A shift strategy for superquadratic convergence of the dqds algorithm for computing singular values

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Computation of singular values

Singular value decomposition

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

$$\Sigma = \left(\begin{array}{ccc|c} \sigma_1 & & 0 & \\ & \ddots & & 0 \\ 0 & & \sigma_r & \\ \hline & 0 & & \end{array}\right)$$

Singular values

U, V: Orthogonal matrices

(Application: least square method, Image compression, etc.)

Step 1 $A \xrightarrow{\text{orthogonal transformation}}$ bidiagonal matrix B

Step 2 Computing singular values of B : $(\sigma_1, \ldots, \sigma_r)$

(e.g.) dqds algorithm is used

History of the method of computing singular values (relevant to the dqds)

- QR method (Golub – Kahan, 1965)
- QR method was improved (Demmel–Kahan, 1990)
- dqds algorithm (Fernando – Parlett, 1994)

  differential **q**uotient **d**ifference with **s**hifts
  - High speed, high accuracy
  - DLASQ routine in LAPACK (Parlett-Marques, 2000)

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- The dqds algorithm
- Our shift strategy for superquadratic convergence of the dqds algorithm
  - Algorithm, Convergence theorem, numerical experiment, Practical implementation
- Conclusions

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Notation and normalization

$$B = \begin{pmatrix} a_1 & b_1 & & 0 \\ & a_2 & \ddots & \\ & & \ddots & b_{m-1} \\ 0 & & & a_m \end{pmatrix} \quad m$$

m

Suppose that

$$a_k, b_k > 0$$

Singular values

$$\sigma_1 > \cdots > \sigma_m > 0$$

(There is no loss of generality in this assumption)

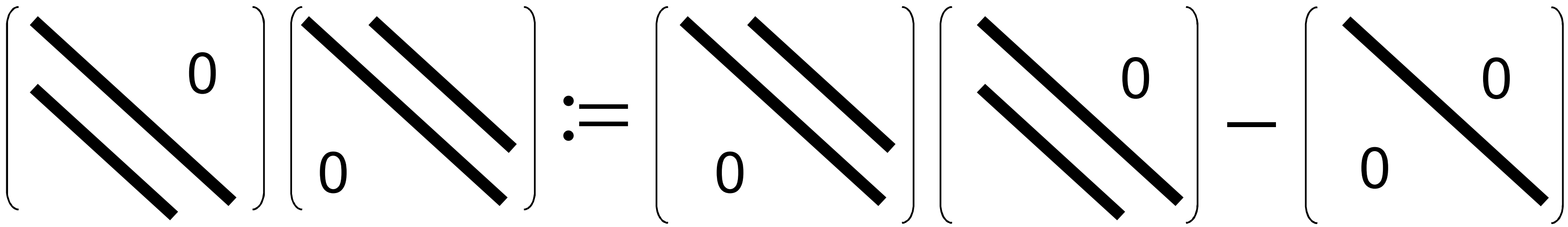
The dqds compute the singular values of B

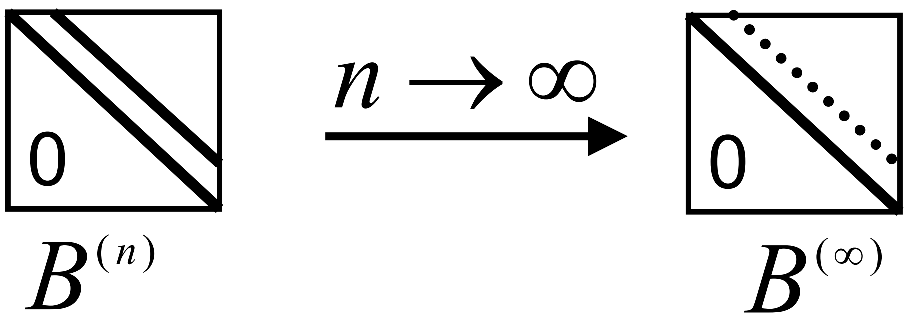
The dqds algorithm (Fernando – Parlett, 1994)

Initialization: $B^{(0)} := B$

Iterations: $(B^{(n+1)})^{\mathrm{T}} B^{(n+1)} := B^{(n)} (B^{(n)})^{\mathrm{T}} - s^{(n)} I$

shift (to accelerate convergence)





The diagonal elements are the singular values

The dqds algorithm (Fernando – Parlett, 1994)

Initialization:

$$q_k^{(0)} = (a_k)^2, e_k^{(0)} = (b_k)^2$$

Iterations:

for $n := 0, 1, \cdots$ do

choose $s^{(n)} \geq 0$

$d_1^{(n+1)} := q_1^{(n)} - s^{(n)}$

for $k := 1, \cdots, m-1$ 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

dqds algorithm:

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

shift (to accelerate convergence)

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

Theorem (Convergence of the dqds)

(Aishima et. al. , 2008, SIMAX)

$\sigma_{\min}^{(n)}$:Smallest singular value of $B^{(n)}$

Shift $0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2$

⇒

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

$$\lim_{n\to\infty} e_k^{(n)} = 0 \ ,$$

$$\lim_{n\to\infty} q_k^{(n)} = \sigma_k^2 - \sum_{n=0}^{\infty} s^{(n)}$$

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

(Singular values $\sigma_1 > \cdots > \sigma_m$)

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(Singular values $\sigma_1 > \cdots > \sigma_m$)

Convergence of the lower right elements are fast

Deflation strategy

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

Convergence of the lower right elements are fast

- $e_{m-1}^{(N)} \approx 0$ then terminate
- approximate $\sigma_m^2 \approx q_m^{(N)} + \sum_{n=0}^{N-1} s^{(n)}$
- repeat deflation
- $\sigma_m, \sigma_{m-1}, \ldots, \sigma_1$ can be computed

Convergence rate of the dqds

Convergence rate of the dqds is the convergence rate of $e_{m-1}^{(n)}$

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

- $s^{(n)} \approx (\sigma_{\min}^{(n)})^2 \Rightarrow$ Accelerate the convergence !
- But the value of $\sigma_{\min}^{(n)}$ is unknown

A strict lower bound of $(\sigma_{\min}^{(n)})^2$ is used for the shift in the implementation of the dqds in LAPACK (DLASQ routine)

Theorem (superquadratic convergence)

(Aishima et. al. , 2010, JCAM)

The dqds in the LAPACK routine is executed

⇒

$$\lim_{n\to\infty} \frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^2} = 0 \qquad B^{(n)} = \begin{pmatrix} \sqrt{q_1^{(n)}} & \sqrt{e_1^{(n)}} & & \\ & \sqrt{q_2^{(n)}} & \ddots & \\ & & \ddots & \sqrt{e_{m-1}^{(n)}} \\ & & & \sqrt{q_m^{(n)}} \end{pmatrix}$$

Superquadratic convergence !

We propose another new superquadratic shift strategy

Direct approach for superquadratic convergence

- The shift strategy in the dqds in LAPACK (DLASQ routine)
  - Shifts are chosen such that $s^{(n)} \approx (\sigma_{\min}^{(n)})^2,\ s^{(n)} < (\sigma_{\min}^{(n)})^2$ based on the perturbation theory. As a result, superquadratic convergence is indirectly achieved

- Our proposed shift strategy
  - Superquadratic convergence: $\dfrac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^2} \approx 0$ is directly and intuitively achieved !

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Motivation

Initialization:

$$q_k^{(0)} = (a_k)^2, e_k^{(0)} = (b_k)^2$$

Iterations:

for $n := 0, 1, \cdots$ do
  choose $s^{(n)} \geq 0$
  $d_1^{(n+1)} := q_1^{(n)} - s^{(n)}$
  for $k := 1, \cdots, m-1$ 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

From the dqds algorithm we see

$$\frac{e_{m-1}^{(n+2)}}{(e_{m-1}^{(n+1)})^2}$$

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

$$= \frac{1}{q_{m-1}^{(n+2)}} \left(\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n+1)}} - 1 \right)$$

$$= \frac{q_{m-1}^{(n+1)}}{q_{m-1}^{(n+2)}} \left(\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n+1)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n+1)}} \right)$$

$$= \frac{q_{m-1}^{(n+1)}}{q_{m-1}^{(n+2)}} \left(\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n+1)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n)} - e_{m-2}^{(n+1)} + e_{m-1}^{(n)} - s^{(n)}} \right)$$

We want to make it 0 for superquadratic convergence

Motivation

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

- We see $\frac{q_{m-1}^{(n+1)}}{q_{m-1}^{(n+2)}} \to 1$ from the global convergence theorem
- We hope that the shift $s^{(n)}$ is chosen such that

$$\frac{q_m^{(n)} - s^{(n)}}{e_{m-1}^{(n)} q_m^{(n)}} - \frac{1}{q_{m-1}^{(n)} - \boxed{e_{m-2}^{(n+1)}} + e_{m-1}^{(n)} - s^{(n)}} \approx 0$$

Unknown

- Hence, we set the shift $s^{(n)}$ that satisfies the following equation:

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

Replace

Motivation

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

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

⇕

Quadratic equation: $(s^{(n)})^2 - X^{(n)} s^{(n)} + Y^{(n)} = 0$

where $X^{(n)} = q_{m-1}^{(n)} + q_m^{(n)} - e_{m-2}^{(n)} + e_{m-1}^{(n)}$, $Y^{(n)} = 4 q_m^{(n)} (q_{m-1}^{(n)} - e_{m-2}^{(n)})$

Solution: $s^{(n)} = \frac{1}{2}(X^{(n)} \pm \sqrt{(X^{(n)})^2 - Y^{(n)}})$

Superquadratic convergence is expected !

Proposed shift strategy

- Quadratic equation: $(s^{(n)})^2 - X^{(n)} s^{(n)} + Y^{(n)} = 0$

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

- One solution: $\lambda^{(n)} := \frac{1}{2}(X^{(n)} - \sqrt{(X^{(n)})^2 - Y^{(n)}})$
- Condition of convergence $0 \le s^{(n)} < (\sigma_{\min}^{(n)})^2$

Shift strategy (Q)

$$s^{(n)} = \begin{cases} \lambda^{(n)} & \text{If} \quad 0 < \lambda^{(n)} < (\sigma_{\min}^{(n)})^2 \\ \text{Other shifts} & \text{Otherwise} \end{cases}$$

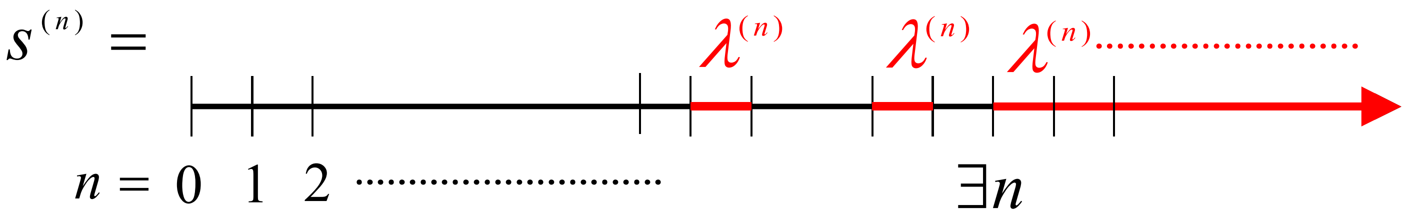
Theoretical analysis

Lemma (shifts in the final phase)

Shift strategy (Q) is used

$s^{(n)} = \lambda^{(n)}$ (superquadratic convergence shift)

for all sufficiently large n



Theoretical analysis

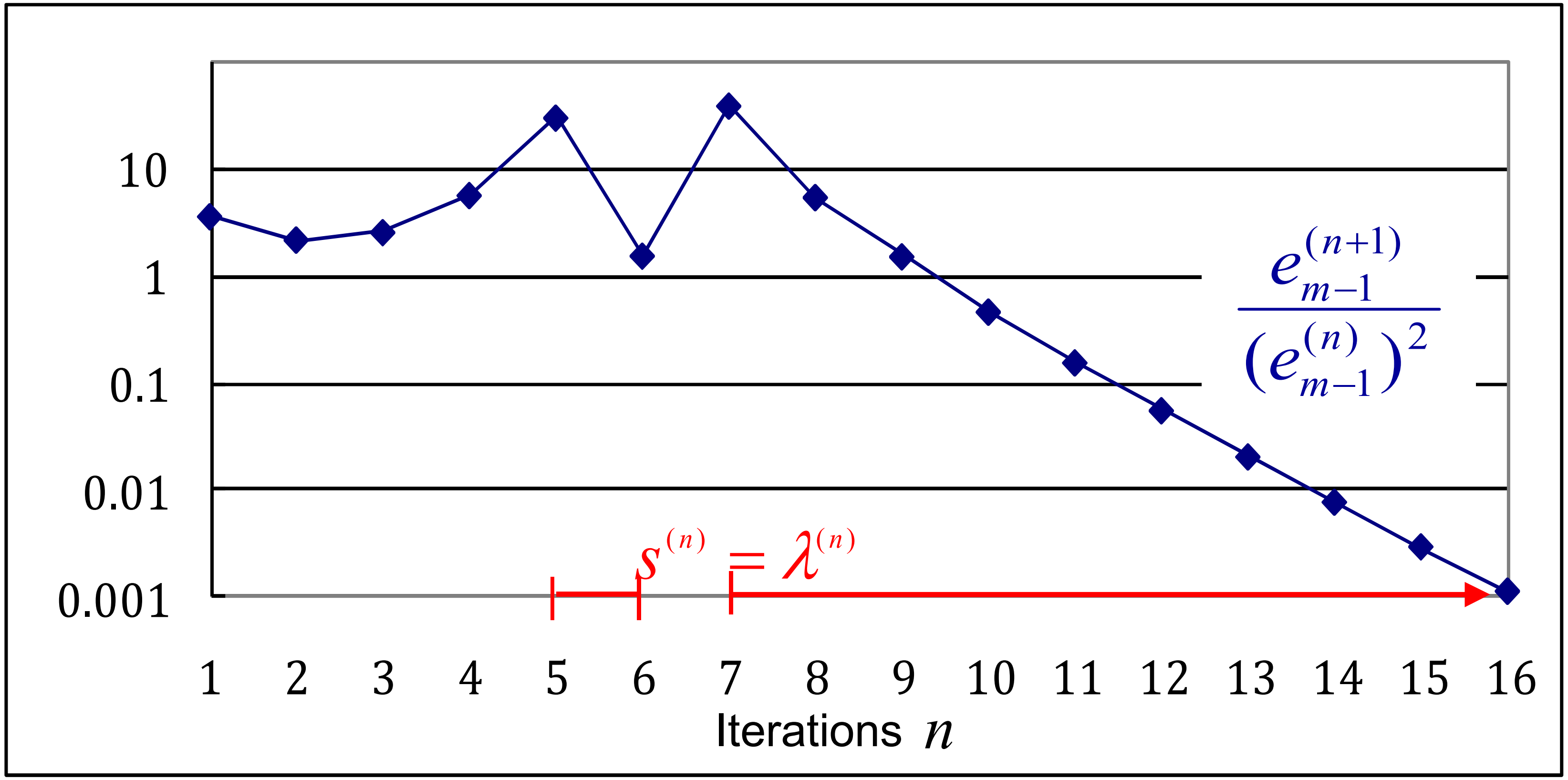
Theorem (superquadratic convergence)

Shift strategy (Q) is used

$$\Rightarrow \quad \lim_{n \to \infty} \frac{e_{m-1}^{(n+1)}}{\left(e_{m-1}^{(n)}\right)^2} = 0 \qquad B^{(n)} = \begin{pmatrix} \sqrt{q_1^{(n)}} & \sqrt{e_1^{(n)}} & & \\ & \sqrt{q_2^{(n)}} & \ddots & \\ & & \ddots & \sqrt{e_{m-1}^{(n)}} \\ & & & \sqrt{q_m^{(n)}} \end{pmatrix}$$

Superquadratic convergence !

A numerical experiment to illustrate the superquadratic convergence



$$\frac{e_{m-1}^{(n+1)}}{(e_{m-1}^{(n)})^2} \longrightarrow 0\text{: Superquadratic convergence}$$

The arbitrary-precision arithmetic library “exflib” , Fortran77

Practical implementation

Shift strategy (Q)

$$s^{(n)} = \begin{cases} \lambda^{(n)} & \text{If} \quad 0 < \lambda^{(n)} < (\sigma_{\min}^{(n)})^2 \\ \underline{\text{Other shifts}} & \text{Otherwise} \end{cases}$$

We employ the LAPACK shift strategy

- The ratio of cpu time to compute all singular values: (Our algorithm)/(LAPACK) is from 0.8 to 1.3 (almost same)

Test matrices are the same matrices in [Parlett-Marques, 2000, LAA]

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Conclusions

- A new shift strategy for superquadratic convergence was proposed
- Superquadratic convergence theorem was shown
- A numerical experiment to illustrate the superquadratic convergence was shown
- Practical implementation similar to LAPACK routine was given