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Kensuke Aishima   Takayasu Matsuo
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DEPARTMENT OF MATHEMATICAL INFORMATICS
GRADUATE SCHOOL OF INFORMATION SCIENCE AND TECHNOLOGY
THE UNIVERSITY OF TOKYO
BUNKYO-KU, TOKYO 113-8656, JAPAN

WWW page: http://www.i.u-tokyo.ac.jp/mi/mi-e.htm

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Kensuke Aishima Takayasu Matsuo
Kazuo Murota Masaaki Sugihara

Department of Mathematical Informatics
Graduate School of Information Science and Technology
The University of Tokyo
Kensuke_Aishima@mist.i.u-tokyo.ac.jp

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Abstract

A novel shift strategy is proposed for the differential quotient difference with shift (dqds) algorithm for the computation of singular values of bidiagonal matrices. While maintaining global convergence, the proposed shift realizes asymptotic superquadratic convergence of the dqds algorithm.

1 Introduction

Every $n \times m$ real matrix A of rank 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 bidiagonal matrices are based on the QR algorithm [3, 16]. Demmel and Kahan's improvement [4] upon the QR algorithm, awarded the second SIAM prize in numerical linear algebra, is open to the public as DBDSQR in LAPACK [2, 10].

In relation to the study of this algorithm, the differential quotient difference (dqd) algorithm was proposed by Fernando–Parlett [8] 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 [2, 10, 13]. The dqds is integrated into Multiple Relatively Robust Representations (MR^3) algorithm [5, 6, 7].

As for theoretical analysis about the dqds algorithm, locally quadratic or cubic convergence, and global convergence has been discussed in [8, 14] under certain assumptions. A recent paper of the present authors [1] has shown a general theorem for global convergence and revealed the asymptotic rate of 1.5 for the Johnson bound shift.

The objective of this paper is to propose a novel shift strategy for the dqds algorithm and to give a theoretical proof that the proposed shift realizes asymptotic superquadratic convergence while maintaining global convergence.

2 Problem setting

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

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

to which the dqds algorithm is applied.

Following [8], we assume

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

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 on 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 [8] for details). Finally it is easy to see that the singular values are invariant if b_k is replaced by $|b_k|$.

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 [8].

3 The dqds algorithm

In this section, we describe the dqds. We first 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 [9, 15]. Recall that the pqd algorithm consists of the so-called *rhombus rules* (Figure 1).

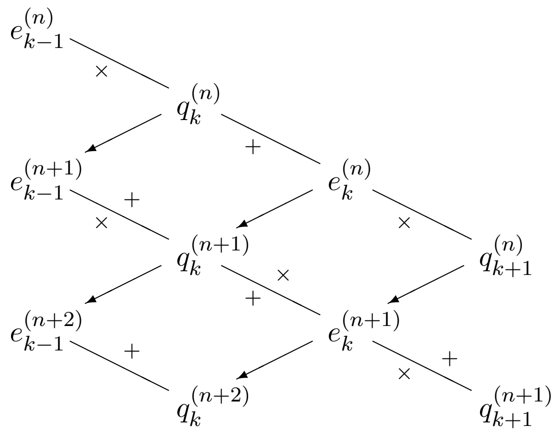

Figure 1: The rhombus rules

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":

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

to simplify the expression of the algorithm. Put

$$B^{(n)} = \begin{pmatrix} b_1^{(n)} & b_2^{(n)} & & \\ & b_3^{(n)} & \ddots & \\ & & \ddots & b_{2m-2}^{(n)} \\ & & & b_{2m-1}^{(n)} \end{pmatrix}, \tag{3}$$

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

$$q_k^{(n)} = (b_{2k-1}^{(n)})^2 \quad (k = 1, 2, \ldots, m;\ n = 0, 1, \ldots), \tag{4}$$

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

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

$$(B^{(n+1)})^{\mathrm{T}} B^{(n+1)} = B^{(n)} (B^{(n)})^{\mathrm{T}} - s^{(n)} I, \tag{6}$$

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

$$(B^{(n)})^{\mathrm{T}} B^{(n)} = W^{(n)} \left((B^{(0)})^{\mathrm{T}} B^{(0)} - \sum_{l=0}^{n-1} s^{(l)} I \right) (W^{(n)})^{-1}, \tag{7}$$

where $W^{(n)} = (B^{(n-1)} \cdots B^{(0)})^{-\mathrm{T}}$ is a nonsingular matrix. Therefore the eigenvalues of $(B^{(n)})^{\mathrm{T}} B^{(n)}$ are the same as those of $(B^{(0)})^{\mathrm{T}} B^{(0)} - \sum_{l=0}^{n-1} s^{(l)} I$. If $s^{(n)} < (\sigma_{\min}^{(n)})^2$ in each iteration n, where $\sigma_{\min}^{(n)}$ is the smallest singular value of $B^{(n)}$, $B^{(n)}$ converges to a diagonal matrix as $n \to \infty$, and then, by (7), the singular values of B can be obtained from the diagonal elements of $B^{(n)}$ with sufficiently large n (see Theorem 4.1). Moreover, if $s^{(n)} < (\sigma_{\min}^{(n)})^2$, the variables in the pqds algorithm are always positive so that the algorithm does not break down (see Lemma 4.1).

The dqds algorithm is obtained from the pqds algorithm by introducing auxiliary quantities $d_k^{(n+1)}$ defined as follows [8]:

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

The resulting algorithm is presented as Algorithm 3.2.

Algorithm 3.2 The dqds algorithm

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

```
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)
end for
```

Generally, the dqds algorithm outperforms the pqds algorithm in numerical stability. Since the variables of the dqds algorithm are positive 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. However we will work with the pqds in place of the dqds in the following convergence analysis.

4 Fundamental facts about convergence

Some relevant facts about the dqds algorithm are reviewed in this section. We begin with the fundamental convergence theorem. Recall that $\sigma_1 > \sigma_2 > \cdots > \sigma_m$ are singular values of B and $\sigma_{\min}^{(n)}$ denotes the smallest singular value of $B^{(n)}$.

Theorem 4.1 (Convergence of the dqds algorithm [1])**.** Suppose the matrix B satisfies Assumption (A), and the shift in the dqds algorithm (or in the pqds algorithm) satisfies $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$ for all $n = 0, 1, 2, \ldots$. Then

$$\sum_{n=0}^{\infty} s^{(n)} \leq {\sigma_m}^2. \tag{8}$$

Moreover,

$$\lim_{n\to\infty} e_k^{(n)} = 0 \quad (k = 1, 2, \ldots, m-1), \tag{9}$$

$$\lim_{n\to\infty} q_k^{(n)} = {\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)} \quad (k = 1, 2, \ldots, m). \tag{10}$$

In matrix form, we have

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

■

Remark 4.1. As mentioned in Section 1, global convergence has also been discussed in [8] and [14]. Those results, however, are not sufficient for our rigorous argument below, where we need the guarantee of global convergence for an arbitrary matrix B satisfying Assumption (A) and for any choice of shift in the range $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$. The theorem in [8] is restricted to the case of $s^{(n)} = 0$, and the theorem in [14] is restricted to generic (or nondegenerate) cases although it deals with general shifts satisfying $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$.

The variables are guaranteed to remain positive, as follows. This fact is crucial to the proof of the convergence theorem above as well as to numerical stability of the algorithm.

Lemma 4.1. Suppose the dqds algorithm is applied to the matrix B satisfying Assumption (A). If $s^{(l)} < (\sigma_{\min}^{(l)})^2$ for $l = 0, 1, \ldots, n$, then $(B^{(l+1)})^{\mathrm{T}} B^{(l+1)}$ are positive definite for $l = 0, 1, \ldots, n$, and hence $q_k^{(l+1)} > 0$ $(k = 1, \ldots, m)$ and $e_k^{(l+1)} > 0$ $(k = 1, \ldots, m-1)$ for $l = 0, 1, \ldots, n$.

Proof. For completeness we give a proof based on [1]. The proof is by induction on n. Under 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 (6), 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 $q_k^{(n+1)} > 0$ because of (4). By the 6th line of Algorithm 3.1, we have $e_k^{(n+1)} > 0$. □

The asymptotic rate of convergence of the dqds algorithm is given by the following lemma.

Lemma 4.2 ([1])**.** Under the same assumption as in Theorem 4.1, we have

$$\lim_{n \to \infty} \frac{e_k^{(n+1)}}{e_k^{(n)}} = \frac{{\sigma_{k+1}}^2 - \sum_{n=0}^{\infty} s^{(n)}}{{\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)}} < 1 \qquad (k = 1, \ldots, m-1). \tag{11}$$

Therefore, $e_k^{(n)}$ $(k = 1, \ldots, m-2)$ are of linear convergence as $n \to \infty$. The bottommost element $e_{m-1}^{(n)}$ is of superlinear convergence if $\sigma_m^2 - \sum_{n=0}^{\infty} s^{(n)} = 0$. ■

In Theorem 4.1 the condition $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$ imposed on the shift is not easy to verify, since $\sigma_{\min}^{(n)}$ is not known to us. To make use of the theorem in designing effective shift strategies we have to translate this condition to another form that is suitable for computational verification.

The following lemma shows that this is in fact possible and the condition can be checked by running one iteration of the dqds algorithm.

Lemma 4.3. For a fixed n, assume $e_k^{(n)} > 0$ $(k = 1, \ldots, m-1)$ and $q_k^{(n)} > 0$ $(k = 1, \ldots, m)$, and apply Algorithm 3.1 with shift $s^{(n)}$ to compute $q_k^{(n+1)}$ $(k = 1, \ldots, m)$. Then $s^{(n)} < (\sigma_{\min}^{(n)})^2$ if and only if $q_k^{(n+1)} > 0$ $(k = 1, \ldots, m)$.

Proof. First suppose that $s^{(n)} < (\sigma_{\min}^{(n)})^2$ is true. Then by (6) we have $b_{2k-1}^{(n+1)} \neq 0$ $(k = 1, \ldots, m)$, which are diagonal elements of $B^{(n+1)}$. Therefore we have $q_k^{(n+1)} > 0$ $(k = 1, \ldots, m)$ from (4).

Conversely suppose that $q_k^{(n+1)} > 0$ $(k = 1, \ldots, m)$. Then the diagonal elements of $B^{(n+1)}$ are positive by (4). Furthermore, by the 6th line of Algorithm 3.1 we see $e_k^{(n+1)} > 0$ $(k = 1, \ldots, m-1)$, and hence $B^{(n+1)}$ is a real matrix by (5). Therefore $(B^{(n+1)})^{\mathrm{T}} B^{(n+1)}$ is positive definite, and hence we have $s^{(n)} < (\sigma_{\min}^{(n)})^2$ from (6). □

The above arguments suggest the following scheme to set the shift in the 2nd line of Algorithm 3.1.

1. Somehow choose a candidate value for the shift, say $\hat{s}^{(n)}$.
2. Check for the condition $\hat{s}^{(n)} < (\sigma_{\min}^{(n)})^2$ on the basis of Lemma 4.3.
3. Set $s^{(n)} := \hat{s}^{(n)}$ if the condition is satisfied; otherwise set $s^{(n)} := 0$.

Note that the assumption of Lemma 4.3 is satisfied for $n = 0$ by Assumption (A). By Lemma 4.1 the assumption of Lemma 4.3 will be met for all n if the condition $0 \leq s^{(n)} < (\sigma_{\min}^{(n)})^2$ is satisfied. Theorem 4.1, on the other hand, guarantees the convergence, whereas Lemma 4.2 shows that the convergence rate is at least linear.

5 Shift for superquadratic convergence

Our shift strategy is proposed in this section. It leads to asymptotic superquadratic convergence, as will be shown later in Theorem 6.1.

Let us start with the motivation of our shift strategy. From Algorithm 3.1 we see

$$\begin{aligned}
\frac{e_{m-1}^{(n+2)}}{(e_{m-1}^{(n+1)})^2} &= \frac{q_m^{(n+1)}}{e_{m-1}^{(n+1)} q_{m-1}^{(n+2)}} \\
&= \frac{1}{q_{m-1}^{(n+2)}} \left(\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n+1)}} - 1 \right) \\
&= \frac{q_{m-1}^{(n+1)}}{q_{m-1}^{(n+2)}} \left(\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n+1)}} \right) \\
&= \frac{q_{m-1}^{(n+1)}}{q_{m-1}^{(n+2)}} \left(\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n)} - e_{m-2}^{(n+1)} + e_{m-1}^{(n)} - s^{(n)}} \right)
\end{aligned} \quad (12)$$

where the first equality is due to the 6th line (with $k = m-1$ and n replaced by $n+1$), the second is to the 8th line, the third is to the 6th line (with $k = m-1$), and the last is to the 5th line (with $k = m-1$).

The ideal choice of the shift $s^{(n)}$ would be such that the right-hand side of (12) vanishes, but this is impossible since the right-hand side involves $e_{m-2}^{(n+1)}$, a value to be determined in the future. As a feasible substitute we replace $e_{m-2}^{(n+1)}$ with $e_{m-2}^{(n)}$ and determine $s^{(n)}$ from the equation

$$\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - s^{(n)}} = 0. \quad (13)$$

Since $e_{m-2}^{(n)}$ is expected to be close to $e_{m-2}^{(n+1)}$, at least for large n, we can reasonably expect that $e_{m-1}^{(n+2)}/(e_{m-1}^{(n+1)})^2$ tends to zero as $n \to \infty$. This would mean superquadratic convergence, although we also have to take care of the condition $0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2$ for convergence, as dictated in Theorem 4.1.

We propose the following procedure to determine the shift $s^{(n)}$. First we take $\lambda^{(n)}$ such that

$$\frac{q_m^{(n)} - \lambda^{(n)}}{e_{m-1}^{(n)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - \lambda^{(n)}} = 0. \tag{14}$$

This amounts to solving a quadratic equation:

$$(\lambda^{(n)})^2 - (q_{m-1}^{(n)} + q_m^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)})\lambda^{(n)} + (q_{m-1}^{(n)} - e_{m-2}^{(n)})q_m^{(n)} = 0 \tag{15}$$

to set

$$\lambda^{(n)} = \frac{1}{2}\left(X^{(n)} - \sqrt{(X^{(n)})^2 - 4q_m^{(n)}(q_{m-1}^{(n)} - e_{m-2}^{(n)})}\right), \tag{16}$$

where

$$X^{(n)} = q_{m-1}^{(n)} + q_m^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)}.$$

Note that we have chosen the smaller root if $X^{(n)} > 0$, which is the case for large n. Then the shift is determined as follows.

$$s^{(n)} = \begin{cases} \lambda^{(n)} & \text{if } \lambda^{(n)} \text{ is real and } \ 0 \le \lambda^{(n)} < (\sigma_{\min}^{(n)})^2, \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

Before we can implement this shift strategy, we have to be able to see if $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ is true or not, without computing the value of $(\sigma_{\min}^{(n)})^2$. Fortunately we can do this by virtue of Lemma 4.3 as follows, where we assume that $\lambda^{(n)}$ is a positive real number.

Algorithm to check for $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$

$\hat{e}_0 := 0$
for $k := 1, \cdots, m-1$ **do**
  $\hat{q}_k := q_k^{(n)} - \hat{e}_{k-1} + e_k^{(n)} - \lambda^{(n)}$
  if $\hat{q}_k \le 0$ **then**
    $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ is false
    return
  end if
  $\hat{e}_k := e_k^{(n)} q_{k+1}^{(n)} / \hat{q}_k$
end for
$\hat{q}_m := q_m^{(n)} - \hat{e}_{m-1} - \lambda^{(n)}$
if $\hat{q}_m^{(n)} \le 0$ **then**
  $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ is false

else
  $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ is true
end if
return

It is emphasized here that the shift determined by (17) is a valid choice in the sense of Theorem 4.1, and hence the variables are convergent. In the next section, we shall establish a theorem for asymptotic superquadratic convergence. It will be shown in particular that $s^{(n)} = \lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ holds true for all sufficiently large n.

6 Theorem of superquadratic convergence

In this section, we prove that the asymptotic superquadratic convergence is realized by the shift strategy proposed in the previous section. Recall that the general convergence theorem (Theorem 4.1) applies to the dqds algorithm with our shift strategy (17).

First, we show that the use of $\lambda^{(n)}$ is effective for all sufficiently large n.

Lemma 6.1. In the shift strategy (17) we have $s^{(n)} = \lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ for all sufficiently large n.

Proof. The proof consists of showing two facts: (i) $\lambda^{(n)}$ given by (16) is a positive real number for all sufficiently large n, and (ii) $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ for all sufficiently large n.

(i) For the discriminant $D^{(n)}$ of the quadratic equation (15) we have

$$\begin{aligned}&\lim_{n\to\infty} D^{(n)}\\&= \lim_{n\to\infty}\left((q_{m-1}^{(n)} + q_m^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)})^2 - 4(q_{m-1}^{(n)} - e_{m-2}^{(n)})q_m^{(n)}\right)\\&= ({\sigma_{m-1}}^2 - {\sigma_m}^2)^2 > 0.\end{aligned}$$

Hence $\lambda^{(n)}$ is real for all sufficiently large n. In (15) we have

$$\begin{aligned}&\lim_{n\to\infty}(q_{m-1}^{(n)} + q_m^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)}) = q_{m-1}^{(\infty)} + q_m^{(\infty)} > 0,\\&\lim_{n\to\infty}(q_{m-1}^{(n)} - e_{m-2}^{(n)})q_m^{(n)} = q_{m-1}^{(\infty)}q_m^{(\infty)} \geq 0\end{aligned}$$

from Theorem 4.1, where $q_k^{(\infty)} = {\sigma_k}^2 - \sum_{n=0}^{\infty} s^{(n)}$ denotes the limit of $q_k^{(n)}$ as $n \to \infty$ given in (10). The above inequalities mean that, for all sufficiently large n, the sum and product of the two roots of (15) are positive, and hence $\lambda^{(n)} > 0$. We can also see that

$$\lim_{n\to\infty} \lambda^{(n)} = q_m^{(\infty)}. \tag{18}$$

(ii) We prove $\lambda^{(n)} < (\sigma_{\min}^{(n)})^2$ on the basis of Lemma 4.3. As observed at the end of Section 4, we can assume that $q_k^{(n)} > 0$ $(k = 1, \ldots, m)$ and $e_k^{(n)} > 0$ $(k = 1, \ldots, m-1)$. Then, by Lemma 4.3, it suffices to show $q_k^{(n+1)} > 0$ $(k = 1, \ldots, m)$ when $\lambda^{(n)}$ is used as the shift $s^{(n)}$.

In the 5th line of Algorithm 3.1 we have

$$\lim_{n\to\infty} q_k^{(n+1)} = \lim_{n\to\infty} \left(q_k^{(n)} - e_{k-1}^{(n+1)} + e_k^{(n)} - \lambda^{(n)} \right) = q_k^{(\infty)} - q_m^{(\infty)} > 0$$

for $k = 1, \ldots, m-1$ by (18). Hence $q_k^{(n+1)} > 0$ $(k = 1, \ldots, m-1)$ for all sufficiently large n. Note that this implies $e_k^{(n+1)} > 0$ $(k = 1, \ldots, m-1)$ by the 6th line of Algorithm 3.1.

The remaining case of $k = m$ can be treated as follows. We see

$$\begin{aligned}
q_m^{(n+1)} &= q_m^{(n)} - e_{m-1}^{(n+1)} - \lambda^{(n)} \\
&= \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - \lambda^{(n)}} - e_{m-1}^{(n+1)} \\
&= \frac{q_{m-1}^{(n+1)} e_{m-1}^{(n+1)}}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - \lambda^{(n)}} - e_{m-1}^{(n+1)} \\
&= \left(\frac{q_{m-1}^{(n)} - e_{m-2}^{(n+1)} + e_{m-1}^{(n)} - \lambda^{(n)}}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - \lambda^{(n)}} - 1 \right) e_{m-1}^{(n+1)} \\
&= \frac{(e_{m-2}^{(n)} - e_{m-2}^{(n+1)}) e_{m-1}^{(n+1)}}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - \lambda^{(n)}}, \qquad (19)
\end{aligned}$$

where the first equality is due to the 8th line of Algorithm 3.1, the second is to (14), the third is to the 6th line (with $k = m-1$) and the fourth is to the 5th line (with $k = m-1$). On the right-hand side of the last equality, the numerator is positive for all sufficiently large n by Lemma 4.2 and the denominator is positive for all sufficiently large n, since

$$\lim_{n\to\infty} \left(q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - \lambda^{(n)} \right) = q_{m-1}^{(\infty)} - q_m^{(\infty)} > 0.$$

Therefore we obtain $q_m^{(n+1)} > 0$ for all sufficiently large n. □

For the convergence of the diagonal elements we can show the following.

Lemma 6.2. With the shift strategy (17) in the dqds algorithm we have

$$\sum_{n=0}^{\infty} s^{(n)} = {\sigma_m}^2, \qquad (20)$$

$$\lim_{n\to\infty} q_k^{(n)} = {\sigma_k}^2 - {\sigma_m}^2 \quad (k = 1, \ldots, m-1); \qquad \lim_{n\to\infty} q_m^{(n)} = 0. \qquad (21)$$

Proof. By Lemma 6.1, the equality of (18), and (8) in Theorem 4.1, we have $\lim_{n\to\infty} q_m^{(n)} = 0$. This, together with (10), proves (20) and (21). $\square$

We now state the main theorem of this paper, which shows the superquadratic convergence of the dqds algorithm with our shift strategy. In view of (2) we introduce the notation

$$r_m^{(n)} = q_m^{(n)} + \sum_{l=0}^{n-1} s^{(l)} - {\sigma_m}^2 \tag{22}$$

to represent the error in the approximated smallest eigenvalue of $B^{\mathrm{T}}B$.

Theorem 6.1 (Superquadratic convergence of the dqds)**.** In the dqds algorithm with the shift strategy (17) we have

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^2} = 0, \tag{23}$$

$$\lim_{n\to\infty} \frac{q_m^{(n+1)}}{(q_m^{(n)})^2} = \frac{1}{{\sigma_{m-2}}^2 - {\sigma_m}^2}, \tag{24}$$

$$\lim_{n\to\infty} \frac{r_m^{(n+1)}}{(r_m^{(n)})^2} = 0. \tag{25}$$

Therefore $e_{m-1}^{(n)}$ and $r_m^{(n)}$ are of superquadratic convergence, and $q_m^{(n)}$ is of quadratic convergence. Moreover, we have

$$\lim_{n\to\infty} \frac{r_m^{(n)}}{e_{m-1}^{(n)}} = 0. \tag{26}$$

Proof. By Lemma 6.1 the shift is equal to $\lambda^{(n)}$ for all sufficiently large n, and accordingly we assume $s^{(n)} = \lambda^{(n)}$ below. By the first equality of (12) and (19) (with $\lambda^{(n)} = s^{(n)}$) we have

$$\begin{aligned} \frac{e_{m-1}^{(n+2)}}{(e_{m-1}^{(n+1)})^2} &= \frac{q_m^{(n+1)}}{e_{m-1}^{(n+1)} q_{m-1}^{(n+2)}} \\ &= \frac{e_{m-2}^{(n)} - e_{m-2}^{(n+1)}}{q_{m-1}^{(n+2)}(q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - s^{(n)})}. \end{aligned}$$

Hence, with the aid of (11) and (20) as well as $\lim_{n\to\infty} s^{(n)} = 0$, we see

$$\begin{aligned} \lim_{n\to\infty} \frac{e_{m-1}^{(n+2)}}{e_{m-2}^{(n+1)}(e_{m-1}^{(n+1)})^2} &= \lim_{n\to\infty} \frac{e_{m-2}^{(n)}/e_{m-2}^{(n+1)} - 1}{q_{m-1}^{(n+2)}(q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - s^{(n)})} \\ &= \frac{({\sigma_{m-2}}^2 - {\sigma_m}^2)/({\sigma_{m-1}}^2 - {\sigma_m}^2) - 1}{({\sigma_{m-1}}^2 - {\sigma_m}^2)^2} \\ &= \frac{{\sigma_{m-2}}^2 - {\sigma_{m-1}}^2}{({\sigma_{m-1}}^2 - {\sigma_m}^2)^3}. \end{aligned} \tag{27}$$

This implies

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

We also have

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

from the 6th line of Algorithm 3.1. Therefore we have

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

where (28) is used in the first equality, and Lemma 6.2 and (27) are used in the third equality.

Finally, we prove (25) and (26). Adding both sides of the 5th line of Algorithm 3.1 over n with $k = m$, we have

$$q_m^{(n)} = q_m^{(0)} - \sum_{l=0}^{n-1} e_{m-1}^{(l+1)} - \sum_{l=0}^{n-1} s^{(l)}. \tag{29}$$

Letting $n \to \infty$ and noting $\sum_{l=0}^{\infty} e_{m-1}^{(l+1)}$ is convergent (see [1] for the detail), we have also

$$q_m^{(\infty)} = q_m^{(0)} - \sum_{l=0}^{\infty} e_{m-1}^{(l+1)} - \sum_{l=0}^{\infty} s^{(l)},$$

and hence, from (10) in Theorem 4.1,

$${\sigma_m}^2 = q_m^{(\infty)} + \sum_{l=0}^{\infty} s^{(l)} = q_m^{(0)} - \sum_{l=0}^{\infty} e_{m-1}^{(l+1)}. \tag{30}$$

Therefore we see

$$r_m^{(n)} = q_m^{(n)} + \sum_{l=0}^{n-1} s^{(l)} - {\sigma_m}^2 = \sum_{l=n+1}^{\infty} e_{m-1}^{(l)} \tag{31}$$

by (22), (29) and (30). It then follows from (31) that

$$\lim_{n\to\infty} \frac{r_m^{(n)}}{e_{m-1}^{(n+1)}} = \lim_{n\to\infty} \frac{1}{e_{m-1}^{(n+1)}} \sum_{l=1}^{\infty} e_{m-1}^{(n+l)} = 1.$$

Hence we obtain

$$\begin{aligned} \lim_{n\to\infty} \frac{r_m^{(n+1)}}{(r_m^{(n)})^2} &= \lim_{n\to\infty} \frac{e_{m-1}^{(n+2)}}{(e_{m-1}^{(n+1)})^2} = 0, \\ \lim_{n\to\infty} \frac{r_m^{(n)}}{e_{m-1}^{(n)}} &= \lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{e_{m-1}^{(n)}} = 0 \end{aligned}$$

from (23). □

Note that the critical variables for convergence are $e_{m-1}^{(n)}$ and $r_m^{(n)}$; the former is used for the convergence criterion and the latter represents the error in the approximation of ${\sigma_m}^2$. Furthermore, when the iteration is stopped at the nth loop, the equation (26) indicates that $r_m^{(n)}$ is small enough compared to $e_{m-1}^{(n)}$. This property is useful in practice. Theorem 6.1 does not say anything about other variables, but this is already sufficient from the algorithmic point of view, since whenever the lower right elements, $e_{m-1}^{(n)}$ and $q_m^{(n)}$, converge to zero, the deflation is applied to reduce the matrix size.

Remark 6.1. Our shift strategy gives a concrete example of the ideal shift for the quadratic convergence discussed in Fernando–Parlett [8].

Their analysis went as follows. From the 5th and the 6th line of Algorithm 3.1, we see

$$\begin{aligned} e_{m-1}^{(n+1)} q_m^{(n+1)} &= e_{m-1}^{(n+1)} \left(q_m^{(n)} - e_{m-1}^{(n+1)} - s^{(n)} \right) \\ &= \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}} \left(q_m^{(n)} - \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}} - s^{(n)} \right). \end{aligned} \tag{32}$$

Hence, if we can choose a shift $s^{(n)}$ that satisfies the condition

$$\left| q_m^{(n)} - s^{(n)} - \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}} \right| \le \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}}, \tag{33}$$

we will have

$$\frac{|e_{m-1}^{(n+1)} q_m^{(n+1)}|}{(e_{m-1}^{(n)} q_m^{(n)})^2} \le \frac{1}{(q_{m-1}^{(n+1)})^2}. \tag{34}$$

If, furthermore, the shift is almost ideal in the sense that

$$s^{(n)} \simeq (\sigma_{\min}^{(n)})^2, \tag{35}$$

then $q_{m-1}^{(n+1)} \simeq \sigma_{m-1}{}^2 - \sigma_m{}^2$, and thus (34) approximately yields the quadratic convergence of $e_{m-1}^{(n)} q_m^{(n)}$ in this single step, where it is noted that $e_{m-1}^{(n)} q_m^{(n)}$ is the lower right subdiagonal element of $(B^{(n)})^{\mathrm{T}} B^{(n)}$.

Our shift in fact asymptotically realizes this ideal situation. Lemma 6.1 shows that for all sufficiently large n the shift $s^{(n)} = \lambda^{(n)}$ is effective, and we also see that

$$\begin{aligned} \left| q_m^{(n)} - s^{(n)} - \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}} \right| &= \left| q_m^{(n)} - s^{(n)} - e_{m-1}^{(n+1)} \right| \\ &= \left| \frac{(e_{m-2}^{(n)} - e_{m-2}^{(n+1)}) e_{m-1}^{(n+1)}}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - s^{(n)}} \right| \\ &= \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}} \left| \frac{e_{m-2}^{(n)} - e_{m-2}^{(n+1)}}{q_{m-1}^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)} - s^{(n)}} \right| \\ &\leq \frac{e_{m-1}^{(n)} q_m^{(n)}}{q_{m-1}^{(n+1)}} \end{aligned}$$

for all sufficiently large n, where the first equality is due to the 6th line of Algorithm 3.1 (with $k = m - 1$), the second equality is to (19), the third equality is to the 6th line of Algorithm 3.1 (with $k = m - 1$) and to the positivity of variables in our shift strategy, and the inequality is to Theorem 4.1. Therefore the condition (33) is met by our shift for all sufficiently large n. The second condition (35) is also satisfied by our shift because both $s^{(n)}$ and $\sigma_{\min}^{(n)}$ asymptotically tend to zero (see Lemma 6.2).

Actually, Theorem 6.1 for our shift gives a sharper estimate:

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

Thus the convergence of $e_{m-1}^{(n)} q_m^{(n)}$ has turned out to be *superquadratic* in our algorithm.

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