(\sqrt{e_{k-1}^{(n)}} + \sqrt{e_k^{(n)}} \right) \right\}, \tag{18}$$

$$s^{(n)} = \left(\max\{\lambda^{(n)},\ 0\} \right)^2. \tag{19}$$

This choice of the shift guarantees the condition $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$ in each iteration n, and hence the dqds is convergent by Theorem 4.1. The precise rate of convergence can be revealed through a scrutiny of the shift.

The next lemma shows that the Johnson bound $\lambda^{(n)}$ is determined solely by $q_m^{(n)}$ and $e_{m-1}^{(n)}$ when n is large enough. As a corollary of this fact we see that $q_m^{(n)}$ approaches zero.

Lemma 5.2. *Under Assumption* (A)*, consider the dqds with the shift* (19)*. For all sufficiently large n, we have*

$$\lambda^{(n)} = \sqrt{q_m^{(n)}} - \frac{1}{2}\sqrt{e_{m-1}^{(n)}}. \tag{20}$$

That is to say, the minimum of the right-hand side of (18) *is attained at $k = m$.*

Proof. Let $k < m$ and consider the identity

$$\left[\sqrt{q_k^{(n)}} - \frac{1}{2}\left(\sqrt{e_{k-1}^{(n)}} + \sqrt{e_k^{(n)}}\right)\right] - \left[\sqrt{q_m^{(n)}} - \frac{1}{2}\left(\sqrt{e_{m-1}^{(n)}} + \sqrt{e_m^{(n)}}\right)\right]$$
$$= \left(\sqrt{q_k^{(n)}} - \sqrt{q_m^{(n)}}\right) - \frac{1}{2}\left(\sqrt{e_{k-1}^{(n)}} + \sqrt{e_k^{(n)}} - \sqrt{e_{m-1}^{(n)}} - \sqrt{e_m^{(n)}}\right).$$

From Theorem 4.1, the first term on the right-hand side remains positive:

$$\lim_{n\to\infty}\left(\sqrt{q_k^{(n)}} - \sqrt{q_m^{(n)}}\right) = \sqrt{{\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)}} - \sqrt{{\sigma_m}^2 - \sum_{n=0}^{\infty} s^{(n)}} > 0,$$

while the second term vanishes since $\lim_{n\to\infty} e_k^{(n)} = 0$ for each k. Thus the minimum on the right-hand side of (18) is attained at $k = m$. □

Lemma 5.3. *Under the same assumption as in Lemma* 5.2*, we have*

$$\sum_{n=0}^{\infty} s^{(n)} = {\sigma_m}^2, \tag{21}$$

$$\lim_{n\to\infty} q_k^{(n)} = {\sigma_k}^2 - {\sigma_m}^2 \quad (k = 1, \ldots, m-1); \qquad \lim_{n\to\infty} q_m^{(n)} = 0. \tag{22}$$

Proof. By (20) and (11), $\lim_{n\to\infty} \lambda^{(n)} = \lim_{n\to\infty} \sqrt{q_m^{(n)}} \geq 0$, and hence

$$\lim_{n\to\infty} s^{(n)} = \lim_{n\to\infty} (\max\{\lambda^{(n)}, 0\})^2 = \lim_{n\to\infty} q_m^{(n)}.$$

Since $\lim_{n\to\infty} s^{(n)} = 0$ by (10), we have $\lim_{n\to\infty} q_m^{(n)} = 0$. This, together with (12), proves (21) and (22). □

The next lemma shows $\lambda^{(n)} > 0$ for all sufficiently large n.

Lemma 5.4 (Positivity of the Johnson bound in the dqds)**.** *Under the same assumption as in Lemma* 5.2*, there exists an integer* N *such that* $\lambda^{(n)} > 0$ *for all* $n > N$*.*

Proof. The proof consists of showing two facts: (i) For every integer N', there exists $n > N'$ such that $\lambda^{(n)} > 0$; (ii) There exists an integer N'' such that $\lambda^{(n)} > 0$ with $n > N''$ implies $\lambda^{(n+1)} > 0$.

(i) The proof is done by contradiction. Suppose that there exists some N' satisfying $\lambda^{(n)} = 0$ ($\forall n > N'$). Then $s^{(n)} = 0$ ($\forall n > N'$), and by (12) in Theorem 4.1, we have

$$\lim_{n\to\infty} q_m^{(n)} = {\sigma_m}^2 - \sum_{n=0}^{\infty} s^{(n)} = {\sigma_m}^2 - \sum_{n=0}^{N'} s^{(n)} > 0,$$

which contradicts Lemma 5.3.

(ii) Assume $\lambda^{(n)} > 0$ for some large n such that (20) holds. In this case, $s^{(n)} = (\lambda^{(n)})^2$, and

$$\begin{aligned} q_m^{(n+1)} &= q_m^{(n)} - e_{m-1}^{(n+1)} - s^{(n)} \\ &= \sqrt{e_{m-1}^{(n)} q_m^{(n)}} - e_{m-1}^{(n+1)} - \frac{1}{4} e_{m-1}^{(n)} \\ &> \frac{1}{2}\sqrt{e_{m-1}^{(n)} q_m^{(n)}} - e_{m-1}^{(n+1)} \\ &= \sqrt{e_{m-1}^{(n+1)}} \left(\frac{1}{2}\sqrt{q_{m-1}^{(n+1)}} - \sqrt{e_{m-1}^{(n+1)}} \right), \end{aligned} \tag{23}$$

where the 5th line of Algorithm 3.1 is used in the first equality, (20) in the second equality, the assumption $\lambda^{(n)} > 0$ (i.e., $\sqrt{q_m^{(n)}} > \frac{1}{2}\sqrt{e_{m-1}^{(n)}}$) in the inequality, and the 6th line of Algorithm 3.1 in the last equality. From (23) it follows that

$$\lambda^{(n+1)} > 0 \iff q_m^{(n+1)} > \frac{1}{4} e_{m-1}^{(n+1)} \iff \sqrt{q_{m-1}^{(n+1)}} > \frac{5}{2}\sqrt{e_{m-1}^{(n+1)}}.$$

Since $\lim_{n\to\infty} q_{m-1}^{(n+1)} > 0$ and $\lim_{n\to\infty} e_{m-1}^{(n+1)} = 0$, there exists an integer N'' such that the last inequality holds for all $n > N''$. □

Using Lemma 5.2 and Lemma 5.4, we see that for sufficiently large n the shift is given as follows.

Lemma 5.5 (Shift in the dqds)**.** *Under the same assumption as in Lemma* 5.2 *we have*

$$s^{(n)} = (\lambda^{(n)})^2 = q_m^{(n)} - \sqrt{e_{m-1}^{(n)} q_m^{(n)}} + \frac{1}{4} e_{m-1}^{(n)} \ > 0 \tag{24}$$

for all sufficiently large n*.*

We are now in the position to prove that the rate of convergence of the dqds is 1.5. The next theorem refers only to the lower right two elements of $B^{(n)}$. This is sufficient from the practical point of view since whenever the lower right elements converge to zero, the deflation is applied to reduce the matrix size.

Theorem 5.1 (Rate of convergence of the dqds)**.** *Suppose the dqds algorithm with the Johnson bound is applied to a matrix B that satisfies Assumption* (A)*. Then we have*

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}} = \frac{1}{\sqrt{{\sigma_{m-1}}^2 - {\sigma_m}^2}}, \tag{25}$$

$$\lim_{n\to\infty} \frac{q_m^{(n+1)}}{(q_m^{(n)})^{3/2}} = \frac{1}{\sqrt{{\sigma_{m-1}}^2 - {\sigma_m}^2}}. \tag{26}$$

That is, the rate of convergence is 1.5*. Hence, by* (4)*, the lower right two elements of $B^{(n)}$, i.e., $b_{2m-2}^{(n)}$ and $b_{2m-1}^{(n)}$, converge to* 0 *with the rate of* 1.5*. Moreover, we have*

$$\lim_{n\to\infty} \frac{\sqrt{e_{m-1}^{(n)}}}{q_m^{(n)}} = \frac{1}{\sqrt{{\sigma_{m-1}}^2 - {\sigma_m}^2}}. \tag{27}$$

Proof. First, we compute the rate of convergence of $e_{m-1}^{(n)}$. By Lemma 5.5 the shift is determined by (24) for sufficiently large n, and we have

$$q_m^{(n+1)} = \sqrt{e_{m-1}^{(n)} q_m^{(n)}} - e_{m-1}^{(n+1)} - \frac{1}{4} e_{m-1}^{(n)}$$

from the second equality in (23). By using this, together with

$$q_m^{(n+1)} = q_{m-1}^{(n+2)} e_{m-1}^{(n+2)} / e_{m-1}^{(n+1)}, \qquad q_m^{(n)} = q_{m-1}^{(n+1)} e_{m-1}^{(n+1)} / e_{m-1}^{(n)}, \tag{28}$$

which can be seen from the 6th line of Algorithm 3.1, we obtain

$$\frac{e_{m-1}^{(n+2)}}{(e_{m-1}^{(n+1)})^{3/2}} = \frac{\sqrt{q_{m-1}^{(n+1)}}}{q_{m-1}^{(n+2)}} \left(1 - \frac{\sqrt{e_{m-1}^{(n+1)}}}{\sqrt{q_{m-1}^{(n+1)}}} - \frac{1}{4\sqrt{q_{m-1}^{(n+1)}}} \cdot \frac{e_{m-1}^{(n)}}{\sqrt{e_{m-1}^{(n+1)}}} \right). \tag{29}$$

We prove that the value in the parentheses on the right-hand side of (29) converges to 1. First, note $\lim_{n\to\infty} q_{m-1}^{(n+1)} > 0$ by (22). By (11), $\lim_{n\to\infty} e_{m-1}^{(n+1)} = 0$, and hence the second term in the parentheses converges to 0. As for the third term, we see

$$e_{m-1}^{(n+1)} = \frac{e_{m-1}^{(n)}}{q_{m-1}^{(n+1)}} \cdot q_m^{(n)} \geq \frac{\sqrt{q_{m-1}^{(n)}} - 2\sqrt{e_{m-1}^{(n)}}}{2 q_{m-1}^{(n+1)}} \left(e_{m-1}^{(n)} \right)^{3/2}$$

from (28) and (23) (with $n+1$ replaced by n). Thus

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n)}}{\sqrt{e_{m-1}^{(n+1)}}} \le \lim_{n\to\infty} \left(\frac{\sqrt{q_{m-1}^{(n)}} - 2\sqrt{e_{m-1}^{(n)}}}{2q_{m-1}^{(n+1)}} \right)^{-1/2} \left(e_{m-1}^{(n)}\right)^{1/4} = 0,$$

and hence the value in the parentheses on the right-hand side of (29) converges to 1. Moreover, from (22), we have

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}} = \lim_{n\to\infty} \frac{\sqrt{q_{m-1}^{(n+1)}}}{q_{m-1}^{(n+2)}} = \frac{1}{\sqrt{{\sigma_{m-1}}^2 - {\sigma_m}^2}}. \tag{30}$$

Next, by the second equation in (28), and by (22) and (30), we see

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

Finally, using this relation, we obtain

$$\begin{aligned} \lim_{n\to\infty} \frac{q_m^{(n+1)}}{(q_m^{(n)})^{3/2}} &= \lim_{n\to\infty} \frac{q_m^{(n+1)}}{\sqrt{e_{m-1}^{(n+1)}}} \left(\frac{q_m^{(n)}}{\sqrt{e_{m-1}^{(n)}}} \right)^{-3/2} \left(\frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}} \right)^{1/2} \\ &= ({\sigma_{m-1}}^2 - {\sigma_m}^2)^{1/2-3/4-1/4} \\ &= ({\sigma_{m-1}}^2 - {\sigma_m}^2)^{-1/2}. \end{aligned}$$

□

6 A numerical experiment

In this section, a simple numerical experiment is presented to illustrate the theory. Let us consider an $m \times m$ symmetric tridiagonal matrix

$$A = \begin{pmatrix} a & b & & 0 \\ b & a & \ddots & \\ & \ddots & \ddots & b \\ 0 & & b & a \end{pmatrix} \tag{31}$$

is considered. The eigenvalues are

$$a + 2b\cos\left(\frac{\pi k}{m+1}\right) \quad (k = 1, \ldots, m).$$

The dqds algorithm is then applied to the bidiagonal matrix B obtained by the Cholesky decomposition of A. The parameters are taken as $m = 10$, $a = 1.0$ and $b = 0.2$.

In view of Theorem 5.1, we define

$$\alpha^{(n)} = \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^{3/2}}, \qquad \beta^{(n)} = \frac{q_m^{(n+1)}}{(q_m^{(n)})^{3/2}},$$

which should converge to the constant $\sqrt{({\sigma_{m-1}}^2 - {\sigma_m}^2)^{-1}}$ according to the theory. The result is shown in Figure 2. The solid line shows $\alpha^{(n)}$, the chained line shows $\beta^{(n)}$ and the dashed line shows $\sqrt{({\sigma_{m-1}}^2 - {\sigma_m}^2)^{-1}} = 4.60$ in this problem setting. Both solid line and chained line approach to the dashed line in Figure 2.

On the other hand, $e_{m-1}^{(n)}$ and $q_m^{(n)}$ are plotted in the single logarithmic graph Figure 3. The solid line shows $e_{m-1}^{(n)}$ and the chained line shows $q_m^{(n)}$. The variables $e_{m-1}^{(n)}$ and $q_m^{(n)}$ converge to zero. By Figure 2 and Figure 3 we can say that the rate of convergence is 1.5. Table 1 presents the index $k = k^*$ that attains the minimum on the right-hand side of (18). If $\lambda^{(n)} < 0$, then k^* is defined to be 0. The result shows that $k^* = m$ for $n \geq 2$, which is consistent with Lemma 5.5.

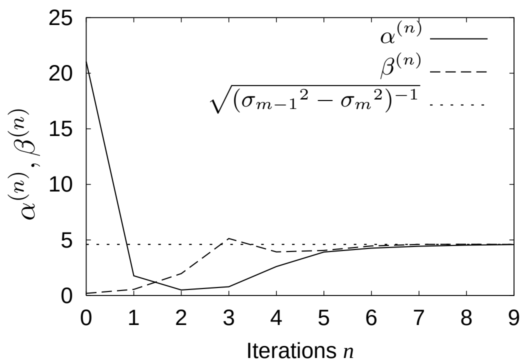

Figure 2: The dqds algorithm: $a = 1$, $b = 0.2$

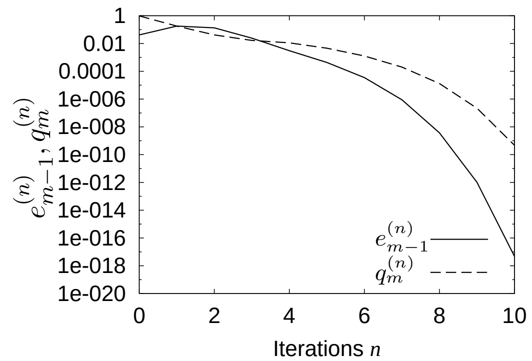

Figure 3: The dqds algorithm: $a = 1$, $b = 0.2$

Table 1: Critical index k^* for the Johnson bound (18) in the dqds algorithm

n	0	1	2	3	4	5	6	7	8	9
k^*	9	9	10	10	10	10	10	10	10	10

7 Conclusion

In this article, we have examined theoretically the convergence of the dqds algorithm for computing singular values of bidiagonal matrices. Under a natural condition on the shift, we have proved the convergence. Moreover, we have proved that the asymptotic rate of convergence of the dqds algorithm with the Johnson bound is 1.5. A simple numerical experiment has confirmed the theoretical result on the asymptotic rate.

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