

A Divide-and-Conquer Method for the Takagi Factorization

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Abstract

This paper presents a divide-and-conquer method for computing the Takagi factorization, or symmetric singular value decomposition, of a complex symmetric and tridiagonal matrix. An analysis of accuracy shows that our method produces accurate Takagi values and orthogonal Takagi vectors. Our preliminary numerical experiments have confirmed our analysis and demonstrated that our divide-and-conquer method is much more efficient than the implicit QR method even for moderately large matrices.

1 Introduction

The Takagi factorization of a complex symmetric $n \times n$ matrix A can be written as

$$A = V\Sigma V^T,$$

where V is a unitary matrix, V^T is the transpose of V and Σ is a diagonal matrix with non-negative diagonal elements. The columns of V are called the Takagi vectors of A and the diagonal elements of Σ are its Takagi values. Since $V^T = \bar{V}^H$, where \bar{V} denotes the complex conjugate of V , the Takagi factorization is a symmetric form of the singular value decomposition (SVD). The Takagi values are the singular values, the Takagi vectors are the left singular vectors and the complex conjugates of the Takagi vectors are the right singular vectors. A standard algorithm for computing the Takagi factorization consists of two stages. The first stage reduces a complex symmetric matrix A to a complex symmetric tridiagonal matrix through Lanczos method with partial orthogonalization [5, 8] as the following

$$A = PTP^T \equiv P \begin{bmatrix} a_1 & b_1 & & 0 \\ b_1 & \ddots & \ddots & \\ & \ddots & \ddots & b_{n-1} \\ 0 & & b_{n-1} & a_n \end{bmatrix} P^T, \quad (1)$$

where P is a unitary matrix of order n and T is an $n \times n$ tridiagonal matrix. The second stage computes the Takagi factorization of $T = Q\Sigma Q^T$. The combination of the two stages

gives

$$A = P(Q\Sigma Q^T)P^T = V\Sigma V^T,$$

where $V = PQ$.

In this paper, we focus on the computation of the Takagi factorization of a complex symmetric tridiagonal matrix T by the divide-and-conquer method based on rank-one tearings of TT^H . It is known that the divide-and-conquer method is the most efficient method for computing the eigenvalues and eigenvectors of a Hermitian matrix. The Takagi vectors of T , that is the columns of Q , are the eigenvectors of the semi-positive definite Hermitian matrix TT^H , since $TT^H = Q\Sigma Q^T \bar{Q}\Sigma Q^H = Q\Sigma^2 Q^H$. However, it is not always true that an eigenvector of TT^H is a Takagi vector of T . For example, let

$$T = \begin{bmatrix} 1 & \sqrt{-1} \\ \sqrt{-1} & 1 \end{bmatrix},$$

It is easy to see that the eigenvalue decomposition of TT^H is

$$TT^H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Obviously, the unit vectors are not the Takagi vectors of T since T is not diagonal. In fact, using the algorithm in [6], we can get the Takagi factorization:

$$T = Q\Sigma Q^T = \begin{bmatrix} \frac{\sqrt{2+\sqrt{2}}}{2} & \frac{\sqrt{2-\sqrt{2}}}{2}\sqrt{-1} \\ \frac{\sqrt{2-\sqrt{2}}}{2}\sqrt{-1} & \frac{\sqrt{2+\sqrt{2}}}{2} \end{bmatrix} \begin{bmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} \frac{\sqrt{2+\sqrt{2}}}{2} & \frac{\sqrt{2-\sqrt{2}}}{2}\sqrt{-1} \\ \frac{\sqrt{2-\sqrt{2}}}{2}\sqrt{-1} & \frac{\sqrt{2+\sqrt{2}}}{2} \end{bmatrix}.$$

The basic idea of our method is to apply the divide-and-conquer method to TT^H to get its eigenvectors and eigenvalues. The square roots of the eigenvalues of TT^H are the Takagi values of T . We then transform the eigenvectors of TT^H into the Takagi vectors of T . However, explicitly computing TT^H is too expensive and also destroys the tridiagonal structure of T . We will introduce an implicit method for computing the eigenvalue decomposition of TT^H .

The rest of the paper is organized as follows. Section 2 describes a divide-and-conquer method for computing the eigenvalue decomposition of TT^H without explicitly forming TT^H . However, as mentioned above, the eigenvectors of TT^H may not be the Takagi vectors of T . In Section 3, We will propose a method for transforming the eigenvectors of TT^H into the Takagi vectors of T . We analyze the sensitivity of Takagi vectors of T in Section 4. Finally, the results of our preliminary numerical experiments are given in Section 5 to show the stability, accuracy, and efficiency of our algorithm.

2 Divide-and-Conquer Scheme

2.1 Dividing the matrix

Let the Takagi factorization of the complex symmetric tridiagonal matrix T in (1) be

$$Q^H T \bar{Q} = \Sigma = \text{diag}(\sigma_1, \dots, \sigma_n) \quad \text{or} \quad T = Q \Sigma Q^T.$$

In the first step, we tear the tridiagonal matrix T into two tridiagonal submatrices of half size. For simplicity, we assume that n is a power of 2 and $m = n/2$, then

$$T = \begin{bmatrix} T_1 & b_m \mathbf{e}_m \mathbf{e}_1^T \\ b_m \mathbf{e}_1 \mathbf{e}_m^T & T_2 \end{bmatrix} \quad (2)$$

where

$$T_1 = \begin{bmatrix} a_1 & b_1 & & 0 \\ b_1 & \ddots & \ddots & \\ & \ddots & \ddots & b_{m-1} \\ 0 & & b_{m-1} & a_m \end{bmatrix}, \quad T_2 = \begin{bmatrix} a_{m+1} & b_{m+1} & & 0 \\ b_{m+1} & \ddots & \ddots & \\ & \ddots & \ddots & b_{n-1} \\ 0 & & b_{n-1} & a_n \end{bmatrix}$$

and \mathbf{e}_1 and \mathbf{e}_m are unit vectors, $[1, 0, \dots, 0]$ and $[0, \dots, 0, 1]$ respectively. Now, we establish the relations between the eigenvalues and eigenvectors of $T_i T_i^H$ and those of $T T^H$ as follows. From (2), we get

$$\begin{aligned} T T^H &= \begin{bmatrix} T_1 & b_m \mathbf{e}_m \mathbf{e}_1^T \\ b_m \mathbf{e}_1 \mathbf{e}_m^T & T_2 \end{bmatrix} \begin{bmatrix} T_1^H & \bar{b}_m \mathbf{e}_m \mathbf{e}_1^T \\ \bar{b}_m \mathbf{e}_1 \mathbf{e}_m^T & T_2^H \end{bmatrix} \\ &= \begin{bmatrix} T_1 T_1^H + |b_m|^2 \mathbf{e}_m \mathbf{e}_m^T & b_m \mathbf{e}_m \mathbf{e}_1^T T_2^H + \bar{b}_m T_1 \mathbf{e}_m \mathbf{e}_1^T \\ \bar{b}_m T_2 \mathbf{e}_1 \mathbf{e}_m^T + b_m \mathbf{e}_1 \mathbf{e}_m^T T_1^H & T_2 T_2^H + |b_m|^2 \mathbf{e}_1 \mathbf{e}_1^T \end{bmatrix} \\ &= \begin{bmatrix} T_1 T_1^H & 0 \\ 0 & T_2 T_2^H \end{bmatrix} + \begin{bmatrix} |b_m|^2 \mathbf{e}_m \mathbf{e}_m^T & b_m \mathbf{e}_m \mathbf{e}_1^T T_2^H \\ \bar{b}_m T_2 \mathbf{e}_1 \mathbf{e}_m^T & 0 \end{bmatrix} \\ &\quad + \begin{bmatrix} 0 & \bar{b}_m T_1 \mathbf{e}_m \mathbf{e}_1^T \\ b_m \mathbf{e}_1 \mathbf{e}_m^T T_1^H & |b_m|^2 \mathbf{e}_1 \mathbf{e}_1^T \end{bmatrix} \\ &= \begin{bmatrix} T_1 T_1^H & 0 \\ 0 & T_2 (I_m - \mathbf{e}_1 \mathbf{e}_1^T) T_2^H \end{bmatrix} + \begin{bmatrix} b_m \mathbf{e}_m \\ T_2 \mathbf{e}_1 \end{bmatrix} \begin{bmatrix} \bar{b}_m \mathbf{e}_m^T & \mathbf{e}_1^T T_2^H \end{bmatrix} \\ &\quad + \begin{bmatrix} 0 & \bar{b}_m T_1 \mathbf{e}_m \mathbf{e}_1^T \\ b_m \mathbf{e}_1 \mathbf{e}_m^T T_1^H & |b_m|^2 \mathbf{e}_1 \mathbf{e}_1^T \end{bmatrix} \\ &= \begin{bmatrix} T_1 (I_m - \mathbf{e}_m \mathbf{e}_m^T) T_1^H & 0 \\ 0 & T_2 (I_m - \mathbf{e}_1 \mathbf{e}_1^T) T_2^H \end{bmatrix} + \begin{bmatrix} b_m \mathbf{e}_m \\ T_2 \mathbf{e}_1 \end{bmatrix} \begin{bmatrix} \bar{b}_m \mathbf{e}_m^T & \mathbf{e}_1^T T_2^H \end{bmatrix} \\ &\quad + \begin{bmatrix} T_1 \mathbf{e}_m \\ b_m \mathbf{e}_1 \end{bmatrix} \begin{bmatrix} \mathbf{e}_m^T T_1^H & \bar{b}_m \mathbf{e}_1^T \end{bmatrix} \\ &= \begin{bmatrix} T_1 (I_m - \mathbf{e}_m \mathbf{e}_m^T) T_1^H & 0 \\ 0 & T_2 (I_m - \mathbf{e}_1 \mathbf{e}_1^T) T_2^H \end{bmatrix} + \mathbf{z}_1 \mathbf{z}_1^H + \mathbf{z}_2 \mathbf{z}_2^H, \end{aligned} \quad (3)$$

where

$$\mathbf{z}_1 = \begin{bmatrix} b_m \mathbf{e}_m \\ T_2 \mathbf{e}_1 \end{bmatrix} \quad \text{and} \quad \mathbf{z}_2 = \begin{bmatrix} T_1 \mathbf{e}_m \\ b_m \mathbf{e}_1 \end{bmatrix}.$$

From (3), if the eigenvalue decompositions

$$T_1 T_1^H = U_1 \Sigma_1^2 U_1^H \quad \text{and} \quad T_2 T_2^H = U_2 \Sigma_2^2 U_2^H \quad (4)$$

of the semi-positive definite Hermitian matrices $T_1 T_1^H$ and $T_2 T_2^H$ are available, we can find the eigenvalue decomposition of TT^H by four rank-one modifications. Thus, if the Takagi factorizations of T_1 and T_2 are available, we can compute the Takagi values of T and the eigenvectors of TT^H by four rank-one modifications. Later in Section 3, we will show how to transform the eigenvectors into the Takagi vectors.

Theorem 2.1 in [2] characterizes the eigenvalues and eigenvectors of the real rank-one modification. We generalize it to the complex case. The proof is similar to the proof in [2].

Theorem 2.1 *Suppose $D^2 = \text{diag}(d_1^2, \dots, d_n^2)$, $d_1^2 > d_2^2 > \dots > d_n^2$, $\mathbf{z} \in C^n$ is a vector with no zero entries, and $\rho > 0$, then the eigenvalues of the matrix $D^2 + \rho \mathbf{z} \mathbf{z}^H$ are the n roots $\delta_1^2 > \delta_2^2 > \dots > \delta_n^2$ of the rational function*

$$w(\delta^2) = 1 + \rho \mathbf{z}^H (D^2 - \delta^2 I)^{-1} \mathbf{z} = 1 + \rho \sum_{j=1}^n \frac{|z_j|^2}{d_j^2 - \delta^2}. \quad (5)$$

The corresponding eigenvectors, $\mathbf{g}_1, \mathbf{g}_2, \dots, \mathbf{g}_n$ of $D^2 + \rho \mathbf{z} \mathbf{z}^H$ are given by

$$\mathbf{g}_j = (D^2 - \delta_j^2 I)^{-1} \mathbf{z} / \|(D^2 - \delta_j^2 I)^{-1} \mathbf{z}\|_2, \quad (6)$$

and d_j^2 strictly separate the eigenvalues δ_j^2 :

$$d_n^2 < \delta_n^2 < d_{n-1}^2 < \delta_{n-1}^2 < \dots < d_1^2 < \delta_1^2 < d_1^2 + \rho \mathbf{z}^H \mathbf{z}.$$

Proof. Let (δ^2, \mathbf{g}) be an eigenpair of $D^2 + \rho \mathbf{z} \mathbf{z}^H$, then it satisfies

$$(D^2 + \rho \mathbf{z} \mathbf{z}^H) \mathbf{g} = \delta^2 \mathbf{g},$$

which implies that $(D^2 - \delta^2 I) \mathbf{g} = -\rho \mathbf{z} \mathbf{z}^H \mathbf{g}$. We will show that $D^2 - \delta^2 I$ is nonsingular. Suppose it is singular, then we can find $\delta = d_i$, for some i . Consequently, the i th component $[(D^2 - \delta^2 I) \mathbf{g}]_i = -z_i \mathbf{z}^H \mathbf{g} = 0$, implying that $\mathbf{z}^H \mathbf{g} = 0$. It then follows that $(D^2 - \delta^2 I) \mathbf{g} = -\rho \mathbf{z} \mathbf{z}^H \mathbf{g} = 0$, that is, $(d_j^2 - \delta^2) g_j = 0$ for all $j \neq i$. Thus, we have $\mathbf{z}^H \mathbf{g} = z_i g_i = 0$, which shows that $z_i = 0$. It contradicts the assumption. Therefore, we have

$$\mathbf{z}^H \mathbf{g} \neq 0 \quad \text{and} \quad \mathbf{g} = \rho \mathbf{z} \mathbf{z}^H \mathbf{g} (D^2 - \delta^2 I)^{-1} \mathbf{z}.$$

The rest of the proof is the same as the proof of Theorem 2.1 in [2]. \square

The above theorem shows that if all diagonal entries of D^2 are nonnegative and satisfy the assumptions in Theorem 2.1, then the eigenvalues computed by this rank-one modification

are also nonnegative and satisfy the strict interlacing property. For now, we assume that all entries in Σ_1^2 and Σ_2^2 are distinct and there is no zero entry in the rank-one modification vector \mathbf{z} . In the next subsection, we will remove these assumptions.

Now, from Theorem 2.1, we can get the eigenvalues of TT^H from (4) via four rank-one modifications. First, we compute the rank-one modifications $T_1T_1^H - T_1\mathbf{e}_m\mathbf{e}_m^T T_1^H$ and $T_2T_2^H - T_2\mathbf{e}_1\mathbf{e}_1^T T_2^H$ to obtain the eigenvalue decompositions

$$T_1T_1^H - T_1\mathbf{e}_m\mathbf{e}_m^T T_1^H = \hat{U}_1\hat{\Sigma}_1^2\hat{U}_1^H \quad \text{and} \quad T_2T_2^H - T_2\mathbf{e}_1\mathbf{e}_1^T T_2^H = \hat{U}_2\hat{\Sigma}_2^2\hat{U}_2^H. \quad (7)$$

Applying the above equations to (3), we have

$$TT^H = \begin{bmatrix} \hat{U}_1 & \\ & \hat{U}_2 \end{bmatrix} \left(\begin{bmatrix} \hat{\Sigma}_1^2 & \\ & \hat{\Sigma}_2^2 \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{u}}_1 \\ \hat{\mathbf{u}}_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{u}}_1 \\ \hat{\mathbf{u}}_2 \end{bmatrix}^H + \begin{bmatrix} \hat{\mathbf{v}}_1 \\ \hat{\mathbf{v}}_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{v}}_1 \\ \hat{\mathbf{v}}_2 \end{bmatrix}^H \right) \begin{bmatrix} \hat{U}_1 & \\ & \hat{U}_2 \end{bmatrix}^H, \quad (8)$$

where $\hat{\mathbf{u}}_1 = b_m\hat{U}_1^H\mathbf{e}_m$, $\hat{\mathbf{u}}_2 = \hat{U}_2^HT_2\mathbf{e}_1$, $\hat{\mathbf{v}}_1 = \hat{U}_1^HT_1\mathbf{e}_m$, and $\hat{\mathbf{v}}_2 = b_m\hat{U}_2^H\mathbf{e}_1$. We then do the rank-one modification using the first two terms in the parenthesis to get the eigenvalue decomposition:

$$\begin{bmatrix} \hat{\Sigma}_1^2 & \\ & \hat{\Sigma}_2^2 \end{bmatrix} + \begin{bmatrix} \hat{\mathbf{u}}_1 \\ \hat{\mathbf{u}}_2 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{u}}_1 \\ \hat{\mathbf{u}}_2 \end{bmatrix}^H = \tilde{G}\Delta^2\tilde{G}^H \quad (9)$$

Thus, we can rewrite (8) as

$$TT^H = \begin{bmatrix} \hat{U}_1 & \\ & \hat{U}_2 \end{bmatrix} \tilde{G}(\Delta^2 + \tilde{\mathbf{v}}\tilde{\mathbf{v}}^H)\tilde{G}^H \begin{bmatrix} \hat{U}_1 & \\ & \hat{U}_2 \end{bmatrix}^H \quad (10)$$

where $\tilde{\mathbf{v}}^H = [\hat{\mathbf{v}}_1 \ \hat{\mathbf{v}}_2]^H\tilde{G}^H$. Finally, applying the rank-one modification to the matrices in the parenthesis in (10), we get the eigenvalue decomposition:

$$TT^H = \begin{bmatrix} \hat{U}_1 & \\ & \hat{U}_2 \end{bmatrix} \tilde{G}G\Sigma^2G^H\tilde{G}^H \begin{bmatrix} \hat{U}_1 & \\ & \hat{U}_2 \end{bmatrix}^H \equiv U\Sigma^2U^H. \quad (11)$$

2.2 Deflation

In this subsection, we remove the assumptions of distinct diagonal entries d_i and no zero entries in the modification vector \mathbf{z} . We first consider the case when \mathbf{z} has zero entries. It can be easily verified that (d_i^2, \mathbf{e}_i) is an eigenpair of $D^2 + \rho\mathbf{z}\mathbf{z}^H$ if $z_i = 0$. In this case, the problem can be deflated by one for each zero entry in \mathbf{z} . Next, we consider the case when there are two equal diagonal elements in D^2 , say, $d_i^2 = d_j^2$. Let P be a Givens rotation such that

$$P \begin{bmatrix} d_i \\ d_j \end{bmatrix} = \begin{bmatrix} * \\ 0 \end{bmatrix},$$

then

$$P \left(\begin{bmatrix} d_i^2 & 0 \\ 0 & d_j^2 \end{bmatrix} + \begin{bmatrix} z_i \\ z_j \end{bmatrix} \begin{bmatrix} z_i \\ z_j \end{bmatrix}^H \right) P^H = P \left(\begin{bmatrix} d_i^2 & 0 \\ 0 & d_j^2 \end{bmatrix} + \begin{bmatrix} * \\ 0 \end{bmatrix} \begin{bmatrix} * \\ 0 \end{bmatrix}^H \right) P^H$$

Thus, when $d_i^2 = d_j^2$ for some $i \neq j$, we can assume $z_i = 0$ or $z_j = 0$. So, the case of equal diagonal elements in D is reduced to the case of zero entries in \mathbf{z} . The procedure is described in the following algorithm.

Algorithm 2.2 Assume that D^2 is a diagonal matrix with nonnegative elements sorted in decreasing order, $\mathbf{z} \in C^n$ and $\rho > 0$, then this algorithm computes the eigenvalues and eigenvectors of $D^2 + \rho \mathbf{z} \mathbf{z}^H$.

1. Check the diagonal elements of D , for each pair (i, j) such that $d_i^2 = d_j^2$ and $i \neq j$, find a Givens matrix to transform $[z_i, z_j]^T$ to $[*, 0]^T$;
2. Order \mathbf{z} into the form $\begin{bmatrix} 0 \\ \hat{\mathbf{z}} \end{bmatrix}$ and order D into $\begin{bmatrix} D_1 & \\ & D_2 \end{bmatrix}$ accordingly;
3. Apply the rank-one update to $D_2^2 + \rho \hat{\mathbf{z}} \hat{\mathbf{z}}^H$ to get the eigenvalue decomposition $(D_2^2 + \rho \hat{\mathbf{z}} \hat{\mathbf{z}}^H) = \tilde{G}_2 \tilde{\Delta}^2 \tilde{G}_2^H$;
4. The eigenvalue decomposition of $D^2 + \rho \mathbf{z} \mathbf{z}^H$ is given by

$$D^2 + \rho \mathbf{z} \mathbf{z}^H = \begin{bmatrix} I_p & \\ & \tilde{G}_2 \end{bmatrix} \begin{bmatrix} D_1^2 & \\ & \tilde{\Delta}^2 \end{bmatrix} \begin{bmatrix} I_p & \\ & \tilde{G}_2 \end{bmatrix}^H,$$

where p is the number of zero entries in \mathbf{z} after step 1.

Due to the rounding errors, we regard two elements d_i^2 and d_j^2 equal if they are sufficiently close. In other words, if the difference between d_i^2 and d_j^2 is less than a predetermined tolerance, tol , then we set them equal. How do we determine the tolerance? In our deflation procedure, when d_i^2 and d_j^2 are numerically equal, we find a Givens rotation to transform $[z_i, z_j]^T$ into $[*, 0]^T$. Let $c = \bar{z}_i / \sqrt{|z_i|^2 + |z_j|^2}$ and $s = -\bar{z}_j / \sqrt{|z_i|^2 + |z_j|^2}$, then

$$\begin{bmatrix} c & -s \\ \bar{s} & \bar{c} \end{bmatrix} \begin{bmatrix} d_i^2 & \\ & d_j^2 \end{bmatrix} \begin{bmatrix} \bar{c} & s \\ -\bar{s} & c \end{bmatrix} = \begin{bmatrix} d_i^2 & \\ & d_j^2 \end{bmatrix} + E$$

where

$$E = (d_i^2 - d_j^2) \begin{bmatrix} -|s|^2 & cs \\ \bar{c}\bar{s} & |s|^2 \end{bmatrix}.$$

We set the tolerance tol so that $\|E\|_F \leq \epsilon \|\text{diag}(d_i^2, d_j^2)\|_F$ when $|d_i^2 - d_j^2| \leq tol$, where ϵ is the machine precision. Taking the Frobenius norm on E and $\text{diag}(d_i^2, d_j^2)$, we get

$$\|E\|_F = \sqrt{2} |s| |d_i^2 - d_j^2| \quad \text{and} \quad \|\text{diag}(d_i^2, d_j^2)\|_F \leq \sqrt{2} d_{\max}^2,$$

where $d_{\max} = \max(d_i, d_j)$, and then set the tolerance

$$tol = \frac{d_{\max}^2}{|s|} \epsilon.$$

3 Takagi Factorization

As described in the previous section, given the Takagi factorizations of T_1 and T_2 in (2), we can compute the eigenvalue decomposition $TT^H = U\Sigma^2U^H$ through four rank-one modifications. Let $T = Q\Sigma Q^T$ be the Takagi factorization of T . It is obvious that the Takagi values of T are the square roots of the eigenvalues of TT^H . What remains is to convert the eigenvectors of TT^H into the Takagi vectors of T . First, in the case when the eigenvalues are distinct, the eigenvectors of TT^H are uniquely defined up to a scalar, which implies that the Takagi vector \mathbf{q}_i is a scalar multiple of \mathbf{u}_i . Let $T\bar{\mathbf{u}}_i = \xi\sigma_i\mathbf{u}_i$ for some scalar ξ such that $|\xi| = 1$, and define

$$\mathbf{q}_i \equiv \sqrt{\text{sign}(\xi)}\mathbf{u}_i = \sqrt{\xi}\mathbf{u}_i, \quad (12)$$

where $\text{sign}(x) = x/|x|$ if $x \neq 0$, otherwise $\text{sign}(x) = 1$. Then

$$T\bar{\mathbf{q}}_i = \sqrt{\text{sign}(\xi)}T\bar{\mathbf{u}}_i = \sqrt{\xi}\xi\sigma_i\mathbf{u}_i = \sqrt{\xi}\xi\sigma_i\sqrt{\xi}\mathbf{q}_i = |\xi|^2\sigma_i\mathbf{q}_i = \sigma_i\mathbf{q}_i$$

as desired. Specifically, ξ can be obtained by $\xi = \text{sign}(\mathbf{u}_i^H T\bar{\mathbf{u}}_i)$.

Next, in the case of multiple eigenvalues, $T\bar{\mathbf{u}}_i$ may not equal $\xi\sigma_i\mathbf{u}_i$. We construct

$$\mathbf{q}_i = \alpha_i(T\bar{\mathbf{u}}_i + \sigma_i\mathbf{u}_i), \quad (13)$$

where $\alpha_i = 1/\|T\bar{\mathbf{u}}_i + \sigma_i\mathbf{u}_i\|_2$. Then

$$T\bar{\mathbf{q}}_i = \alpha_i T(\overline{T\bar{\mathbf{u}}_i + \sigma_i\mathbf{u}_i}) = \alpha_i(T\bar{T}\mathbf{u}_i + \sigma_i T\bar{\mathbf{u}}_i) = \alpha_i(\sigma_i^2\mathbf{u}_i + \sigma_i T\bar{\mathbf{u}}_i) = \sigma_i\mathbf{q}_i.$$

Finally, we check the orthogonality of the Takagi vectors of T converted from the eigenvectors of TT^H . It is obvious that the orthogonality is maintained among the Takagi vectors corresponding to distinct Takagi values because of the orthogonality of the eigenvectors corresponding to distinct eigenvalues. Now, assume that $\mathbf{q}_i, \dots, \mathbf{q}_{i+k}$ are the Takagi vectors corresponding to a multiple Takagi value σ_i of multiplicity k . The construction of \mathbf{q}_i shows that the subspace spanned by $\mathbf{q}_i, \dots, \mathbf{q}_{i+k}$ is same as the one spanned by $\mathbf{u}_i, \dots, \mathbf{u}_{i+k}$ since $\mathbf{q}_i, \dots, \mathbf{q}_{i+k}$ are the eigenvectors associated with σ_i^2 . Thus, \mathbf{q}_{i+t} ($t = 1, \dots, k$) are orthogonal to \mathbf{q}_j , the Takagi vector corresponding to σ_j , if $\sigma_j \neq \sigma_i$. However, the Takagi vectors corresponding to the same Takagi value may lose their orthogonality. So, the modified Grand-Schmidt orthogonalization is applied to these vectors to restore the orthogonality. Suppose that \mathbf{q}_{i+t} is one of the Takagi vectors corresponding to σ_i computed from (13), then we orthogonalize it against the previous $t - 1$ vectors $\mathbf{q}_i, \dots, \mathbf{q}_{i+t-1}$ as follows:

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for  $j = 1 : t - 1$ 
     $\mathbf{q}_{i+t} = \mathbf{q}_{i+t} - \mathbf{q}_{i+j}^H \mathbf{q}_{i+t} \mathbf{q}_{i+j}$ ;
end

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Now, we give the divide-and-conquer algorithm for computing the Takagi factorization of a complex symmetric tridiagonal matrix.

Algorithm 3.1 *Given a complex symmetric and tridiagonal matrix T , this algorithm computes the Takagi factorization $T = Q\Sigma Q^T$. There are two stages in this algorithm. The first stage computes the eigenvalue decomposition $TT^H = U\Sigma^2U^H$; the second stage computes the Takagi vectors \mathbf{q}_i of T from the eigenvectors \mathbf{u}_i of TT^H .*

1. Partition T as (2). If T_1 and T_2 are small enough, directly compute the eigenvalue decompositions

$$T_1T_1^H = U_1\Sigma_1U_1^H \quad \text{and} \quad T_2T_2^H = U_2\Sigma_2U_2^H.$$

If T_1 and T_2 are large, apply this algorithm to T_1 and T_2 ;

2. Apply the rank-one modification Algorithm 2.2 to $T_1T_1^H - T_1\mathbf{e}_m\mathbf{e}_m^T T_1^H$ and $T_2T_2^H - T_2\mathbf{e}_1\mathbf{e}_1^T T_2^H$ to obtain their eigenvalue decompositions (7). Thus, TT^H has the form (8);
3. Compute the eigenvalue decomposition (9) using Algorithm 2.2. Then, TT^H has the form (10);
4. Apply Algorithm 2.2 again to the rank-one modification in the parenthesis in (10) to compute the eigenvalue decomposition

$$\Delta^2 + \tilde{\mathbf{v}}\tilde{\mathbf{v}}^H = G\Sigma^2G^H.$$

5. At this point, we get the eigenvalue decomposition $TT^H = U\Sigma^2U^H$. The Takagi values of T are the square roots of the eigenvalues of TT^H ;
6. For a single Takagi value, its corresponding Takagi vector \mathbf{q}_i is computed using (12); for a multiple Takagi value, its Takagi vector \mathbf{q}_i is computed using (13) and then orthogonalized against the previously computed Takagi vectors corresponding to the same Takagi value by the modified Gram-Schmidt orthogonalization.

4 Orthogonality of Takagi Vectors

In the previous section, we presented a divide-and-conquer algorithm for computing the Takagi factorization of T . It is based on the rank-one update of the eigenvalue decomposition of a Hermitian matrix. Rank-one modification Theorem 2.1 is applied four times to get the eigenvalue decomposition if we have the decompositions of $T_1T_1^H$ and $T_2T_2^H$. Due to the rounding errors, the orthogonality of the eigenvectors may be lost after rank-one modifications. In this section, we present an analysis of the orthogonality of the computed eigenvectors and discuss the circumstances under which the orthogonality can be maintained. For simplicity, we assume that the given matrix in the rank-one modification is already deflated.

First, we derive a formula for the eigenvectors \mathbf{g}_j in Theorem 2.1. Differentiating the both sides of the function $w(t)$ in (5) with respect to t , we get

$$\|(D^2 - \delta^2 I)^{-1}\|_2^2 = \sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \delta^2)^2} = \frac{1}{\rho} |w'(\delta^2)|.$$

Then (6) can be rewritten as

$$\mathbf{g}_j = \left(\frac{z_1}{d_1^2 - \delta_j^2}, \frac{z_2}{d_2^2 - \delta_j^2}, \dots, \frac{z_n}{d_n^2 - \delta_j^2} \right) \frac{\sqrt{\rho}}{\sqrt{w'(\delta_j^2)}}. \quad (14)$$

Let $\hat{\delta}_i^2$ be a computed root of w in (5). In the following, by extending the results in [4], we show that if the relative error in $d_j^2 - \hat{\delta}_i^2$ is small for all i and j , then the computed eigenvectors $\hat{\mathbf{g}}_i$ have good orthogonality.

Theorem 4.1 Denote $\hat{\delta}_i^2$ and $\hat{\delta}_k^2$ as the computed roots of w in (5). Let the relative errors in $d_j^2 - \hat{\delta}_i^2$ and $d_j^2 - \hat{\delta}_k^2$ be θ_i and θ_k respectively, that is,

$$d_j^2 - \hat{\delta}_i^2 = (d_j^2 - \delta_i^2)(1 + \theta_i) \quad \text{and} \quad d_j^2 - \hat{\delta}_k^2 = (d_j^2 - \delta_k^2)(1 + \theta_k),$$

and $|\theta_i|, |\theta_k| \leq \tau \ll 1$ for all j , then

$$|\hat{\mathbf{g}}_i^H \hat{\mathbf{g}}_k| = |\mathbf{g}_i^H E \mathbf{g}_k| \leq \tau(2 + \tau) \left(\frac{1 + \tau}{1 - \tau} \right)^2,$$

where $\hat{\mathbf{g}}_i$ and $\hat{\mathbf{g}}_k$ are computed eigenvectors using (14) and E is a diagonal matrix whose i th diagonal entry is

$$E_{ii} = \frac{\theta_i + \theta_k + \theta_i \theta_k}{(1 + \theta_i)(1 + \theta_k)} \left(\frac{w'(\delta_i^2)w'(\delta_k^2)}{w'(\hat{\delta}_i^2)w'(\hat{\delta}_k^2)} \right)^{1/2}.$$

Proof. From (14), we have

$$\begin{aligned} & -\hat{\mathbf{g}}_i^H \hat{\mathbf{g}}_k \\ &= - \left(\sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \delta_k^2)(d_j^2 - \delta_i^2)(1 + \theta_i)(1 + \theta_k)} \right) \frac{\rho}{(w'(\hat{\delta}_i^2)w'(\hat{\delta}_k^2))^{1/2}} \\ &= \left(\sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \delta_k^2)(d_j^2 - \delta_i^2)} - \sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \delta_k^2)(d_j^2 - \delta_i^2)(1 + \theta_i)(1 + \theta_k)} \right) \frac{\rho}{(w'(\hat{\delta}_i^2)w'(\hat{\delta}_k^2))^{1/2}} \end{aligned}$$

since $\mathbf{g}_i^H \mathbf{g}_k = 0$. Thus, we have

$$|\hat{\mathbf{g}}_i^H \hat{\mathbf{g}}_k|$$

$$\begin{aligned}
&= \left| \sum_{j=1}^n \left(\frac{|z_j|^2}{(d_j^2 - \delta_k^2)(d_j^2 - \delta_i^2)} \right) \left(1 - \frac{1}{(1 + \theta_i)(1 + \theta_k)} \right) \frac{\rho}{(w'(\hat{\delta}_i^2)w'(\hat{\delta}_k^2))^{1/2}} \right| \\
&= \left| \sum_{j=1}^n \left(\frac{|z_j|^2}{(d_j^2 - \delta_k^2)(d_j^2 - \delta_i^2)} \right) \left(\frac{\theta_i + \theta_k + \theta_i\theta_k}{(1 + \theta_i)(1 + \theta_k)} \right) \left(\frac{w'(\delta_i^2)w'(\delta_k^2)}{w'(\hat{\delta}_i^2)w'(\hat{\delta}_k^2)} \right)^{1/2} \frac{\rho}{(w'(\delta_i^2)w'(\delta_k^2))^{1/2}} \right| \\
&= |\mathbf{g}_i^H E \mathbf{g}_k| \leq \|E\|_2,
\end{aligned}$$

where E is a diagonal matrix, whose diagonal elements are

$$E_{ii} = \frac{\theta_i + \theta_k + \theta_i\theta_k}{(1 + \theta_i)(1 + \theta_k)} \left(\frac{w'(\delta_i^2)w'(\delta_k^2)}{w'(\hat{\delta}_i^2)w'(\hat{\delta}_k^2)} \right)^{1/2}. \quad (15)$$

On the other hand, it is easy to show that

$$\frac{w'(\delta_i^2)}{w'(\hat{\delta}_i^2)} = \frac{\sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \delta_i^2)^2}}{\sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \delta_i^2)^2(1 + \theta_i)^2}} \leq (1 + \tau)^2. \quad (16)$$

Substituting $w'(\delta_i^2)/w'(\hat{\delta}_i^2)$ in (15) with (16), we have

$$\max(E_{ii}) \leq \frac{\tau + \tau + \tau^2}{(1 - \tau)^2} (1 + \tau)^2 = \tau(2 + \tau) \left(\frac{1 + \tau}{1 - \tau} \right)^2.$$

It completes the proof. \square

Apparently, if the roots δ_i^2 of w are computed in high accuracy, then the relative errors in $d_j^2 - \hat{\delta}_i^2$ are small, provided that the eigenvalues δ_i^2 are not clustered. Consequently, from the above theorem, the computed eigenvectors $\hat{\mathbf{g}}_i$ have good orthogonality. In the following, we show how to compute the roots δ_i^2 accurately.

From Theorem 2.1, the eigenvalues of a rank-one modification are the zeros of the function $w(t)$ in (5). There are many zero finding methods, for example, the rational interpolation strategy in [1] and bisection and its variations [7, 9]. We adopt the rational interpolation strategy in our algorithm. In a zero finding method, accurate function evaluation is crucial. In the following, we reformulate the function $w(t)$ in (5) into a new function, which can be evaluated accurately.

Theorem 2.1 shows that each root δ_i^2 of the function $w(\delta^2)$ is located in (d_i^2, d_{i-1}^2) . First, we consider the case when $\delta^2 \in (d_i^2, (d_{i-1}^2 + d_i^2)/2)$ and let $\zeta_j = (d_j^2 - d_i^2)/\rho$,

$$\psi_i(\mu) = \sum_{j=1}^{i-1} \frac{|z_j|^2}{\zeta_j - \mu} \quad \text{and} \quad \varphi_i(\mu) = \sum_{j=i}^n \frac{|z_j|^2}{\zeta_j - \mu}$$

where $\mu = (\delta^2 - d_i^2)/\rho \in (0, \zeta_{i-1}/2)$. Thus, the equation $w(\delta^2) = 0$ can be rewritten as

$$w(\rho\mu + d_i^2) = 1 + \psi_i(\mu) + \varphi_i(\mu) \equiv f_i(\mu) = 0.$$

An important property of $f_i(\mu)$ is that the difference $|\zeta_j - \mu|$ can be computed to high relative accuracy for any $\mu \in (0, \zeta_{i-1}/2)$ [3]. It then assures that the function $f_i(\mu)$ can be evaluated for any $\mu \in (0, \zeta_{i-1}/2)$ and $d_j^2 - \delta^2 = d_j^2 - d_i^2 - (\delta^2 - d_i^2) = \rho(\zeta_j - \mu)$ is in high relative accuracy, which guarantees the good orthogonality of the computed eigenvectors.

Now we consider the case when $\delta^2 \in [(d_{i-1}^2 + d_i^2)/2, d_{i-1}^2)$ and let $\zeta_j = (d_j^2 - d_{i-1}^2)/\rho$,

$$\psi_i(\mu) = \sum_{j=1}^{i-1} \frac{|z_j|^2}{\zeta_j - \mu} \quad \text{and} \quad \varphi_i(\mu) = \sum_{j=i}^n \frac{|z_j|^2}{\zeta_j - \mu}$$

where $\mu = (\delta^2 - d_{i-1}^2)/\rho \in [\zeta_i/2, 0)$. So, the equation $w(\delta^2) = 0$ can be rewritten as

$$w(\rho\mu + d_{i-1}^2) = 1 + \psi_i(\mu) + \varphi_i(\mu) \equiv f_i(\mu) = 0.$$

Also, the difference $\zeta_j - \mu$ can be computed to high relative accuracy.

Finally, we consider the case when $i = 1$. Let $\zeta_j = (d_j^2 - d_1^2)/\rho$,

$$\psi_1(\mu) = 0, \quad \text{and} \quad \varphi_1(\mu) = \sum_{j=1}^n \frac{|z_j|^2}{\zeta_j - \mu}.$$

We want to find a root $\mu = (\delta^2 - d_1^2)/\rho$ in $(0, \|\mathbf{z}\|^2)$. Similar to the previous cases, for any $\mu \in (0, \|\mathbf{z}\|^2)$, the ratio $|z_i|^2/(\zeta_j - \mu)$ can be computed to high relative accuracy.

So far, we have reformulated the problem of finding the zeros of $w(t)$ into the problem of finding the zeros of $f_i(\mu)$ which can be accurately evaluated. Now, we propose a stopping criterion for $f_i(\mu)$ so that using this stopping criterion we can obtain accurate computed eigenvalues $\hat{\delta}_i^2$.

From the definitions of $\psi_i(\mu)$ and $\varphi_i(\mu)$, we have $\psi_i(\mu) \geq 0$ and $\varphi_i(\mu) \leq 0$. We define the stopping criterion as

$$|f_i(\mu)| \leq \epsilon n (|\psi_i(\mu)| + |\varphi_i(\mu)| + 1). \quad (17)$$

In the following, we show that using this criterion, the computed roots $\hat{\delta}_i^2$ of $w(\delta^2)$ are accurate.

Since $w(\delta_i^2) = 0$, we have

$$\begin{aligned} w(\hat{\delta}_i^2) &= w(\hat{\delta}_i^2) - w(\delta_i^2) = \rho \sum_{j=1}^n \frac{|z_j|^2}{d_j^2 - \hat{\delta}_i^2} - \rho \sum_{j=1}^n \frac{|z_j|^2}{d_j^2 - \delta_i^2} \\ &= \rho(\hat{\delta}_i^2 - \delta_i^2) \sum_{j=1}^n \frac{|z_j|^2}{(d_j^2 - \hat{\delta}_i^2)(d_j^2 - \delta_i^2)} \end{aligned}$$

According to the stopping criterion, since $f_i(\mu)$ can be evaluated accurately, we have

$$|w(\hat{\delta}_i^2)| \leq \epsilon n \left(1 + \rho \left| \sum_{j=1}^n \frac{|z_j|^2}{d_j^2 - \hat{\delta}_i^2} \right| \right) \leq \rho \epsilon n \left(\sum_{j=1}^n \frac{|z_j|^2}{|d_j^2 - \hat{\delta}_i^2|} + \sum_{j=1}^n \frac{|z_j|^2}{|d_j^2 - \delta_i^2|} \right)$$

since $1 = -\rho \sum_{j=1}^n \frac{|z_j|^2}{d_j^2 - \delta_i^2}$. Without loss of generality, we assume δ_i^2 and $\hat{\delta}_i^2$ are in the same interval, say (d_i^2, d_{i-1}^2) . It follows that $(d_j^2 - \delta_i^2)(d_j^2 - \hat{\delta}_i^2) > 0$. So,

$$\begin{aligned} |w(\hat{\delta}_i^2)| &= \rho |\hat{\delta}_i^2 - \delta_i^2| \sum_{j=1}^n \frac{|z_j|^2}{|(d_j^2 - \hat{\delta}_i^2)(d_j^2 - \delta_i^2)|} \leq \rho \epsilon n \left(\sum_{j=1}^n \frac{|z_j|^2}{|d_j^2 - \hat{\delta}_i^2|} + \sum_{j=1}^n \frac{|z_j|^2}{|d_j^2 - \delta_i^2|} \right) \\ &\leq \rho \epsilon n (4\|D^2 + \rho \mathbf{z}\mathbf{z}^H\|_2 + |\hat{\delta}_i^2 - \delta_i^2|) \sum_{j=1}^n \frac{|z_j|^2}{|(d_j^2 - \hat{\delta}_i^2)(d_j^2 - \delta_i^2)|}, \end{aligned}$$

since $|d_j^2 - \hat{\delta}_i^2| + |d_j^2 - \delta_i^2| \leq 2|d_j^2 - \delta_i^2| + |\hat{\delta}_i^2 - \delta_i^2| \leq 4\|D^2 + \rho \mathbf{z}\mathbf{z}^H\|_2 + |\hat{\delta}_i^2 - \delta_i^2|$. From the above equation, we can get the upper bound for $|\hat{\delta}_i^2 - \delta_i^2|$:

$$|\hat{\delta}_i^2 - \delta_i^2| \leq \frac{4\epsilon n \|D^2 + \rho \mathbf{z}\mathbf{z}^H\|_2}{1 - \epsilon n}. \quad (18)$$

In conclusion, we apply the rational interpolation zero finding method to $f_i(\mu)$ using the stopping criterion (17). We then can obtain accurate eigenvalues δ_i^2 . Provided that the eigenvalues are not clustered, it results the high relative accuracy of the difference $d_i^2 - \hat{\delta}_i^2$, which implies good orthogonality of the computed eigenvectors of TT^H .

5 Numerical Examples

We programmed our divide-and-conquer Algorithm 3.1 in Matlab and tested it on three types of complex symmetric and tridiagonal matrices. Our experiments were carried out on a SUN SPARC Ultra 10. The complex symmetric and tridiagonal matrices with predetermined Takagi values were generated as follows. First, a random vector uniformly distributed on $(0, 1]$ was generated and sorted in descending order as a Takagi value vector d . Then a random unitary matrix was generated as a Takagi vector matrix V . The product $A = V\Sigma V^T$, where $\Sigma = \text{diag}(d)$, was computed as a complex symmetric matrix. Finally, a complex symmetric and tridiagonal T was obtained by applying the Lanczos method with partial orthogonalization [8] to A . Denoting \hat{Q} and \hat{d} as the computed Takagi vector matrix and Takagi value vector respectively, the error in the computed Takagi factorization was measured by

$$\gamma_t = \|\hat{Q}\hat{\Sigma}\hat{Q}^T - T\|_2, \quad \text{where } \hat{\Sigma} = \text{diag}(\hat{d}).$$

The error in the computed Takagi values was measured by

$$\gamma_v = \|d - \hat{d}\|_2$$

and the orthogonality of the computed Takagi vector matrix \hat{Q} was measured by

$$\gamma_o = \|\hat{Q}\hat{Q}^H - I\|_2.$$

Example	γ_o	γ_v	γ_t
1	6.5453e-13	2.7071e-13	3.7802e-12
2	4.3764e-14	2.9148e-14	4.9324e-13
3	2.4833e-13	3.7276e-14	1.8752e-12
4	3.3486e-13	5.3199e-14	2.0680e-12
5	3.5356e-14	4.8627e-14	3.2510e-13

Table 1: The Takagi factorization of five 64×64 testing matrices with distinct Takagi values

Example	γ_o	γ_v	γ_t
1	3.4502e-12	2.3378e-14	3.3106e-13
2	7.7844e-12	1.4947e-14	5.6152e-13
3	2.3450e-12	1.5453e-14	7.4974e-13
4	4.6577e-10	2.2160e-14	1.2787e-10
5	4.6045e-12	5.1199e-15	4.9863e-13

Table 2: The Takagi factorization of five 64×64 testing matrices with multiple Takagi values of small multiplicity

Example 1 *Five random complex symmetric and tridiagonal matrices of order 64 were generated as described above. In this example, the Takagi values of each matrix were distinct. Table 1 shows that the computed Takagi values and Takagi vectors are accurate.*

Example 2 *Five random complex symmetric and tridiagonal matrices of order 64 were generated. In this example, we set the three largest Takagi values equal and the four smallest Takagi values equal. Table 2 shows the results.*

Example 3 *Five random T of order 64 were generated. In this example, however, we set the 15 largest Takagi values equal. As expected, when the Takagi values are clustered, the computed Takagi vectors may lose orthogonality as shown in the third matrix.*

For performance, we tested our algorithm on random complex symmetric and tridiagonal matrices of five different sizes. For each size, we generated five matrices and ran our divide-and-conquer (DAC) method and the implicit QR (IQR) method [6]. In our method, when the size of the submatrix T_i , for $i = 1, 2$, in (2) is less than or equal to 4, its Takagi factorization is computed directly by the implicit QR method. Table 4 shows the average running time and the average factorization error γ_t of the five matrices of same size. The results in Table 4 demonstrate that our method is significantly more efficient than the implicit QR method even for matrices of moderately large size. We expect the improvement in efficiency is more significant for large matrices.

Example	γ_o	γ_v	γ_t
1	4.6459e-13	4.3785e-15	6.0149e-13
2	1.0763e-13	6.1213e-15	1.5335e-12
3	2.7721e-4	1.2094e-7	2.1865e-4
4	3.2599e-13	1.9481e-13	2.3556e-13
5	1.0308e-13	3.5831e-15	6.4613e-14

Table 3: The Takagi factorization of five 64×64 testing matrices with multiple Takagi values of large multiplicity

matrix size	Running time (sec)		γ_t	
	DAC method	IQR method	DAC method	IQR method
16	0.406	0.568	1.0240e-14	1.0002e-14
32	1.036	1.988	1.6271e-14	1.2533e-14
64	2.882	7.154	4.2004e-13	4.5231e-14
128	9.446	30.674	3.8701e-12	2.7546e-13
256	37.37	158.39	4.9525e-12	9.4915e-13

Table 4: The performance and accuracy comparison of the divide-and-conquer (DAC) method and the implicit QR (IQR) method

Conclusion We have proposed a divide-and-conquer method for the Takagi factorization of a complex symmetric and tridiagonal matrix and presented an analysis, which shows that our method computes accurate Takagi values and vectors provided that the Takagi values are not clustered. Our preliminary experiments have demonstrated that our method produced accurate results even for matrices with Takagi values of moderate multiplicities and is much more efficient than the implicit QR method [6].

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