A Stable Lanczos Tridiagonalization of Complex Symmetric Matrices

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Abstract

We present two orthogonalization schemes for stablizing Lanczos tridiagonalization of a complex symmetric matrix.

Keywords: Complex symmetric matrix, Lanczos algorithm, singular value decomposition (SVD), Takagi factorization.

1 Introduction

For any complex symmetric matrix A of order n, there exist a unitary $Q \in C^{n \times n}$ and an order n nonnegative diagonal $\Sigma = \mathrm{diag}(\sigma_1, ..., \sigma_n)$, where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$, such that

$$A = Q \Sigma Q^{\mathrm{T}} \quad \text{or} \quad Q^{\mathrm{H}} A \bar{Q} = \Sigma.$$

This special form of singular value decomposition (SVD) is called Takagi factorization [4, 8].

The computation of the Takagi factorization consists of two stages: tridiagonalization and diagonalization [1]. A complex symmetric matrix is first reduced to a complex symmetric and tridiagonal form. There are various tridiagonalization schemes. Householder transformations can be used [1]. Unfortunately, when A is sparse or structured, Householder transformations destroy sparsity or structure. Alternatively, Lanczos method can be applied. Since Lanczos algorithm involves only matrix-vector multiplication, sparsity and structures can be exploited to develop fast tridiagonalization algorithms [5].

The second stage, diagonalization of the complex symmetric tridiagonal matrix computed in the first stage, can be implemented by the implicit QR method [1, 5].

This paper presents a stable Lanczos tridiagonalization algorithm for complex symmetric matrices. In Section 2, we describe the Lanczos tridiagonalization algorithm for complex symmetric matrices. Unfortunately, this method is unstable in floating-point arithmetic. A simple selective orthogonalization scheme and a practical partial orthogonalization scheme are proposed in Sections 3 and 4. Finally, Section 5 demonstrates our numerical experiments.

2 Lanczos Tridiagonalization

For an n-by-n complex symmetric A, we can find a unitary $Q \in C^{n \times n}$ such that

$$T = Q^{\mathrm{H}} A \bar{Q} \tag{1}$$

is complex symmetric and tridiagonal. For example, Q may consists of a sequence of Householder transformations [1]. Let

$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ 0 & & \beta_{n-1} & \alpha_n \end{bmatrix} \tag{2}$$

and rewrite (1) as

$$A\bar{Q} = QT. \tag{3}$$

Comparing the jth columns on the both sides of (3), we have

$$A\bar{\mathbf{q}}_j = \beta_{j-1}\mathbf{q}_{j-1} + \alpha_j \mathbf{q}_j + \beta_j \mathbf{q}_{j+1}, \quad \beta_0 \mathbf{q}_0 = 0,$$

which leads to a Lanczos three-term recursion:

$$\beta_j \mathbf{q}_{j+1} = A\bar{\mathbf{q}}_j - \alpha_j \mathbf{q}_j - \beta_{j-1}\mathbf{q}_{j-1}. \tag{4}$$

The orthogonormality of $\mathbf{q}_j$ implies

$$\alpha_j = \mathbf{q}_j^{\mathrm{H}} A \bar{\mathbf{q}}_j.$$

Let $\mathbf{r}_j = A\bar{\mathbf{q}}_j - \alpha_j \mathbf{q}_j - \beta_{j-1}\mathbf{q}_{j-1}$, then $\beta_j = \pm\|\mathbf{r}_j\|_2$ and $\mathbf{q}_{j+1} = \mathbf{r}_j/\beta_j$ if $\mathbf{r}_j \neq 0$. Thus we have a generic Lanczos tridiagonalization algorithm for complex symmetric matrices.

Algorithm 1 (Lanczos Tridiagonalization) *Given a starting vector* $\mathbf{b}$ *and a subroutine for matrix-vector multiplication* $\mathbf{y} = A\mathbf{x}$ *for any* $\mathbf{x}$*, where* A *is an* n*-by-*n *complex symmetric matrix. This algorithm computes the diagonals of the complex symmetric and tridiagonal matrix* T *in (2) and a unitary* Q *such that* $T = Q^{\mathrm{H}} A \bar{Q}$*.*

$\mathbf{q}_0 = 0$; $\beta_0 = 0$;
$\mathbf{q}_1 = \mathbf{b}/\|\mathbf{b}\|_2$;
for $j = 1$ to n
  $\mathbf{y} = A\bar{\mathbf{q}}_j$;
  $\alpha_j = \mathbf{q}_j^{\mathrm{H}} \mathbf{y}$;
  $\mathbf{y} = \mathbf{y} - \alpha_j \mathbf{q}_j - \beta_{j-1} \mathbf{q}_{j-1}$;
  $\beta_j = \|\mathbf{y}\|_2$;
  if $\beta_j = 0$, quit; end
  $\mathbf{q}_{j+1} = \mathbf{y}/\beta_j$;
end.

Since Lanczos method involves only matrix-vector multiplication, fast tridiagonalization can be developed by exploiting the structure of A [5]. Unfortunately, in floating-point arithmetic, the above algorithm suffers from the loss of the orthogonality of the computed Q. To circumvent the problem, we may orthogonalize each $\mathbf{q}_j$ against all previous $\mathbf{q}_{j-1}, ..., \mathbf{q}_1$. This is called complete orthogonalization. For example, Householder matrices [3, Page 483] or Gram-Schmidt scheme [2, Page 375] can be used. Complete orthogonalization, however, is prohibitively expensive. In the following section, we propose a selective orthogonalization scheme.

3 Selective Orthogonalization

Analogous to the Lanczos algorithms for symmetric eigenvalue problem [2], in this section, we present a selective orthogonalization scheme for the Lanczos tridiagonalization of a complex symmetric matrix.

Before discussing the selective orthogonalization, we introduce some notations and definitions. During the kth iteration, α_k, β_k, and $\mathbf{q}_{k+1}$ are computed. Denote

$$Q_k = [\mathbf{q}_1, ..., \mathbf{q}_k]$$

and

$$T_k = \begin{bmatrix} \alpha_1 & \beta_1 & & 0 \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{k-1} \\ 0 & & \beta_{k-1} & \alpha_k \end{bmatrix}.$$

Suppose that

$$T_k = U \Sigma U^{\mathrm{T}} \tag{5}$$

is the Takagi factorization of T_k. We call the singular values or Takagi values on the diagonal of Σ the Takagi-Ritz values and the columns of $Q_k U$ or their complex conjugates the Takagi-Ritz vectors. These values and vectors are approximations of the Takagi values (singular values) and Takagi vectors (left and right singular vectors) of A.

The basic idea behind the selective orthogonalization is to orthogonalize $\mathbf{q}_{k+1}$ against only few selected Takagi-Ritz vectors, rather than all previously computed $\mathbf{q}_i$. What are the criteria for selecting the Takagi-Ritz vectors?

Similar to the case of real symmetric tridiagonalization problem considered by Paige [6]. we will show, for the case of complex symmetric tridiagonalization, that

$$\text{if} \quad |\beta_k u_k| / \|A\|_2 \leq \sqrt{\epsilon} \quad \text{then} \quad |\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}| \geq O(\sqrt{\epsilon}), \tag{6}$$

where $\mathbf{u}$ is a column of U in (5) and u_k is the kth or the last entry of $\mathbf{u}$ and ϵ is the unit of roundoff. A large $|\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}|$, which measures the orthogonality between $\mathbf{q}_{k+1}$ and a Takagi-Ritz vector $Q_k \mathbf{u}$ indicates that $\mathbf{q}_{k+1}$ has a large component in the direction of $Q_k \mathbf{u}$. We then orthogonalize $\mathbf{q}_{k+1}$ against the Takagi-Ritz vector.

Now, we prove the statement (6). Incorporating roundoff errors into the three-term recursion (4), we write

$$\beta_j \mathbf{q}_{j+1} + \mathbf{f}_j = A \bar{\mathbf{q}}_j - \alpha_j \mathbf{q}_j - \beta_{j-1} \mathbf{q}_{j-1}, \quad j = 1, .., k, \tag{7}$$

where $\mathbf{f}_j$ represents roundoff errors. In matrix form,

$$[0, ..., 0, \beta_k \mathbf{q}_{k+1}] + F_k = A \bar{Q}_k - Q_k T_k,$$

where $F_k = [\mathbf{f}_1, ..., \mathbf{f}_k]$, that is

$$A \bar{Q}_k = Q_k T_k + \beta_k \mathbf{q}_{k+1} \mathbf{e}_k^{\mathrm{T}} + F_k$$

where $\mathbf{e}_k = [0, ..., 0, 1]^{\mathrm{T}}$. Premultiplying the above equation with Q_k^{H}, we get

$$Q_k^{\mathrm{H}} A \bar{Q}_k = Q_k^{\mathrm{H}} Q_k T_k + \beta_k Q_k^{\mathrm{H}} \mathbf{q}_{k+1} \mathbf{e}_k^{\mathrm{T}} + Q_k^{\mathrm{H}} F_k.$$

Since $Q_k^{\mathrm{H}} A \bar{Q}_k$ is symmetric,

$$(Q_k^{\mathrm{H}} Q_k T_k - T_k Q_k^{\mathrm{T}} \bar{Q}_k) + \beta_k (Q_k^{\mathrm{H}} \mathbf{q}_{k+1} \mathbf{e}_k^{\mathrm{T}} - \mathbf{e}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k) + (Q_k^{\mathrm{H}} F_k - F_k^{\mathrm{T}} \bar{Q}_k) = 0.$$

Let $Q_k^{\mathrm{H}} Q_k = I + C + C^{\mathrm{H}}$, where C is the strictly lower triangular part of $Q_k^{\mathrm{H}} Q_k$. We assume that $\mathbf{q}_{j+1}$ is almost orthogonal to $\mathbf{q}_j$ for $j = 1, ..., k$, i.e., $\mathbf{q}_{j+1}^{\mathrm{H}} \mathbf{q}_j = O(\epsilon)$, then both the diagonal and subdiagonal of C are zero. Also, $\mathbf{q}_{k+1}^{\mathrm{H}} \mathbf{q}_k = O(\epsilon)$ implies that the last entry of $\mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k$ is almost zero, which means that $\mathbf{e}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k$ is also strictly lower triangular. Thus $CT_k - T_k \bar{C}$ is the strictly lower triangular part of $Q_k^{\mathrm{H}} Q_k T_k - T_k Q_k^{\mathrm{T}} \bar{Q}_k$ and $\beta_k \mathbf{e}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k$ is the strictly lower triangular part of $\beta_k (Q_k^{\mathrm{H}} \mathbf{q}_{k+1} \mathbf{e}_k^{\mathrm{T}} - \mathbf{e}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k)$. Denoting L as the strictly lower triangular part of $Q_k^{\mathrm{H}} F_k - F_k^{\mathrm{T}} \bar{Q}_k$, we get

$$(CT_k - T_k \bar{C}) - \beta_k \mathbf{e}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k + L = 0. \tag{8}$$

Let $(\sigma, \mathbf{u})$ be a Takagi pair of T_k, then premultiplying and postmultiplying (8) with $\mathbf{u}^{\mathrm{H}}$ and $\bar{\mathbf{u}}$ respectively, we have

$$\sigma(\mathbf{u}^{\mathrm{H}} C \mathbf{u} - \mathbf{u}^{\mathrm{T}} \bar{C} \bar{\mathbf{u}}) - \beta_k \bar{u}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k \bar{\mathbf{u}} + \mathbf{u}^{\mathrm{H}} L \bar{\mathbf{u}} = 0.$$

Consider the real part. Since $\mathrm{Real}(\mathbf{u}^{\mathrm{H}} C \mathbf{u} - \mathbf{u}^{\mathrm{T}} \bar{C} \bar{\mathbf{u}}) = 0$,

$$|\mathrm{Real}(\beta_k \bar{u}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k \bar{\mathbf{u}})| = |\mathrm{Real}(\mathbf{u}^{\mathrm{H}} L \bar{\mathbf{u}})|.$$

The right side

$$|\mathrm{Real}(\mathbf{u}^{\mathrm{H}} L \bar{\mathbf{u}})| \leq |\mathbf{u}^{\mathrm{H}} L \bar{\mathbf{u}}| \leq \|L\|_2 = O(\|F\|_2) = O(\epsilon \|A\|_2).$$

The left side

$$\begin{aligned} & |\mathrm{Real}(\beta_k \bar{u}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k \bar{\mathbf{u}})| \\ = \; & |\beta_k (\mathrm{Real}(u_k) \, \mathrm{Real}(\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}) - \mathrm{Im}(u_k) \, \mathrm{Im}(\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}))|. \end{aligned}$$

Thus

$$|\beta_k (\mathrm{Real}(u_k) \, \mathrm{Real}(\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}) - \mathrm{Im}(u_k) \, \mathrm{Im}(\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}))| = O(\epsilon \|A\|_2).$$

If $|\beta_k u_k| / \|A\|_2 \leq \sqrt{\epsilon}$, then $|\beta_k \mathrm{Real}(u_k)| / \|A\|_2 \leq \sqrt{\epsilon}$ and $|\beta_k \mathrm{Im}(u_k)| / \|A\|_2 \leq \sqrt{\epsilon}$. Consequently,

$$\begin{aligned} O(\epsilon \|A\|_2) &= |\beta_k \mathrm{Real}(\bar{u}_k \mathbf{q}_{k+1}^{\mathrm{T}} \bar{Q}_k \bar{\mathbf{u}})| \\ &\leq \sqrt{\epsilon} \|A\|_2 (|\mathrm{Real}(\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u})| + |\mathrm{Im}(\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u})|) \\ &\approx \sqrt{\epsilon} \|A\|_2 |\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}|, \end{aligned}$$

which implies that $|\mathbf{q}_{k+1}^{\mathrm{H}} Q_k \mathbf{u}| \geq O(\sqrt{\epsilon})$.

Finally, we present the following Lanczos algorithm with a simple selective orthogonalization scheme. We use the largest singular value σ_1 of T_k as an approximation of $\|A\|_2$ and Gram-Schmidt method for orthogonalization.

Algorithm 2 (Selective Orthogonalization) *Given a starting vector* $\mathbf{b}$ *and a subroutine for matrix-vector multiplication* $\mathbf{y} = A\mathbf{x}$ *for any* $\mathbf{x}$*, where* A *is an* n*-by-*n *complex symmetric matrix. This algorithm computes the diagonals of the complex symmetric and tridiagonal matrix* T *in (2) and a unitary* Q *such that* $T = Q^{\mathrm{H}} A \bar{Q}$.

$\mathbf{q}_0 = 0$; $\beta_0 = 0$;
$\mathbf{q}_1 = \mathbf{b}/\|\mathbf{b}\|_2$;
for $j = 1$ to n
    $\mathbf{y} = A\bar{\mathbf{q}}_j$;
    $\alpha_j = \mathbf{q}_j^{\mathrm{H}}\mathbf{y}$;
    $\mathbf{y} = \mathbf{y} - \alpha_j \mathbf{q}_j - \beta_{j-1}\mathbf{q}_{j-1}$;
    $\beta_j = \|\mathbf{y}\|_2$;
    Compute Takagi factorization $T_j = U\Sigma U^{\mathrm{T}}$;
    for $k = 1$ to j
        if $|\beta_j U(j,k)| \leq \sigma_1\sqrt{\epsilon}$
            $\mathbf{v} = Q_j \mathbf{u}_k$;
            $\mathbf{y} = \mathbf{y} - (\mathbf{v}^{\mathrm{H}}\mathbf{y})\mathbf{v}$;
        end
    end
    $\beta_j = \|\mathbf{y}\|_2$;
    if $\beta_j = 0$, quit; end
    $\mathbf{q}_{j+1} = \mathbf{y}/\beta_j$;
end.

This selective orthogonalization scheme has two drawbacks. First, it requires the Takagi factorization of T_j for each iteration. Second, it orthogonalizes $\mathbf{q}_{j+1}$ against only selected Takagi-Ritz vectors. What is wrong with the selective orthogonalization? Suppose that $\mathbf{q}_k^{\mathrm{H}}\mathbf{q}_{j+1}$ has exceeded the threshold, usually some neighboring $\mathbf{q}_i^{\mathrm{H}}\mathbf{q}_{j+1}$ have grown to about the threshold [7]. If we reorthogonalize $\mathbf{q}_{j+1}$ only against $\mathbf{q}_k$, then its effect will be wiped out immediately by the neighboring terms. In the next section, we apply the partial reorthogonalization [7] to complex symmetric case to overcome these two drawbacks.

4 Partial Orthogonalization

To avoid the calculation of the Takagi-Ritz vectors and values, we check the orthogonalities $\mathbf{q}_k^{\mathrm{H}}\mathbf{q}_{j+1}$ of Takagi vectors, instead of Takagi-Ritz vectors. In this section, we first establish a recursion on the estimates for the orthogonalities of Takagi vectors. This recursion provides an efficient way of monitoring the orthogonality. Based on the recursion, we propose a re-orthogonalization algorithm.

From (7), we have

$$\begin{aligned}\beta_j \mathbf{q}_{j+1} &= A\bar{\mathbf{q}}_j - \alpha_j \mathbf{q}_j - \beta_{j-1}\mathbf{q}_{j-1} - \mathbf{f}_j \\ \beta_k \mathbf{q}_{k+1} &= A\bar{\mathbf{q}}_k - \alpha_k \mathbf{q}_k - \beta_{k-1}\mathbf{q}_{k-1} - \mathbf{f}_k.\end{aligned}$$

Premultiplying the above two equations with $\mathbf{q}_k^{\mathrm{H}}$ and $\mathbf{q}_j^{\mathrm{H}}$ respectively and denoting $\omega_{k,j} = \mathbf{q}_k^{\mathrm{H}}\mathbf{q}_j$, we get

$$\begin{aligned}\beta_j \omega_{k,j+1} &= \mathbf{q}_k^{\mathrm{H}} A\bar{\mathbf{q}}_j - \alpha_j \omega_{k,j} - \beta_{j-1}\omega_{k,j-1} - \mathbf{q}_k^{\mathrm{H}}\mathbf{f}_j \\ \beta_k \omega_{j,k+1} &= \mathbf{q}_j^{\mathrm{H}} A\bar{\mathbf{q}}_k - \alpha_k \omega_{j,k} - \beta_{k-1}\omega_{j,k-1} - \mathbf{q}_j^{\mathrm{H}}\mathbf{f}_k.\end{aligned}$$

Since A is symmetric, $\mathbf{q}_k^{\mathrm{H}} A\bar{\mathbf{q}}_j = \mathbf{q}_j^{\mathrm{H}} A\bar{\mathbf{q}}_k$. Thus, subtracting the above two equations and noting that $\omega_{k,j} = \bar{\omega}_{j,k}$, we have the following recursion on the orthogonalities of the Takagi vectors:

$$\beta_j \omega_{k,j+1} = \beta_k \bar{\omega}_{k+1,j} + \alpha_k \bar{\omega}_{k,j} - \alpha_j \omega_{k,j} + \beta_{k-1}\bar{\omega}_{k-1,j} - \beta_{j-1}\omega_{k,j-1} + \mathbf{q}_j^{\mathrm{H}}\mathbf{f}_k - \mathbf{q}_k^{\mathrm{H}}\mathbf{f}_j. \tag{9}$$

The above equation shows that we need $\omega_{k-1,j}$, $\omega_{k,j}$ and $\omega_{k+1,j}$ computed in iteration j and $\omega_{k,j-1}$ in iteration $j-1$ to calculate $\omega_{k,j+1}$. Obviously, we define $\omega_{0,j} = 0$ and $\omega_{j,j} = 1$ for all j. Thus, we also define

$$\psi_j := \omega_{j,j+1} \tag{10}$$

as a random variable whose value will be discussed later. The problem is that the round-off error term $\mathbf{q}_j^{\mathrm{H}}\mathbf{f}_k - \mathbf{q}_k^{\mathrm{H}}\mathbf{f}_j$ in (9) is unknown. Again, we define

$$\theta_{k,j} := \mathbf{q}_j^{\mathrm{H}}\mathbf{f}_k - \mathbf{q}_k^{\mathrm{H}}\mathbf{f}_j, \tag{11}$$

as a random variable whose value will be discussed soon. Using these notations, we get

$$\omega_{k,j+1} = \beta_j^{-1}(\beta_k \bar{\omega}_{k+1,j} + \alpha_k \bar{\omega}_{k,j} - \alpha_j \omega_{k,j} + \beta_{k-1}\bar{\omega}_{k-1,j} - \beta_{j-1}\omega_{k,j-1}) + \theta_{k,j}, \tag{12}$$

for $k = 1, ..., j-1$, with

$$\beta_0 = \omega_{0,j} = 0, \quad \omega_{j,j+1} = \psi_j \quad \text{and} \quad \omega_{j+1,j+1} = 1.0$$

How do we choose the values for ψ_j in (10) and $\theta_{k,j}$ in (11)? Based on the statistical study by Simon [7], let ϵ be the machine precision, we propose that

$$\psi_j = n\epsilon \frac{\beta_1}{\beta_j}(\Psi_\mathrm{r} + i\Psi_\mathrm{i}), \quad \Psi_\mathrm{r},\ \Psi_\mathrm{i} \in N(0, 0.6), \tag{13}$$

where $N(0,v)$ means normal distribution with zero mean and variance v, and

$$\theta_{k,j} = \epsilon(\beta_k + \beta_j)(\Theta_\mathrm{r} + i\Theta_\mathrm{i}), \quad \Theta_\mathrm{r},\ \Theta_\mathrm{i} \in N(0, 0.6). \tag{14}$$

To aleviate the problem caused by isolated reorthogonalization, when $\omega_{k,j+1}$ exceeds the threshold $\sqrt{\epsilon}$ for some k, we reorthogonalize $\mathbf{q}_{j+1}$ against all the previous Takagi vectors $\mathbf{q}_k$, $k = 1, ..., j$. Moreover, we always perform a reorthogonalization in the subsequent iteration. Theoretically, after the reorthogonalization, $\omega_{k,j+1} = 0$, $k = 1, ..., j$. To incorporate the rounding errors, we set

$$\omega_{k,j+1} = \epsilon(\Omega_\mathrm{r} + i\Omega_\mathrm{i}), \quad \Omega_\mathrm{r},\ \Omega_\mathrm{i} \in N(0, 1.5). \tag{15}$$

Finally, we have the following algorithm for the partial reorthogonalization.

Algorithm 3 (Partial Orthogonalization) *Given a starting vector* $\mathbf{b}$ *and a subroutine for matrix-vector multiplication* $\mathbf{y} = A\mathbf{x}$ *for any* $\mathbf{x}$*, where* A *is an n-by-n complex symmetric matrix. This algorithm computes the diagonals of the complex symmetric and tridiagonal matrix* T *in (2) and a unitary* Q *such that* $T = Q^\mathrm{H} A \bar{Q}$.

$\mathbf{q}_0 = 0$; $\beta_0 = 0$; $\omega_{1,1} = 1$;
$\mathbf{q}_1 = \mathbf{b}/\|\mathbf{b}\|_2$;
for $j = 1$ to n
    $\mathbf{y} = A\bar{\mathbf{q}}_j$;
    $\alpha_j = \mathbf{q}_j^\mathrm{H}\mathbf{y}$;
    $\mathbf{y} = \mathbf{y} - \alpha_j \mathbf{q}_j - \beta_{j-1}\mathbf{q}_{j-1}$;
    $\beta_j = \|\mathbf{y}\|_2$;
    Compute $\omega_{k,j+1}$ for $k = 1, ..., j-1$ using (12);
    Set $\omega_{j,j+1}$ to ψ_j using (13);
    Set $\omega_{j+1,j+1} = 1$;
    if $\max_{1 \le k \le j}(|\omega_{k,j+1}|) > \sqrt{\epsilon}$

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            Orthogonalize y against q_1, ..., q_j;
            Perform orthogonalization in the next iteration;
            Reset ω_{k,j+1} using (15);
            Recalculate β_j = ||y||_2;
        end
        if β_j = 0, quit; end
        q_{j+1} = y/β_j;
end.
```

5 Experiments

Algorithms 1, 2 and 3 were programmed in MATLAB. The random complex symmetric matrices in the following examples were generated as follows. First, a set of n random numbers with a normal Gaussian distribution with zero mean and variance 1 was generated. Their absolute values were chosen as the singular values $\sigma_1, ..., \sigma_n$. Then, a random unitary matrix Q of order n was generated to form a complex symmetric matrix $A = Q\Sigma Q^{\mathrm{T}}$. All starting vectors $\mathbf{b}$ were $[1, ..., 1]^{\mathrm{T}}$.

Example 1. A 40-by-40 random complex symmetric matrix was generated. We ran 19 iterations in Algorithm 2 and computed the Takagi-Ritz values. The jth, $j = 1, ..., 19$, column in Figure 1 plots the j Takagi-Ritz values in the jth iteration. The 21st column shows the Takagi values or the singular values of A. This example shows that the Takagi-Ritz values quickly converge to the Takagi values or the singular values of A, especially the large ones.

Example 2. We ran 30 iterations in Algorithm 1 (without orthogonalization) for a 40-by-40 random complex symmetric matrix and computed $|\beta_k U(k,1)|$ and $|\mathbf{q}_{k+1}^{\mathrm{H}}(Q_k \mathbf{u}_1)|$ in iteration k, $k = 1, ..., 30$. In Figure 2, a "+" in the kth column is $|\beta_k U(k,1)|$ and an "o" is $|\mathbf{q}_{k+1}^{\mathrm{H}}(Q_k \mathbf{u}_1)|$. The figure depicts that these two values are related approximately by

$$|\beta_k U(k,1)| = \frac{O(\epsilon)}{|\mathbf{q}_{k+1}^{\mathrm{H}}(Q_k \mathbf{u}_1)|}.$$

Example 3. Various sizes of random complex symmetric matrices were generated and ran on Algorithm 2 (with selective orthogonalization). The orthogonality of Q was measured by $\|I - Q^{\mathrm{H}}Q\|_{\mathrm{F}}/n^2$ and the error in the tridiagonalization was measured by $\|Q^{\mathrm{H}}A\bar{Q} - T\|_{\mathrm{F}}/n^2$. Table 1 shows the

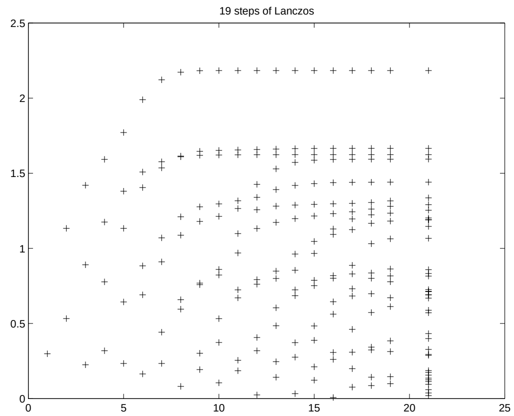

Figure 1: Takagi-Ritz values of a 40-by-40 complex symmetric matrix A. Column j shows the j Takagi-Ritz values computed in the jth iteration of Algorithm 2. The 21st column shows the 40 Takagi values of A.

size n	number of vectors selected for orthogonalization	orthogonality $\|I - Q^{\mathrm{H}}Q\|_{\mathrm{F}}/n^2$	factorization $\|Q^{\mathrm{H}}A\bar{Q} - T\|_{\mathrm{F}}/n^2$
20	11	$2.02E-11$	$1.29E-10$
40	73	$1.16E-10$	$2.60E-09$
100	1122	$1.86E-11$	$2.35E-09$
200	6162	$1.07E-08$	$1.15E-06$

Table 1: Efficiency and accuracy of Algorithm 2.

results. For comparison, without orthogonalization, typically, Q completely loses orthogonality around size $n = 20$.

Example 4. In comparison with the selective orthogonalization in Example 3, various sizes of random complex symmetric matrices were generated and ran on Algorithm 3 (with partial orthogonalization). The measurements of the orthogonality of Q and the error in the tridiagonalization are the same as those in Example 3. Table 2 shows the results.

Example 5. Algorithm 2 was applied to a random 1000-by-1000 complex symmetric matrix A for 30 iterations. The four largest Takagi-Ritz values and their corresponding vectors were computed as approximations of the Takagi values and vectors of A. Table 3 shows the accuracy of the approximations. A small $1 - |\mathbf{q}_i^{\mathrm{H}}\hat{\mathbf{q}}_i|$ indicates that $\mathbf{q}_i$ and $\hat{\mathbf{q}}_i$ are either in the same

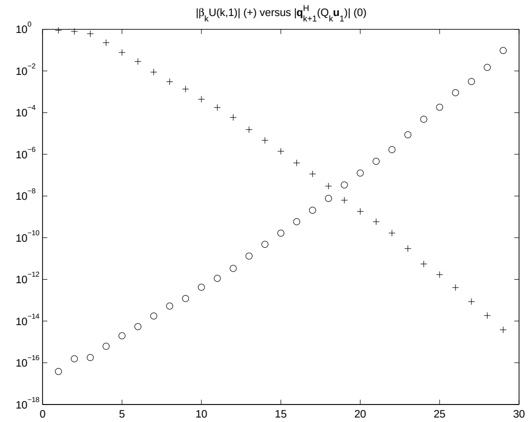

Figure 2: Algorithm 1 is applied to a 40-by-40 complex symmetric matrix. Column k plots $|\beta_k U(k,1)|$ (a "+") and $|\mathbf{q}_{k+1}^{\mathrm{H}}(Q_k \mathbf{u}_1)|$ (an "o") computed in the kth iteration, $k = 1, ..., 30$.

direction or in the opposite directions. This example shows that Algorithm 2 is very effective in computing approximations of the largest singular values and vectors of complex symmetric matrices.

Conclusion. In this paper, we have presented a simple selective orthogonalization scheme and a practical partial orthogonalization scheme for the Lanczos tridiagonalization of a complex symmetric matrix. Experimental results show that the partial orthogonalization scheme effectively stablizes the Lanczos tridiagonalization.

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size n	number of vectors selected for orthogonalization	orthogonality $\|I - Q^{\rm H}Q\|_{\rm F}/n^2$	factorization $\|Q^{\rm H}A\bar{Q} - T\|_{\rm F}/n^2$
20	54	$6.00E-11$	$7.17E-12$
40	245	$7.78E-11$	$8.56E-12$
100	1579	$2.81E-11$	$1.85E-12$
200	6407	$3.40E-11$	$1.00E-12$
500	46204	$2.95E-14$	$2.35E-13$
1000	193605	$2.12E-14$	$2.05E-13$
2000	816276	$4.78E-15$	$9.11E-14$

Table 2: Efficiency and accuracy of Algorithm 3.

i	1	2	3	4
$\|\hat{\sigma}_i - \sigma_i\|$	$1.90E-8$	$1.71E-6$	$7.27E-4$	$7.40E-3$
$1 - \|\mathbf{q}_i^{\rm H}\hat{\mathbf{q}}_i\|$	$1.59E-8$	$3.33E-6$	$1.10E-3$	$1.11E-1$

Table 3: Errors in the largest four computed Takagi-Ritz values $\hat{\sigma}_i$ and Takagi-Ritz vectors $\hat{\mathbf{q}}_i$ against the exact Takagi values σ_i and vectors $\mathbf{q}_i$ after 30 iterations of Algorithm 2 on a 1000-by-1000 complex symmetric matrix.

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