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An application of the Kato-Temple inequality on matrix eigenvalues to the dqds algorithm for singular values

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Abstract

Choice of suitable shifts strongly influences performance of numerical algorithms with shift for computing matrix eigenvalues or singular values. On the dqds (differential quotient difference with shifts) algorithm for singular values, a new shift strategy is proposed in this paper. The new shift strategy includes shifts obtained from an application of the Kato-Temple inequality on matrix eigenvalues. The dqds algorithm with the new shift strategy is shown to have a better performance in iteration number than that of the subroutine DLASQ in LAPACK.

Keywords dqds algorithm, shift strategy, implementation

Research Activity Group Algorithms for Matrix / Eigenvalue Problems and their Applications

1. Introduction

Singular value decomposition (SVD) can be adapted to a wide field of applications. In this paper, we consider the dqds (differential quotient difference with shifts) algorithm [1] as a singular value computation algorithm. Before execution of the dqds algorithm, an input matrix is transformed into an upper bidiagonal matrix $B^{(0)}$ by sequential application of the well-known Householder transforms. The dqds algorithm corresponds to the Cholesky transform with shift

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

for $n = 0, 1, 2, \dots$, where $s^{(n)}$ and I are shift (non-negative) and the unit matrix, respectively. It is known that the square of a lower bound of the minimal singular value of $B^{(n)}$ can be used as a shift [1]. In the DLASQ subroutine in LAPACK [2], a shift strategy by Parlett and Marques [3] is implemented. This is called *the aggressive shift*. The aggressive shift is based on heuristic and estimates the quantity of shift $s^{(n)}$ from a part of elements of $B^{(n)}$ and values of $d_{m-2}^{(n)}$, $d_{m-1}^{(n)}$, $d_m^{(n)}$, $\min_{1\le i\le m-2} d_k^{(n)}$, $\min_{1\le i\le m-1} d_k^{(n)}$ and $\min_{1\le i\le m} d_k^{(n)}$ in Algorithm 1. Note that $\min_{1\le k\le m}\{d_k^{(n)} + s^{(n)}\}$ is an upper bound of the minimal eigenvalue of $(B^{(n+1)})^\top B^{(n+1)}$ [1]. In this paper, we propose a new shift strategy for the dqds algorithm. We use the generalized Newton shift of order 2, the Laguerre shift, the forward Kato-Temple shift, the backward Kato-Temple shift and the Gerschgorin shift shown in Section 3. These shifts share almost part of computation except the Gerschgorin shift. Our shift strategy is not heuristic since it always gives a lower bound of the minimal singular value by exact computation.

This paper is organized as follows. In Section 2, the dqds algorithm is briefly reviewed. In Section 3, lower bounds of the minimal singular value of upper bidiagonal matrix $B^{(n)}$, which are considered in our new shift strategy, are introduced. Application of the Kato-Temple inequality is also described in this section. In Section 4, a new shift strategy for the dqds algorithm is presented. In Section 5, a numerical experiment is shown. Performance of singular value computation by the dqds algorithm with our new shift strategy is compared to that by DLASQ.

2. The dqds algorithm

In this section, we describe the dqds algorithm briefly. Let $B^{(n)}$ $(n = 0, 1, 2, \dots)$ be an $m \times m$ upper bidiagonal matrix. For $i = 1, \dots, m$, let the (i, i) element of $B^{(n)}$ be given as $(q_i^{(n)})^{1/2}$, where all the $q_i^{(n)}$ are positive. Similarly, for $i = 1, \dots, m-1$, let the $(i, i+1)$ element of $B^{(n)}$ be given as $(e_i^{(n)})^{1/2}$, where all the $e_i^{(n)}$ are positive. The dqds algorithm is described as in Algorithm 1.

Algorithm 1 The dqds algorithm

for $n = 0, 1, 2, \dots$ **do:**
  Set the shift $s^{(n)} (\ge 0)$
  $d_1^{(n+1)} \leftarrow q_1^{(n)} - s^{(n)}$
  for $k = 1, \dots, m-1$ **do:**
    $q_k^{(n+1)} \leftarrow d_k^{(n+1)} + e_k^{(n)}$
    $e_k^{(n+1)} \leftarrow e_k^{(n)} q_{k+1}^{(n)} / q_k^{(n+1)}$
    $d_{k+1}^{(n+1)} \leftarrow (d_k^{(n+1)} q_{k+1}^{(n)} / q_k^{(n+1)}) - s^{(n)}$
  end for
  $q_m^{(n+1)} \leftarrow d_m^{(n+1)}$
end for

3. Lower bounds of the smallest singular value of $B^{(n)}$

Let the smallest singular value of $B^{(n)}$ and the smallest eigenvalue of $B^{(n)}(B^{(n)})^\top$ be denoted by $\sigma_{\min}^{(n)}$ and $\lambda_{\min}^{(n)}$, respectively. Note that $\lambda_{\min}^{(n)} = (\sigma_{\min}^{(n)})^2$. Let $J_M(B^{(n)})$ $(M = 1, 2, \dots)$ denote the trace

$$J_M(B^{(n)}) = \mathrm{Tr}(\{[B^{(n)}(B^{(n)})^\top]^M\}^{-1}).$$

Let $Y(B^{(n)})$ be

$$Y(B^{(n)}) = m \cdot \frac{J_2(B^{(n)})}{(J_1(B^{(n)}))^2} - 1. \tag{1}$$

Since $e_i^{(n)} > 0$ $(i = 1, \dots, m-1)$, all the eigenvalues $\lambda_i^{(n)}$ $(i = 1, \dots, m)$ of $(B^{(n)})^\top B^{(n)}$ are simple. Since it holds $J_M(B^{(n)}) = \sum_{i=1}^m [(\lambda_i^{(n)})^{-M}]$, we have

$$(J_1(B^{(n)}))^2 Y(B^{(n)}) = \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \left(\frac{1}{\lambda_i^{(n)}} - \frac{1}{\lambda_j^{(n)}} \right)^2.$$

Therefore, $Y(B^{(n)})$ is positive. In von Matt [4], a lower bound of $\sigma_{\min}^{(n)}$ using $J_1(B^{(n)})$ and $J_2(B^{(n)})$ is given as

$$\Theta_{\mathrm{L}}^{(n)} = \left(\frac{1}{J_1(B^{(n)})} \cdot \frac{m}{1 + \left[(m-1)Y(B^{(n)})\right]^{\frac{1}{2}}} \right)^{\frac{1}{2}} \le \sigma_{\min}^{(n)}. \tag{2}$$

Though $\Theta_{\mathrm{L}}^{(n)}$ is called *Laguerre's shift* in [4], let us call $(\Theta_{\mathrm{L}}^{(n)})^2$ *the Laguerre shift* in this paper. In [5], a sequence of lower bounds of $\sigma_{\min}^{(n)}$ are given as

$$\Theta_{\mathrm{gN},M}^{(n)} = (J_M(B^{(n)}))^{-\frac{1}{2M}} < \sigma_{\min}^{(n)} \quad (M = 1, 2, \dots). \tag{3}$$

In [6], $(\Theta_{\mathrm{gN},M}^{(n)})^2$ is named *the generalized Newton shift of order M*.

Next, we give lower bounds of $\lambda_{\min}^{(n)}$ utilizing the Kato-Temple inequality [7, pp.182–183]. We consider the interlacing theorem [8, pp.186–187]. Let A and x be an $m \times m$ real symmetric matrix and an m real vector with $x^\top x = 1$, respectively. For x, let ρ be a Rayleigh quotient of A, namely, $\rho = x^\top A x$. Among eigenvalues of A, assume that only one eigenvalue λ is included in an open interval $(\underline{\lambda}, \bar{\lambda})$ and others are not included in this interval. In addition to this assumption, assume that ρ is included in the interval $(\underline{\lambda}, \bar{\lambda})$. Then, it holds

$$\rho - \frac{\varepsilon^2}{\bar{\lambda} - \rho} \le \lambda \le \rho + \frac{\varepsilon^2}{\rho - \underline{\lambda}},$$

where $\varepsilon^2 = \|Ax - \rho x\|_2^2$. Let us take x as $x = (0, \dots, 0, 1)^\top$. Let $\hat{B}^{(n)}$ be the $(m-1) \times (m-1)$ principal submatirix of $B^{(n)}$. Let $\hat{B}^{(n)}(\hat{B}^{(n)})^\top$ be denoted by $\hat{A}$. For $i = 1, \dots, m$, let the (i, i) elements of $[(B^{(n)})^\top B^{(n)}]^{-1}$, $[B^{(n)}(B^{(n)})^\top]^{-1}$, $\{[B^{(n)}(B^{(n)})^\top]^2\}^{-1}$, $[(\hat{B}^{(n)})^\top \hat{B}^{(n)}]^{-1}$, $[\hat{B}^{(n)}(\hat{B}^{(n)})^\top]^{-1}$, $\{[\hat{B}^{(n)}(\hat{B}^{(n)})^\top]^2\}^{-1}$ be denoted by α_i, β_i, γ_i, $\hat{\alpha}_i$, $\hat{\beta}_i$, $\hat{\gamma}_i$, respectively. Let us consider the case of $A = B^{(n)}(B^{(n)})^\top$. Let the smallest eigenvalue of $\hat{A}$ and the second smallest eigenvalue of A be denoted by $\lambda_{\min}(\hat{A})$ and $\lambda_{m-1}(A)$, respectively. We see $\lambda_{m-1}(A) \ge \lambda_{\min}(\hat{A})$. If ζ is a lower bound of $\lambda_{\min}(\hat{A})$ and it holds $\zeta > \rho = q_m^{(n)}$, then ζ can be used as an endpoint of $\bar{\lambda}$ of the open interval. In such cases, we obtain a lower bound of $\lambda_{\min}^{(n)}$

$$\Xi_{\mathrm{KT},+}^{(n)} = q_m^{(n)} \left(1 - \frac{e_{m-1}^{(n)}}{\bar{\lambda} - q_m^{(n)}} \right) \le \lambda_{\min}^{(n)}. \tag{4}$$

In [9, 10], such shifts for the mdLVs algorithm [11] for singular value computation are given. The endpoints $\bar{\lambda}$ given in [9, 10] are different from each other. In this paper, we choose a lower bound $\bar{\lambda}$ of $\lambda_{\min}(\hat{A})$ as

$$\bar{\lambda} = \left(\sum_{i=1}^{m-1} \gamma_i \right)^{-\frac{1}{2}}, \tag{5}$$

which is different from those in [9, 10]. We can show that it holds $\alpha_i > \hat{\alpha}_i$ and $\beta_i = \hat{\beta}_i$ for $i = 1, \dots, m-1$ from the recurrence relations in [5, Remark 4.6]. Then, from the recurrence relations in [6, Theorem 2.2.5], it holds that $\gamma_i > \hat{\gamma}_i$ $(i = 1, \dots, m-1)$. Since the generalized Newton shift of order 2 of $\hat{B}^{(n)}$ is given as $(\sum_{i=1}^{m-1} \hat{\gamma}_i)^{-1/2}$, it holds

$$\lambda_{m-1}(A) \ge \lambda_{\min}(\hat{A}) > \left(\sum_{i=1}^{m-1} \hat{\gamma}_i \right)^{-\frac{1}{2}} > \bar{\lambda}.$$

The lower bound $\Xi_{\mathrm{KT},+}^{(n)}$ in (4) with $\bar{\lambda}$ in (5) is named *the forward Kato-Temple shift*. Next, let us consider the case of $A = [B^{(n)}(B^{(n)})^\top]^{-1}$. Let the largest and the second largest eigenvalues of A be denoted by $\lambda_{\max}(A)$ and $\lambda_2(A)$, respectively. Note that x is not an eigenvector of A. It can readily be shown that $\rho = \beta_m < \lambda_{\max}(A)$. We have

$$\varepsilon^2 = x^\top A^2 x - \rho^2 = \gamma_m - (\beta_m)^2 > 0.$$

Let A_{m-1} be the $(m-1) \times (m-1)$ principal submatrix of A. Let us choose $\underline{\lambda}$ as

$$\underline{\lambda} = \mathrm{Tr} A_{m-1}. \tag{6}$$

It can be readily shown that $\underline{\lambda} > \lambda_2(A)$. If $\rho = \beta_m > \underline{\lambda}$ holds, then we can make an interval $(\underline{\lambda}, \bar{\lambda})$ which satisfies $\lambda_2(A) < \underline{\lambda} < \rho \le \lambda_{\max}(A) < \bar{\lambda}$. In such cases, we obtain a lower bound of $\lambda_{\min}^{(n)}$

$$\Xi_{\mathrm{KT},-}^{(n)} = \left(\beta_m + \frac{\gamma_m - (\beta_m)^2}{\beta_m - \underline{\lambda}} \right)^{-1} \le \lambda_{\min}^{(n)}. \tag{7}$$

Let us call $\Xi_{\mathrm{KT},-}^{(n)}$ *the backward Kato-Temple shift*. This shift is newly introduced in this paper.

Lastly, we consider a lower bound of $\lambda_{\min}^{(n)}$ obtained from application of the Gerschgorin theorem [12] to the matrix $B^{(n)}$. For $i = 1, \dots, m$, let $K_i^{(n)}$ be

$$K_i^{(n)} = (q_i^{(n)} + e_i^{(n)}) - \left[\left(q_i^{(n)} e_{i-1}^{(n)} \right)^{\frac{1}{2}} + \left(q_{i+1}^{(n)} e_i^{(n)} \right)^{\frac{1}{2}} \right],$$

where $q_{m+1}^{(n)} = 0$ and $e_0^{(n)} = e_m^{(n)} = 0$, respectively. Then, a lower bound of $\lambda_{\min}^{(n)}$ is given as

$$\Xi_{\mathrm{G}}^{(n)} = \min_{1 \le i \le m} \{K_i^{(n)}\} \le \lambda_{\min}^{(n)}. \tag{8}$$

See [10] for detail. Let us call $\Xi_{\mathrm{G}}^{(n)}$ *the Gerschgorin shift*.

4. A new shift strategy

In this section, we present a shift strategy for the dqds algorithm. In this strategy, we prepare a "flag". According to value of this flag, we compute a shift in different ways. At the start of singular value computation, the value of this flag is set to "0". Note that the subroutine DLASQ in LAPACK has a function to detect failure of the Cholesky transform with shift. This failure occurs in the following cases:

- The computed shift is no less than the minimal eigenvalue $\lambda_{\min}^{(n)}$ of $B^{(n)}(B^{(n)})^\top$.
- The computed shift is smaller than $\lambda_{\min}^{(n)}$ but very close to it.

When the flag is "0" and this failure occures, the flag is changed to "1" before beginning of the next iteration. The flag "1" is reset to "0" when only deflation occurs. Regardless the value of the flag, when failure of the Cholesky transform with shift occurs, our implementation uses the original retry strategy implemented in LAPACK.

In the case where the value of the flag is "0", we determine shift as $\max\{\Theta_1, \Theta_2, \Theta_3\}$, where Θ_i $(i = 1, 2, 3)$ are given as follows.

- Setting of Θ_1: The quantity $Y(B^{(n)})$, which is theoretically positive, in (1) is computed. When numerically computed $Y(B^{(n)})$ is positive, we compute $(\Theta_{\mathrm{L}}^{(n)})^2$ according to (2) and set $\Theta_1 = (\Theta_{\mathrm{L}}^{(n)})^2$. When numerically computed $Y(B^{(n)})$ is non-positive, we compute $(\Theta_{\mathrm{gN},M}^{(n)})^2$ for $M = 2$ according to (3) and set $\Theta_1 = (\Theta_{\mathrm{gN},2}^{(n)})^2$.
- Setting of Θ_2: We compute $\bar{\lambda}$ in (5). If $\bar{\lambda} > q_m^{(n)}$ holds, then we compute $\Xi_{\mathrm{KT},+}^{(n)}$ in (4) and set $\Theta_2 = \Xi_{\mathrm{KT},+}^{(n)}$. Else, we set $\Theta_2 = 0$.
- Setting of Θ_3: If $\underline{\lambda} \geq \beta_m$, then we set $\Theta_3 = 0$. If the quantity $\gamma_m - (\beta_m)^2$, which is theoretically positive from (1), is numerically non-positive, then we set $\Theta_3 = 0$. If $\underline{\lambda} < \beta_m$ holds and numerically computed $\gamma_m - (\beta_m)^2$ is positive, then we compute $\Xi_{\mathrm{KT},-}^{(n)}$ in (7) and set $\Theta_3 = \Xi_{\mathrm{KT},-}^{(n)}$.

In the case where the value of the flag is "1", we compute the lower bound $\Xi_{\mathrm{G}}^{(n)}$ in (8). If $\Xi_{\mathrm{G}}^{(n)}$ is positive, then we use it as a shift. Else, we do not execute shift of origin, namely, shift is *zero*.

An efficient method to compute quantities $\bar{\lambda}$ in (5), $J_1(B^{(n)})$ and $J_2(B^{(n)})$ is required. The diagonals of $[B^{(n)}(B^{(n)})^T]^{-1}$ and $\{[B^{(n)}(B^{(n)})^T]^2\}^{-1}$ can be obtained through simple recurrence relations. These recurrence relations are found in [5, 6].

5. Numerical experiment

In this section, performance of the dqds algorithm with the new shift strategy introduced in the previous section is compared with that of DLASQ in LAPACK 3.4.0. We use a computer with the Intel(R) Core^{TM} i5-2500@3.30GHz CPU, 8 GB of memory, Linux operating system and gfortran version 4.4.5 compiler. We compile our source code with option -O2.

As input upper bidiagonal matrices, we prepare *random matrices* and *precision test matrices*. The random matrices are upper bidiagonal matrices where all the diagonals and the upper subdiagonals are given from *uniform pseudo-random numbers* in interval $[0, 1]$. The precision test matrices are upper bidiagonal matrices where all the diagonals and the upper subdiagonals are 1. The $m \times m$ precision test matrix has the same singular values with the $m \times m$ upper bidiagonal matrix $\tilde{B}_m$ where all the diagonals and the upper subdiagonals are 1 and -1, respectively. It is well-known that the matrix $\tilde{B}_m$ has singular values expressed by a trigonometric function as

$$\sigma_i = 2\sin\left(\frac{2i-1}{2(2m+1)}\pi\right) \quad (i = 1, \ldots, m).$$

Since singular values of the precision test matrices are exactly given, we can evaluate relative errors of computed singular values of these matrices.

Our shift strategy is implemented into the dqds algorithm by replacing the aggressive shift in DLASQ. The deflation, splitting and stopping criteria are same in both implementations. Moreover, the scaling strategy in DLASQ is also changed in our implementation. In this change, scaling size is changed to be smaller. Possibility of underflow becomes smaller according to increase of scaling size [3]. Therefore, our change of scaling strategy is fair.

Results of experiment are shown in Tables from 1 to 7. On the random matrices, we prepare 10 matrices for each size. Numerical computation is executed once for each matrix. Data of performance are averages among the 10 matrices. On the precision test matrices, numerical computation is executed once for each size of matrix. Errors of singular values shown in Table 5 are averages of absolute values of relative errors on all the singular values. Note that we executed numerical computations for Tables from 1 to 5 and for Tables 6 and 7 independently. Each column for percentage in Tables 6 and 7 represents zero shift, the Laguerre shift, the generalized Newton shift of order 2, the forward Kato-Temple shift, the backward Kato-Temple shift and the Gerschgorin shift, respectively.

We see that

- In all the cases, iteration numbers in our strategy are less than those in DLASQ.
- On the random matrices, except for the case where the matrix size is 10000, the averages of execution time in our strategy are shorter than those in DLASQ.
- On the precision test matrices, execution time in our strategy is longer than that in DLASQ in all the cases. While, the relative errors of the computed singular values in our strategy are smaller than those in DLASQ in all the cases.

On tables from 1 to 4, reversal between the numbers of iterations and the execution time is caused from frequency of splitting.

Table 1. Iteration numbers on random matrices.

Matrix size	DLASQ	Our strategy
10,000	93125.9	71607.1
30,000	283183.2	219723.0
50,000	473910.8	370932.4
100,000	951654.1	746296.4
300,000	2868929.4	2256803.1
500,000	4783286.3	3766986.9
1,000,000	9585259.1	7547005.2

Table 2. Execution time on random matrices (in sec.).

Matrix size	DLASQ	Our strategy
10,000	1.66	1.73
30,000	12.19	11.86
50,000	31.27	30.42
100,000	114.73	107.95
300,000	875.34	800.45
500,000	2203.63	2016.12
1,000,000	8014.09	7185.34

Table 3. Iteration numbers on precision test matrices.

Matrix size	DLASQ	Our strategy
10,000	40020	32833
30,000	119214	93267
50,000	194322	152796
100,000	375526	302480
300,000	1068813	902148
500,000	1741156	1502034
1,000,000	3381461	3001909

Table 4. Execution time on precision test matrices (in sec.).

Matrix size	DLASQ	Our strategy
10,000	2.06	3.00
30,000	18.10	25.73
50,000	48.45	70.80
100,000	185.94	282.14
300,000	1640.02	2692.59
500,000	4519.11	7627.34
1,000,000	17717.18	30834.91

Table 5. Errors of singular values on precision test matrices.

Matrix size	DLASQ	Our strategy
10,000	1.63×10^{-14}	1.36×10^{-15}
30,000	1.05×10^{-14}	2.24×10^{-15}
50,000	1.05×10^{-14}	2.82×10^{-15}
100,000	9.21×10^{-15}	2.45×10^{-15}
300,000	9.47×10^{-15}	3.97×10^{-15}
500,000	1.17×10^{-14}	4.22×10^{-15}
1,000,000	1.01×10^{-14}	4.73×10^{-15}

6. Conclusions

A new shift strategy for the dqds algorithm is presented. This strategy utilizes shifts obtained by applying the Kato-Temple inequality on matrix eigenvalues. In numerical experiment, iteration numbers in the dqds algorithm with our shift strategy are less than those with the aggressive shift in all the cases. We have some more numerical examples on other types of test matrices which show the same tendency. Therefore, it can be expected that the computed singular values with the new shift strategy have higher precision than those with the aggressive shift.

Table 6. Percentage of numbers of iteration with each shift to the total iteration numbers on random matrices.

Matrix size	zero	Lag.	g. N.	KT+	KT−	Ger.
10,000	48.92	43.48	1.92	1.26	1.98	2.44
30,000	50.69	41.55	1.89	1.26	1.99	2.62
50,000	51.52	40.74	1.87	1.23	1.97	2.68
100,000	52.08	40.12	1.87	1.23	1.96	2.74
300,000	52.70	39.48	1.86	1.23	1.96	2.77
500,000	52.84	39.32	1.86	1.22	1.96	2.79
1,000,000	52.97	39.18	1.87	1.23	1.96	2.80

Table 7. Percentage of numbers of iteration with each shift to the total iteration numbers on precision test matrices.

Matrix size	zero	Lag.	g. N.	KT+	KT−	Ger.
10,000	2.56	32.65	3.83	30.44	30.51	0
30,000	1.06	33.04	1.55	32.16	32.20	0
50,000	0.50	33.20	0.82	32.72	32.76	0
100,000	0.23	33.24	0.38	33.06	33.09	0
300,000	0.07	33.31	0.11	33.25	33.26	0
500,000	0.04	33.32	0.06	33.29	33.29	0
1,000,000	0.02	33.32	0.03	33.31	33.31	0

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