# Implementation of the Orthogonal QD Algorithm for Lower Tridiagonal Matrices 

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## 1. Introduction

In 1997, von Matt proposed an algorithm, based on Rutishauser's qd algorithm [1], called orthogonal qd algorithm with shifts (oqds algorithm) for computing the singular values of bidiagonal matrices in which all the transformations consist of Givens rotations [2]. It is shown that the oqds algorithm is also applicable to general triangular matrices [3].

In this paper, we shall consider the application of the oqds algorithm to lower tridiagonal matrices. It allows us to use lower-tridiagonalization as pre-processing instead of bidiagonalization. The lower-tridiagonalization is less computational complexity than the bidiagonalization. Further, we can adopt BLAS Level 2.5 routines with efficient cache reuse which are faster than BLAS Level 2 routines for implementation of the lower-tridiagonalization. The oqds algorithm for lower tridiagonal matrices thus enables us to reduce the total computation time to obtain the singular values of general triangular matrices.
For practical use, we should design good shift strategies for convergence acceleration and good convergence criteria for accurate computation. However, appropriate shift strategies and convergence criteria for lower tridiagonal matrices have not been proposed yet. In this paper, we propose a shift strategy consisting of the generalized Newton shift and associated two methods, Laguerre shift and Kato-Temple shift, and the well known Gerschgorin shift. Moreover, we design new convergence criteria for deflation and splitting required for the implementation of the oqds algorithm. By the criteria, we can do the convergence test for lower tridiagonal matrices. At the end, we show some results of numerical experiments to compare the oqds algorithms for bidiagonal matrices and for lower tridiagonal matrices.

## 2. Orthogonal QD Algorithm for Lower Tridiagonal Matrix

Let

$$
L=\left[\begin{array}{ccccc}
\alpha_{1} & & & & \\
\beta_{1} & \alpha_{2} & & & \\
\gamma_{1} & \beta_{2} & \alpha_{3} & & \\
& \ddots & \ddots & \ddots & \\
& & \gamma_{n-2} & \beta_{n-1} & \alpha_{n}
\end{array}\right]
$$

be an $n$-by- $n$ lower tridiagonal matrix. One step of Cholesky LR method [4] with shift $\sigma^{2}$ transforms the lower tridiagonal
matrix $L$ into the upper tridiagonal matrix $U$ by

$$
\begin{equation*}
L^{T} L-\sigma^{2} I=U^{T} U \tag{2}
\end{equation*}
$$

Then, we set $L:=U^{T}$. By repeating this procedure iteratively, the diagonal elements of the matrix $L$ converge to the singular values of the matrix $L$ and the non-diagonal elements get into zero. The formulation of this algorithm (also containing shift method) for lower didiagonal matrices is called orthogonal qd algorithm with shifts (oqds algorithm). In this paper, we expand this algorithm for lower tridiagonal matrices.

## 3. Shift Strategy

In the implicit Cholesky decomposition, proper choice of the shift value $\sigma$ significantly accelerates convergence of the oqds algorithm. The shift value $\sigma$ must be smaller than the minimum singular value of the matrix $L$ to keep the positivedefiniteness of $U^{T} U$. Therefore, we need a method to estimate the lower bound of the minimum singular value of the lower tridiagonal matrix $L$ or the minimum eigenvalue of $L^{T} L$.

In this section, we discuss four types of lower bounds of the minimum singular value or eigenvalue and design shift method using them.

### 3.1 Gerschgorin Shift

Theorem 3.1 (Gerschgorin [5]). For an n-by-n matrix $A=$ $\left(a_{i j}\right)$, let us define

$$
\begin{equation*}
R_{i}:=\sum_{k \neq i}\left|a_{i k}\right| . \tag{3}
\end{equation*}
$$

Then, for any eigenvalue $\lambda$ of $A$, there exists an integer $i$ such as

$$
\begin{equation*}
\left|\lambda-a_{i i}\right| \leq R_{i} . \tag{4}
\end{equation*}
$$

If the matrix $A$ is positive-definite symmetric, $\min \left(a_{i i}-R_{i}\right)$ gives a lower bound of the eigenvalues since all the eigenvalues of $A$ are positive real number.

### 3.2 Generalized Newton shift

For a positive-definite symmetric matrix $A$ and an arbitrary positive integer $p$, the value of $\left(\operatorname{Tr}\left(A^{-p}\right)\right)^{-1 / p}$ is a lower bound of the eigenvalues of $A$. Then, finding the value of $\operatorname{Tr}\left\{\left(L^{T} L\right)^{-p}\right\}$, we get a lower bound of the singular values of $L$. We consider a method of computing the value of $\operatorname{Tr}\left\{\left(L^{T} L\right)^{-p}\right\}$ in this subsection.

Let $\bar{L}$ be an $n$-by- $n$ lower tridiagonal matrix,

$$
\bar{L}=\left[\begin{array}{ccccc}
\bar{\alpha}_{1} & & & &  \tag{5}\\
\bar{\beta}_{1} & \bar{\alpha}_{2} & & & \\
\bar{\gamma}_{1} & \bar{\beta}_{2} & \bar{\alpha}_{3} & & \\
& \ddots & \ddots & \ddots & \\
& & \bar{\gamma}_{n-2} & \bar{\beta}_{n-1} & \bar{\alpha}_{n}
\end{array}\right]
$$

determined from $L$ with shift $s$ by

$$
\begin{equation*}
\bar{L} \bar{L}^{T}=L L^{T}-s I . \tag{6}
\end{equation*}
$$

The relationships among elements are given by

$$
\begin{gather*}
\bar{\alpha}_{i}^{2}+\bar{\beta}_{i-1}^{2}+\bar{\gamma}_{i-2}^{2}=\alpha_{i}^{2}+\beta_{i-1}^{2}+\gamma_{i-2}^{2}-s  \tag{7}\\
\bar{\beta}_{i-2} \bar{\gamma}_{i-2}+\bar{\alpha}_{i-1} \bar{\beta}_{i-1}=\beta_{i-2} \gamma_{i-2}+\alpha_{i-1} \beta_{i-1}  \tag{8}\\
\bar{\alpha}_{i-2} \bar{\gamma}_{i-2}=\alpha_{i-2} \gamma_{i-2} \tag{9}
\end{gather*}
$$

Differentiating equations (7)-(9) with respect to $s$, we obtain

$$
\begin{gather*}
2 \bar{\alpha}_{i} \bar{\alpha}_{i}^{\prime}+2 \bar{\beta}_{i-1} \bar{\beta}_{i-1}^{\prime}+2 \bar{\gamma}_{i-2} \bar{\gamma}_{i-2}^{\prime}=-1,  \tag{10}\\
\bar{\beta}_{i-2}^{\prime} \bar{\gamma}_{i-2}+\bar{\beta}_{i-2} \bar{\gamma}_{i-2}^{\prime}+\bar{\alpha}_{i-1}^{\prime} \bar{\beta}_{i-1}+\bar{\alpha}_{i-1} \bar{\beta}_{i-1}^{\prime}=0,  \tag{11}\\
\bar{\alpha}_{i-2}^{\prime} \bar{\gamma}_{i-2}+\bar{\alpha}_{i-2} \bar{\gamma}_{i-2}^{\prime}=0 . \tag{12}
\end{gather*}
$$

Note that the $\alpha_{i}, \beta_{i}, \gamma_{i}$ are independent of $s$ but the $\bar{\alpha}_{i}, \bar{\beta}_{i}, \bar{\gamma}_{i}$ are not. Differentiating once more, we get

$$
\begin{align*}
& \begin{array}{l}
2 \bar{\alpha}_{i}^{\prime 2}+2 \bar{\alpha}_{i} \bar{\alpha}_{i}^{\prime \prime}+2 \bar{\beta}_{i-1}^{\prime 2} \\
\quad+2 \bar{\beta}_{i-1} \bar{\beta}_{i-1}^{\prime \prime}+2 \bar{\gamma}_{i-2}^{\prime 2}+2 \bar{\gamma}_{i-2} \bar{\gamma}_{i-2}^{\prime \prime}=0 \\
\bar{\alpha}_{i-2}^{\prime \prime} \bar{\gamma}_{i-2}+2 \bar{\alpha}_{i-2}^{\prime} \bar{\gamma}_{i-2}^{\prime}+\bar{\alpha}_{i-2} \bar{\gamma}_{i-2}^{\prime \prime}=0
\end{array} \\
& \begin{array}{l}
\bar{\beta}_{i-2}^{\prime \prime} \bar{\gamma}_{i-2}+2 \bar{\beta}_{i-2}^{\prime} \bar{\gamma}_{i-2}^{\prime}+\bar{\beta}_{i-2} \bar{\gamma}_{i-2}^{\prime \prime} \\
\\
\quad+\bar{\alpha}_{i-1}^{\prime \prime} \bar{\beta}_{i-1}+2 \bar{\alpha}_{i-1}^{\prime} \bar{\beta}_{i-1}^{\prime}+\bar{\alpha}_{i-1} \bar{\beta}_{i-1}^{\prime \prime}=0
\end{array} \tag{13}
\end{align*}
$$

Let us write the eigenvalues of the matrix $L L^{T}$ by $\lambda_{1}, \lambda_{2}, \cdots, \lambda_{n}$. Then, the characteristic polynomial of the ma$\operatorname{trix} \bar{L} \bar{L}^{T}$

$$
\begin{align*}
f(s) & =\operatorname{det}\left(L L^{T}-s I\right) \\
& =\left(\lambda_{1}-s\right)\left(\lambda_{2}-s\right) \cdots\left(\lambda_{n}-s\right), \tag{16}
\end{align*}
$$

because of the triangularity of the matrix $L$, is expressed by

$$
\begin{equation*}
f(s)=\bar{\alpha}_{1} \bar{\alpha}_{2} \cdots \bar{\alpha}_{n} . \tag{17}
\end{equation*}
$$

Let us define

$$
\begin{align*}
g(s) & :=-\frac{f^{\prime}(s)}{f(s)}=-2 \frac{\bar{\alpha}_{1}^{\prime}}{\bar{\alpha}_{1}}-2 \frac{\bar{\alpha}_{2}^{\prime}}{\bar{\alpha}_{2}}-\cdots-2 \frac{\bar{\alpha}_{n}^{\prime}}{\bar{\alpha}_{n}},  \tag{18}\\
h(s) & :=g^{\prime}(s) \\
& =-2 \frac{\bar{\alpha}_{1}^{\prime \prime} \bar{\alpha}_{1}-\bar{\alpha}_{1}^{\prime 2}}{\bar{\alpha}_{1}^{2}}-\cdots-2 \frac{\bar{\alpha}_{n}^{\prime \prime} \bar{\alpha}_{n}-\bar{\alpha}_{n}^{\prime 2}}{\bar{\alpha}_{n}^{2}} \tag{19}
\end{align*}
$$

so that $g(0)=\operatorname{Tr}\left\{\left(L^{T} L\right)^{-1}\right\}$ and $h(0)=\operatorname{Tr}\left\{\left(L^{T} L\right)^{-2}\right\}$. Each $\bar{\alpha}_{i}$ tends to $\alpha_{i}$ as $s \rightarrow 0$. Hence, we can calculate the value of $\bar{\alpha}_{i}^{\prime}, \bar{\beta}_{i}^{\prime}, \bar{\gamma}_{i}^{\prime}, \bar{\alpha}_{i}^{\prime \prime}, \bar{\beta}_{i}^{\prime \prime}, \bar{\gamma}_{i}^{\prime \prime}$ at $s=0$ from $\alpha_{i}, \beta_{i}, \gamma_{i}$ by using (10)-(15), and then $g(0)$ and $h(0)$ by (18) and (19).

It is clear by the definition of $g(0)$ and $h(0)$ that the values are always nonnegative without numerical error (in infiniteprecision arithmetic). This procedure is a expansion of the method obtaining the traces for didiagonal matrices introduced as a part of Algebraic shift in [3].

### 3.3 Laguerre Shift

If we already have the value of $\operatorname{Tr}\left\{\left(L L^{T}\right)^{-1}\right\}$ and $\operatorname{Tr}\left\{\left(L L^{T}\right)^{-2}\right\}$, we could improve the sharpness of the shift by $O(1)$ operation. Laguerre shift is one of the methods to improve the shift value.

Theorem 3.2 (Laguerre [7]). For an n-by-n positive-definite symmetric penta-diagonal matrix $B=L L^{T}$, let $\theta$ be the following value:

$$
\theta:=\frac{n}{\operatorname{Tr}\left(B^{-1}\right)+\sqrt{(n-1)\left(n \operatorname{Tr}\left(B^{-2}\right)-\operatorname{Tr}\left(B^{-1}\right)^{2}\right)}} .
$$

Then, the $\theta$ is a lower bound of the eigenvalues of $B$ which is greater than $\operatorname{Tr}\left(B^{-1}\right)^{-1}$ and $\operatorname{Tr}\left(B^{-2}\right)^{-1 / 2}$.

If the value $n \operatorname{Tr}\left(B^{-2}\right)-\operatorname{Tr}\left(B^{-1}\right)^{2}$ is negative, Laguerre shift is useless. In that case, we adopt the generalized Newton shift.

### 3.4 Kato-Temple Shift

There is another lowerbound, Kato-temple shift.
Theorem 3.3 (Kato-Temple [8]). For an n-by-n symmetric matrix $A_{n}$, let $A_{n-1}$ denote the submatrix of $A_{n}$ obtained by deleting the last row and column. For any lower bound $\lambda^{*}$ of the eigenvalues of $A_{n-1}$, and for any $x \in \mathbb{R}^{n},\|x\|=1$, let $\rho=x^{T} A x$. Then, if $\rho<\lambda^{*}$, the value

$$
\rho-\frac{\left\|A_{n} x-\rho x\right\|^{2}}{\lambda^{*}-\rho} \leq \lambda_{\min }\left(A_{n}\right)
$$

gives a lower bound of the eigenvalues of $A_{n}$.
We choose $x=(0, \ldots, 0,1)^{T}$. The method requires $\lambda^{*}$ which is a lower bound for the submatrix $A_{n-1}$, but the generalized Newton method enables us to find the lower bound of $A_{n-1}$ in computation of the lower bound of $A_{n}$. Consequently, we obtain one more improved shift value by $O(1)$ operation. The procedure of the proposed shift composed by the generalized Newton, Laguerre and Kato-Temple is shown in Algorithm 1. We adopt the largest value of them.

## 4. Convergence Criteria

It is nontrivial how to assess a series of matrices generated by the iterative process of the oqds algorithm converges sufficiently.Besides, in the implementation of this algorithm, deflation and splitting are required for activating the shift method. In this section, we consider the situation that deflation or splitting is available where the values of subdiagonal and second-subdiagonal elements are so small.

Let us write

$$
\hat{L}:=L-\beta_{k} \mathbf{e}_{k+1} \mathbf{e}_{k}{ }^{T}
$$

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```

Algorithm 1 Proposed shift (algshift( $L$ ))

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```

Algorithm 1 Proposed shift (algshift( $L$ ))
$\alpha_{1}^{\prime}:=-1 /\left(2 \alpha_{1}\right)$
$\alpha_{1}^{\prime}:=-1 /\left(2 \alpha_{1}\right)$
$\beta_{1}^{\prime}:=-\alpha_{1}^{\prime} \beta_{1} / \alpha_{1}$
$\beta_{1}^{\prime}:=-\alpha_{1}^{\prime} \beta_{1} / \alpha_{1}$
$\gamma_{1}^{\prime}:=-\alpha_{1}^{\prime} \gamma_{1} / \alpha_{1}$
$\gamma_{1}^{\prime}:=-\alpha_{1}^{\prime} \gamma_{1} / \alpha_{1}$
$\alpha_{2}^{\prime}:=\left(-\beta_{1} \beta_{1}^{\prime}-0.5\right) / \alpha_{2}$
$\alpha_{2}^{\prime}:=\left(-\beta_{1} \beta_{1}^{\prime}-0.5\right) / \alpha_{2}$
$\beta_{2}^{\prime}:=-\left(\gamma_{1}^{\prime} \beta_{1}+\gamma_{1} \gamma_{1}^{\prime}+\alpha_{2}^{\prime} \beta_{2}\right) / \alpha_{2}$
$\beta_{2}^{\prime}:=-\left(\gamma_{1}^{\prime} \beta_{1}+\gamma_{1} \gamma_{1}^{\prime}+\alpha_{2}^{\prime} \beta_{2}\right) / \alpha_{2}$
$\alpha_{3}^{\prime}:=-\left(1+2 \times \gamma_{1} \gamma_{1}^{\prime}+2 \beta_{2} \beta_{2}^{\prime}\right) /\left(2 \alpha_{3}\right)$
$\alpha_{3}^{\prime}:=-\left(1+2 \times \gamma_{1} \gamma_{1}^{\prime}+2 \beta_{2} \beta_{2}^{\prime}\right) /\left(2 \alpha_{3}\right)$
$\alpha_{1}^{\prime \prime}:=-\alpha_{1}^{\prime 2} / \alpha_{1}$
$\alpha_{1}^{\prime \prime}:=-\alpha_{1}^{\prime 2} / \alpha_{1}$
$\beta_{1}^{\prime \prime}:=-\left(\alpha_{1}^{\prime \prime} \beta_{1}+2 \alpha_{1}^{\prime} \beta_{1}^{\prime}\right) / \alpha_{1}$
$\beta_{1}^{\prime \prime}:=-\left(\alpha_{1}^{\prime \prime} \beta_{1}+2 \alpha_{1}^{\prime} \beta_{1}^{\prime}\right) / \alpha_{1}$
$\gamma_{1}^{\prime \prime}:=-\left(\alpha_{1}^{\prime \prime} \gamma_{1}+2 \alpha_{1}^{\prime} \gamma_{1}^{\prime}\right) / \alpha_{1}$
$\gamma_{1}^{\prime \prime}:=-\left(\alpha_{1}^{\prime \prime} \gamma_{1}+2 \alpha_{1}^{\prime} \gamma_{1}^{\prime}\right) / \alpha_{1}$
$\alpha_{2}^{\prime \prime}:=-\left(\beta_{1}^{\prime 2}+\beta_{1} \beta_{1}^{\prime \prime}+\alpha_{2}^{\prime 2}\right) / \alpha_{2}$
$\alpha_{2}^{\prime \prime}:=-\left(\beta_{1}^{\prime 2}+\beta_{1} \beta_{1}^{\prime \prime}+\alpha_{2}^{\prime 2}\right) / \alpha_{2}$
$\beta_{2}^{\prime \prime}:=-\left(\gamma_{1}^{\prime \prime} \beta_{1}+2 \gamma_{1}^{\prime} \beta_{1}^{\prime}+\gamma_{1} \beta_{1}^{\prime \prime}+\alpha_{2}^{\prime \prime} \beta_{2}+2 \alpha_{2}^{\prime} \beta_{2}^{\prime}\right) / \alpha_{2}$
$\beta_{2}^{\prime \prime}:=-\left(\gamma_{1}^{\prime \prime} \beta_{1}+2 \gamma_{1}^{\prime} \beta_{1}^{\prime}+\gamma_{1} \beta_{1}^{\prime \prime}+\alpha_{2}^{\prime \prime} \beta_{2}+2 \alpha_{2}^{\prime} \beta_{2}^{\prime}\right) / \alpha_{2}$
$\alpha_{3}^{\prime \prime}:=-\left(\gamma_{1}^{\prime 2}+\gamma_{1} \gamma_{1}^{\prime \prime}+\beta_{2}^{\prime 2}+\beta_{2} \beta_{2}^{\prime \prime}+\alpha_{3}^{\prime 2}\right) / \alpha_{3}$
$\alpha_{3}^{\prime \prime}:=-\left(\gamma_{1}^{\prime 2}+\gamma_{1} \gamma_{1}^{\prime \prime}+\beta_{2}^{\prime 2}+\beta_{2} \beta_{2}^{\prime \prime}+\alpha_{3}^{\prime 2}\right) / \alpha_{3}$
for $i=4$ to $N$ do
for $i=4$ to $N$ do
$\gamma_{i-2}^{\prime}:=-\alpha_{i-2}^{\prime} \gamma_{i-2} / \alpha_{i-2}$
$\gamma_{i-2}^{\prime}:=-\alpha_{i-2}^{\prime} \gamma_{i-2} / \alpha_{i-2}$
$\beta_{i-1}^{\prime}:=-\left(\beta_{i-2}^{\prime} \gamma_{i-2}+\beta_{i-2} \gamma_{i-2}^{\prime}+\alpha_{i-1}^{\prime} \beta_{i-1}\right) / \alpha_{i-1}$
$\beta_{i-1}^{\prime}:=-\left(\beta_{i-2}^{\prime} \gamma_{i-2}+\beta_{i-2} \gamma_{i-2}^{\prime}+\alpha_{i-1}^{\prime} \beta_{i-1}\right) / \alpha_{i-1}$
$\alpha_{i}^{\prime}:=-\left(1+2 \beta_{i-1} \beta_{i-1}^{\prime}+2 \gamma_{i-2} \gamma_{i-2}^{\prime}\right) /\left(2 \alpha_{i}\right)$
$\alpha_{i}^{\prime}:=-\left(1+2 \beta_{i-1} \beta_{i-1}^{\prime}+2 \gamma_{i-2} \gamma_{i-2}^{\prime}\right) /\left(2 \alpha_{i}\right)$
$\gamma_{i-2}^{\prime \prime}:=-\left(\alpha_{i-2}^{\prime \prime} \gamma_{i-2}+2 \alpha_{i-2}^{\prime} \gamma_{i-2}^{\prime}\right) / \alpha_{i-2}$
$\gamma_{i-2}^{\prime \prime}:=-\left(\alpha_{i-2}^{\prime \prime} \gamma_{i-2}+2 \alpha_{i-2}^{\prime} \gamma_{i-2}^{\prime}\right) / \alpha_{i-2}$
$\beta_{i-1}^{\prime \prime}:=-\left(\beta_{i-2}^{\prime \prime} \gamma_{i-2}+2 \beta_{i-2}^{\prime} \gamma_{i-2}^{\prime}\right.$
$\beta_{i-1}^{\prime \prime}:=-\left(\beta_{i-2}^{\prime \prime} \gamma_{i-2}+2 \beta_{i-2}^{\prime} \gamma_{i-2}^{\prime}\right.$
$\left.+\beta_{i-2} \gamma_{i-2}^{\prime \prime}+\alpha_{i-1}^{\prime \prime} \beta_{i-1}+2 \alpha_{i-1}^{\prime} \beta_{i-1}^{\prime}\right) / \alpha_{i-1}$
$\left.+\beta_{i-2} \gamma_{i-2}^{\prime \prime}+\alpha_{i-1}^{\prime \prime} \beta_{i-1}+2 \alpha_{i-1}^{\prime} \beta_{i-1}^{\prime}\right) / \alpha_{i-1}$
$\alpha_{i}^{\prime \prime}:=-\left(\alpha_{i}^{\prime 2}+\beta_{i-1}^{\prime}{ }^{2}+\beta_{i-1} \beta_{i-1}^{\prime \prime}+\gamma_{i-2}^{\prime}{ }^{2}+\gamma_{i-2} \gamma_{i-2}^{\prime \prime}\right) / \alpha_{i}$
$\alpha_{i}^{\prime \prime}:=-\left(\alpha_{i}^{\prime 2}+\beta_{i-1}^{\prime}{ }^{2}+\beta_{i-1} \beta_{i-1}^{\prime \prime}+\gamma_{i-2}^{\prime}{ }^{2}+\gamma_{i-2} \gamma_{i-2}^{\prime \prime}\right) / \alpha_{i}$
end for
end for
$\operatorname{tr} 1:=0$
$\operatorname{tr} 1:=0$
for $i=1$ to $N-1$ do
for $i=1$ to $N-1$ do
$\operatorname{tr} 1:=\operatorname{tr} 1-\left(2 \alpha_{i}^{\prime} / \alpha_{i}\right)$
$\operatorname{tr} 1:=\operatorname{tr} 1-\left(2 \alpha_{i}^{\prime} / \alpha_{i}\right)$
end for
end for
$\operatorname{tr} 2:=0$
$\operatorname{tr} 2:=0$
for $i=1$ to $N-1$ do
for $i=1$ to $N-1$ do
$\operatorname{tr} 2:=\operatorname{tr} 2-2\left(\alpha_{i}^{\prime \prime} \alpha_{i}-\alpha_{i}^{\prime 2}\right) / \alpha_{i}^{2}$
$\operatorname{tr} 2:=\operatorname{tr} 2-2\left(\alpha_{i}^{\prime \prime} \alpha_{i}-\alpha_{i}^{\prime 2}\right) / \alpha_{i}^{2}$
end for
end for
$\lambda^{*}:=1 / \operatorname{sqrt}(t r 2)$
$\lambda^{*}:=1 / \operatorname{sqrt}(t r 2)$
$t m p:=n \times t r 2-t r 1^{2}$
$t m p:=n \times t r 2-t r 1^{2}$
if $t m p>0$ then
if $t m p>0$ then
$\lambda^{*}:=\max \left(\lambda^{*}, n /(\operatorname{tr} 1+\sqrt{(n-1) \times \operatorname{tmp}})\right)$
$\lambda^{*}:=\max \left(\lambda^{*}, n /(\operatorname{tr} 1+\sqrt{(n-1) \times \operatorname{tmp}})\right)$
end if
end if
$\operatorname{tr} 1:=\operatorname{tr} 1-\left(2 \alpha_{N}^{\prime} / \alpha_{N}\right)$
$\operatorname{tr} 1:=\operatorname{tr} 1-\left(2 \alpha_{N}^{\prime} / \alpha_{N}\right)$
$\operatorname{tr} 2:=\operatorname{tr} 2-2\left(\alpha_{N}^{\prime \prime} \alpha_{N}-\alpha_{N}^{\prime}{ }^{2}\right) / \alpha_{N}^{2}$
$\operatorname{tr} 2:=\operatorname{tr} 2-2\left(\alpha_{N}^{\prime \prime} \alpha_{N}-\alpha_{N}^{\prime}{ }^{2}\right) / \alpha_{N}^{2}$
shift $:=1 / \operatorname{sqrt}(\operatorname{tr} 2)$
shift $:=1 / \operatorname{sqrt}(\operatorname{tr} 2)$
$x:=(0, \ldots, 0,1)^{T}$
$x:=(0, \ldots, 0,1)^{T}$
$\rho:=x^{T} L_{n-1} x$
$\rho:=x^{T} L_{n-1} x$
if $\rho<\lambda^{*}$ then
if $\rho<\lambda^{*}$ then
shift $:=\max \left(\right.$ shift,$\left.\rho-\left\|A_{n} x-\rho x\right\|^{2} /\left(\lambda^{*}-\rho\right)\right)$
shift $:=\max \left(\right.$ shift,$\left.\rho-\left\|A_{n} x-\rho x\right\|^{2} /\left(\lambda^{*}-\rho\right)\right)$
end if
end if
tmp $:=n \times \operatorname{tr} 2-t r 1^{2}$
tmp $:=n \times \operatorname{tr} 2-t r 1^{2}$
if $t m p>0$ then
if $t m p>0$ then
shift $:=\max ($ shift,$n /(\operatorname{tr} 1+\sqrt{(n-1) \times \operatorname{tmp})})$
shift $:=\max ($ shift,$n /(\operatorname{tr} 1+\sqrt{(n-1) \times \operatorname{tmp})})$
end if
end if
return shift

```
```

    return shift
    ```
```

which is the matrix equal to $L$ except for zero at $(k+1, k)$-entry. Then

$$
\begin{align*}
& L^{T} L=\hat{L}^{T} \hat{L}+E_{1}  \tag{20}\\
& L L^{T}=\hat{L} \hat{L}^{T}+E_{2} \tag{21}
\end{align*}
$$

hold, where

$$
\begin{align*}
E_{1}:=\beta^{2} \mathbf{e}_{k} \mathbf{e}_{k}^{T} & +\alpha_{k+1} \beta_{k}\left(\mathbf{e}_{k} \mathbf{e}_{k+1}^{T}+\mathbf{e}_{k+1} \mathbf{e}_{k}^{T}\right) \\
& +\beta_{k} \gamma_{k-1}\left(\mathbf{e}_{k-1} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k-1}^{T}\right),  \tag{22}\\
E_{2}:=\beta^{2} \mathbf{e}_{k+1} \mathbf{e}_{k+1}^{T} & +\alpha_{k} \beta_{k}\left(\mathbf{e}_{k-1} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k-1}^{T}\right) \\
& +\beta_{k} \gamma_{k}\left(\mathbf{e}_{k+1} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k+1}^{T}\right) . \tag{23}
\end{align*}
$$

Theorem 4.1 (Weyl's monotonicity theorem [9], [10]). For an n-by-n positive-definite matrix $A$, let $\lambda_{i}(A)$ denote the $i$-th largest eigenvalue of $A$. Then, there exist reals $u_{i}$ and $v_{i}$ such that

$$
\begin{align*}
\lambda_{i}\left(L^{T} L\right) & =\lambda_{i}\left(\hat{L}^{T} \hat{L}\right)+u_{i}\left\|E_{1}\right\|_{1},  \tag{24}\\
\lambda_{i}\left(L L^{T}\right) & =\lambda_{i}\left(\hat{L} \hat{L}^{T}\right)+v_{i}\left\|E_{2}\right\|_{1} \tag{25}
\end{align*}
$$

where $\left|u_{i}\right| \leq 1,\left|v_{i}\right| \leq 1$.
From the definitions (22) and (23) of $E_{1}$ and $E_{2}$, we have

$$
\begin{align*}
& \left\|E_{1}\right\|_{1}=\left\|E_{1}\right\|_{\infty}=\left|\beta_{k}\right|\left(\left|\alpha_{k+1}\right|+\left|\beta_{k}\right|+\left|\gamma_{k-1}\right|\right),  \tag{26}\\
& \left\|E_{2}\right\|_{1}=\left\|E_{2}\right\|_{\infty}=\left|\beta_{k}\right|\left(\left|\alpha_{k}\right|+\left|\beta_{k}\right|+\left|\gamma_{k}\right|\right) . \tag{27}
\end{align*}
$$

By Weyl's monotonicity theorem, we thus get the numerical deflation or splitting criterion to neglect a subdiagonal element $\beta_{k}$ :

$$
\begin{equation*}
\sigma^{2}+\left|\beta_{k}\right|\left(\left|\beta_{k}\right|+\min \left(\left|\alpha_{k+1}\right|+\left|\gamma_{k-1}\right|,\left|\alpha_{k}\right|+\left|\gamma_{k}\right|\right)\right) \simeq \sigma^{2} \tag{28}
\end{equation*}
$$

where ' $\simeq$ ' means that the left-hand side and the right-hand side are numerically equal. We assume that $\beta_{k}$ is so small and negligible provided that (28) holds numerically.

Similarly, we get the numerical criterion for neglecting a second-subdiagonal element $\gamma_{k}$. On the setting of

$$
\hat{L}:=L-\gamma_{k} \mathbf{e}_{k+2} \mathbf{e}_{k}^{T},
$$

the perturbation matrices are given by

$$
\begin{aligned}
E_{1}^{\prime}:=\gamma^{2} \mathbf{e}_{k} \mathbf{e}_{k}^{T}+ & \alpha_{k+2} \gamma_{k}\left(\mathbf{e}_{k+2} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k+2}^{T}\right) \\
+ & \beta_{k+1} \gamma_{k}\left(\mathbf{e}_{k+1} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k+1}^{T}\right), \\
E_{2}^{\prime}:=\gamma^{2} \mathbf{e}_{k+2} \mathbf{e}_{k+2}^{T} & +\alpha_{k} \gamma_{k}\left(\mathbf{e}_{k-2} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k-2}^{T}\right) \\
& +\beta_{k} \gamma_{k}\left(\mathbf{e}_{k-1} \mathbf{e}_{k}^{T}+\mathbf{e}_{k} \mathbf{e}_{k-1}^{T}\right) .
\end{aligned}
$$

Then, by evaluating the 1 - and $\infty$-norms of these matrices, we obtain the criterion for neglecting a second-subdiagonal element $\gamma_{k}$ as follows:

$$
\begin{equation*}
\sigma^{2}+\left|\gamma_{k}\right|\left(\left|\gamma_{k}\right|+\min \left(\left|\alpha_{k+2}\right|+\left|\beta_{k+1}\right|,\left|\alpha_{k}\right|+\left|\beta_{k}\right|\right)\right) \simeq \sigma^{2} . \tag{29}
\end{equation*}
$$

For the matrices in iteration, we perform deflation and splitting as follows:

1) If $\beta_{n-1}$ and $\gamma_{n-2}$ in the last row satisfy the criteria (28) and (29), then we deflate the matrix by deleting the last row and column.
2) If $\beta_{k-1}, \gamma_{k-1}$ and $\gamma_{k-2}$ satisfy the criteria (28) and (29), then we split the matrix into two submatrices formed by rows and columns 1 to $k-1$ and $k$ to $n$, respectively.

## 5. Numerical Experiments

Some numerical experiments were performed for the oqds algorithms for bidiagonal matrices and for lower tridiagonal matrices. The singular values of square random matrices were computed by the oqds algorithm for bidiagonal matrices by von Matt and by the oqds algorithm for lower tridiagonal matrices which we propose. It should be noted that: The oqds for bidiagonal matrices were applied to random bidiagonal matrices and the proposed oqds algorithm for lower tridiagonal matrices were applied to random lower tridiagonal matrix. The numerical experiments were performed on a Linux PC with Intel Core i7 920 (Nehalem) 2.66 GHz and DDR3-1066 12GB memory. Table 1 shows the computation time of each algorithm. The first row shows the size of matrices. The second and the third rows show the computation time taken by the oqds algorithm for bidiagonal matrices and for lower tridiagonal matrices, respectively.

Table 1
Computation time (seconds)

| matrix size | 10000 | 20000 | 30000 |
| :---: | :---: | :---: | :---: |
| oqds for bidiagonal | 11.764 | 43.243 | 93.080 |
| proposed oqds for lower tridiagonal | 27.089 | 100.013 | 210.225 |

### 5.1 Discussion

Hence, in order to compute the eigenvalues of matrices of the same size, the oqds algorithm for lower tridiagonal matrices is expected to take a longer computation time than the oqds for bidiagonal matrices. From Table 1, we observe that the computation time in the former algorithm is not extremely longer than the latter algorithm: the former is two or three times slower than the latter.
This observation demonstrates that the oqds algorithm for lower tridiagonal matrices is practically useful for the general dense matrices. Commonly, the computation of the singular values of a dense matrix is twofold:

1) preprocess of reducing into a sparse band matrix.
2) singular computation of the sparse band matrix.

The computation time for preprocess is estimated $O\left(n^{3}\right)$ while for the singular value computation $O\left(n^{2}\right)$. Hence, a vast amount of the computation time is consumed by the preprocess. On the preprocess for dense matrices, it is reported in [11] that the reduction into a lower tridiagonal matrix is about $50 \%$ faster than that into bidiagonal matrices. Therefore, the total time of preprocess into a lower tridiagonal matrix and the oqds for lower tridiagonal matrices is much faster than the time of preprocess into bidiagonal matrices and the oqds for bidiagonal matrices.

## 6. Conclusions

We proposed the oqds algorithm for lower tridiagonal matrices. Though computing singular values of lower tridiagonal matrices takes longer time than bidiagonal matrices, preprocess reducing dense matrices into lower tridiagonal matrices takes less time than into bidiagonal matrices. Not only
simple reduction of computational complexity, we can apply the BLAS Level 2.5 routines to lower tridiagonalization. The BLAS Level 2.5 routines are more cache efficient than BLAS Level 2 routines commonly applied to bidiagonalization. A cache efficient algorithm saves a number of memory accesses which waste a big time. The computation time for preprocess is estimated $O\left(n^{3}\right)$ while for the singular value computation $O\left(n^{2}\right)$, hence, a vast amount of the computation time is consumed by the preprocess. Therefore, if we can compute the singular values of lower tridiagonal matrices not so longer than for bidiagonal matrices, it is expected that total computation time decreases extremely.

For an implementation of this algorithm, we proposed a new shift strategy consisting of the generalized Newton shift and associated two methods, Laguerre shift and Kato-Temple shift, and the well known Gerschgorin shift. Moreover, we design new convergence criteria for deflation and splitting required for the implementation of the oqds algorithm. By the criteria, we can do the convergence test for lower tridiagonal matrices.

As a result, the algorithm computes the singular values of a lower tridiagonal matrix within $O\left(n^{2}\right)$ computation time. Although it takes about two or three times as long time for tridiagonal matrices as for bidiagonal matrices, proposed algorithm is expected to be faster than the conventional methods since the preprocessing requires $O\left(n^{3}\right)$ operations and takes much larger time than the oqds algorithm.
As a future work, we have to perform more experiment to compare the computation time including preprocessing. Furthermore, exact error analysis should be made and we ought to check out the accuracy of the algorithm after improving the implementation and setting proper test matrices which have known eigenvalues.

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