Abstract

We present an algorithm for computing the eigendecomposition of a symmetric rank-one modification of a symmetric matrix whose eigendecomposition is known. Previous algorithms for this problem suffer a potential loss of orthogonality among the computed eigenvectors, unless extended precision arithmetic is used. Our algorithm is based on a novel, backward stable method for computing the eigenvectors. It does *not* require extended precision and is as efficient as previous approaches.

A Stable and Efficient Algorithm for the Rank-one Modification of the Symmetric Eigenproblem [†]

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1. Introduction

Given a real scalar ρ, a real n-vector u, and the eigendecomposition of a real $n \times n$ symmetric matrix B, the rank-one modification of the symmetric eigenproblem is to find the eigendecomposition of the matrix $B + \rho uu^T$.

This is an important problem in numerical linear algebra. Applications include divide-and-conquer algorithms for the symmetric tridiagonal eigenproblem [8, 9, 14, 17], the bidiagonal singular value decomposition (SVD) [2, 3, 4, 13, 18, 19], and the unitary and orthogonal eigenproblems [1, 4, 12]; updating the SVD [6, 16]; and various stationary value problems [10].

The problem can easily be reduced to the following special case (see [7]):

> Given a diagonal matrix $D = diag(d_1, d_2, \ldots, d_n)$ with $d_1 < d_2 < \ldots < d_n$, and a real vector $z = (z_1, z_2, \ldots, z_n)^T$ with $z_j > 0$, find the eigendecomposition
>
> $$D + zz^T = Q\Lambda Q^T$$
>
> of $A \equiv D + zz^T$, where $\Lambda = diag(\lambda_1, \lambda_2, \ldots, \lambda_n)$ with $\lambda_1 < \lambda_2 < \ldots < \lambda_n$, and Q is orthogonal. The diagonal elements of Λ are the eigenvalues of A, and the columns of Q are the corresponding eigenvectors.

From now on we focus on this reduced problem, yet still refer to it as the rank-one modification problem.

Since error is associated with computation, a *numerical eigendecomposition* of $D + zz^T$ is usually defined as a decomposition of the form

$$D + zz^T = \tilde{Q}\tilde{\Lambda}\tilde{Q}^T + O(\epsilon(\|D\|_2 + \|z\|_2^2)) \quad , \tag{1.1}$$

where ϵ is the machine precision, $\tilde{\Lambda} = diag(\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_n)$ with $\tilde{\lambda}_1 < \tilde{\lambda}_2 < \ldots < \tilde{\lambda}_n$, and $\tilde{Q}$ is *numerically orthogonal.* An algorithm that produces such a decomposition is said to be *backward stable* [25].

While the eigenvalues of A are always well-conditioned with respect to a symmetric perturbation, the eigenvectors can be extremely sensitive to such perturbations [11, 23, 25, 26]. That is, $\tilde{\Lambda}$ is guaranteed to be close to Λ, but $\tilde{Q}$ can be very different from Q. Thus one is usually content with a backward stable algorithm.

The problem can be further simplified in light of (1.1). Given any rank-one modification matrix $D + zz^T$, we can use the deflation procedure in [9] to reduce the eigenproblem to one that satisfies

$$d_{j+1} - d_j \geq \tau(\|D\|_2 + \|z\|_2^2) \quad \text{and} \quad z_j \geq \tau\sqrt{\|D\|_2 + \|z\|_2^2} \quad ,$$

where τ is a small multiple of ϵ to be specified later.

The basic tool for the rank-one modification problem is an algorithm developed by Bunch, Nielsen, and Sorensen [7] and inspired by earlier work of Golub [10]. Dongarra and Sorensen [9] propose a more liberal deflation process to make the algorithm more efficient and more stable. We refer to the algorithm in [9] as *Algorithm I*.

While Algorithm I always computes the eigenvalues to high absolute accuracy, in the presence of close eigenvalues it can have difficulties in computing numerically orthogonal eigenvectors [7, 8, 9]. This instability affects all algorithms using rank-one modification techniques.

To overcome this instability, Kahan [20] proposes using extended precision arithmetic to compute some key quantities more accurately. Independently, Sorensen and Tang [24] develop a new version of Algorithm I that uses simulated extended precision and show that it is stable. The problem with extended precision is that it results in machine-dependent software [5, 24].

In this paper we present a new algorithm for solving the rank-one modification problem. Since Algorithm I works well for finding the eigenvalues, the new algorithm uses a similar approach. But it uses a completely different approach to finding the eigenvectors, one that is backward stable. The amount of work is roughly the same as for Algorithm I, yet the new algorithm does not require the use or simulation of extended precision arithmetic. We refer to this new algorithm as *Algorithm II*.

Section 2 introduces Algorithm I and points out how it can fail. Section 3 introduces Algorithm II. Section 4 proves the numerical stability of Algorithm II. Section 5 reviews previous results on the stability of Algorithm I and shows why they require more accuracy than necessary. Section 6 presents some numerical results. Section 7 points out some extensions.

Throughout the paper we assume that the elements of D and z are given in floating point representation. We take the usual model of arithmetic:[1]

$$fl(x \circ y) = (x \circ y)(1 + \xi) \quad ,$$

where x and y are floating point numbers; $\circ$ is one of $+, -, \times$, and $\div$; $fl(x \circ y)$ is the floating point result of the operation $\circ$; and $|\xi| \leq \epsilon$. We also require that

$$fl(\sqrt{x}) = \sqrt{x}(1 + \xi)$$

for any positive floating point number x. For simplicity, we ignore the possibility of overflow and underflow.

[1] This model excludes machines like CRAYs and CDC Cybers that do not have a guard digit. Algorithm II can easily be modified for such machines.

2. How Algorithm I Can Fail

The following lemma characterizes the eigenvalues and eigenvectors of $D + zz^T$.

LEMMA 1 (BUNCH, NIELSEN, AND SORENSEN [7]). *Assume that* $d_1 < d_2 < \ldots < d_n$ *and that* $z_j > 0$. *Then the eigenvalues* $\{\lambda_i\}_{i=1}^n$ *of* $D + zz^T$ *satisfy the* interlacing property

$$d_1 < \lambda_1 < d_2 < \lambda_2 < \ldots < d_n < \lambda_n$$

and are the roots of the secular equation

$$f(\lambda) \equiv 1 + \sum_{j=1}^{n} \frac{z_j^2}{d_j - \lambda} = 0 \quad .$$

For each eigenvalue λ_i, *the corresponding eigenvector is given by*

$$q_i = \left(\frac{z_1}{d_1 - \lambda_i}, \ldots, \frac{z_n}{d_n - \lambda_i} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{n} \frac{z_j^2}{(d_j - \lambda_i)^2}} \quad . \tag{2.1}$$

Algorithm I uses a rational interpolation strategy to solve for $\{\lambda_i\}_{i=1}^n$ (see [7]). For each eigenvalue λ_i, it finds a numerical approximation $\tilde{\lambda}_i$ and approximates q_i by

$$\tilde{q}_i^I = \left(\frac{z_1}{d_1 - \tilde{\lambda}_i}, \ldots, \frac{z_n}{d_n - \tilde{\lambda}_i} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{n} \frac{z_j^2}{(d_j - \tilde{\lambda}_i)^2}} \quad .$$

In other words, the *exact* λ_i is replaced by the *approximation* $\tilde{\lambda}_i$ in (2.1).

In pathological cases, even though $\tilde{\lambda}_i$ is close to λ_i, the approximate ratio $z_j/(d_j - \tilde{\lambda}_i)$ is very different from the exact ratio $z_j/(d_j - \lambda_i)$, resulting in a computed eigenvector very different from the true eigenvector. More importantly, when all the eigenvectors are computed, the resulting eigenvector matrix is far from orthogonal.

3. Algorithm II

3.1. Computing the Eigenvectors

For each eigenvalue λ_i, the corresponding eigenvector is given by

$$q_i = \left(\frac{z_1}{d_1 - \lambda_i}, \ldots, \frac{z_n}{d_n - \lambda_i} \right)^T \Bigg/ \sqrt{\sum_{j=1}^{n} \left(\frac{z_j}{d_j - \lambda_i} \right)^2}$$

(see Lemma 1). Observe that if λ_i was given *exactly*, then we could compute each difference, each ratio, each product, and each sum in this formula to high relative accuracy, and thus compute q_i to component-wise high relative accuracy.

In practice we can only hope to compute an approximation $\tilde{\lambda}_i$ to λ_i. But suppose that we could find a $\tilde{z}$ such that $\{\tilde{\lambda}_i\}_{i=1}^n$ are the *exact* eigenvalues of the *new* rank-one modification matrix $\tilde{A} = D + \tilde{z}\tilde{z}^T$. Since

$$\begin{aligned} A &= D + zz^T \\ &= D + \tilde{z}\tilde{z}^T + zz^T - \tilde{z}\tilde{z}^T \\ &= \tilde{A} + (z - \tilde{z})z^T + z(z - \tilde{z})^T - (z - \tilde{z})(z - \tilde{z})^T \quad , \end{aligned}$$

$\tilde{A}$ will be close to A as long as $\tilde{z}$ is close to z. Moreover, the formula

$$\tilde{q}_i^{II} = \left(\frac{\tilde{z}_1}{d_1 - \tilde{\lambda}_i}, \ldots, \frac{\tilde{z}_n}{d_n - \tilde{\lambda}_i}\right)^T \Bigg/ \sqrt{\sum_{j=1}^n \frac{\tilde{z}_j^2}{(d_j - \tilde{\lambda}_i)^2}} \tag{3.1}$$

gives the *exact* eigenvector corresponding to the eigenvalue $\tilde{\lambda}_i$ of $\tilde{A}$. As we observed before, $\tilde{q}_i^{II}$ can be computed to component-wise high relative accuracy. Thus, when all the eigenvectors of $\tilde{A}$ are computed, the resulting eigenvector matrix will be numerically orthogonal.

We now show why such a $\tilde{z}$ exists. By definition,

$$\det(\tilde{A} - \lambda I) = \prod_{j=1}^n (\tilde{\lambda}_j - \lambda) \quad .$$

On the other hand,

$$\det(\tilde{A} - \lambda I) = \det(D + \tilde{z}\tilde{z}^T - \lambda I) = \left(1 + \sum_{j=1}^n \frac{\tilde{z}_j^2}{d_j - \lambda}\right) \prod_{j=1}^n (d_j - \lambda) \quad .$$

Combining these relations,

$$\prod_{j=1}^n (\tilde{\lambda}_j - \lambda) = \left(1 + \sum_{j=1}^n \frac{\tilde{z}_j^2}{d_j - \lambda}\right) \prod_{j=1}^n (d_j - \lambda) \quad .$$

Setting $\lambda = d_i$, we get

$$\tilde{z}_i^2 = \frac{\prod_j (\tilde{\lambda}_j - d_i)}{\prod_{j \neq i} (d_j - d_i)} \quad . \tag{3.2}$$

If the computed eigenvalues $\{\tilde{\lambda}_i\}_{i=1}^n$ satisfy the interlacing property[2]

$$d_1 < \tilde{\lambda}_1 < d_2 < \tilde{\lambda}_2 < \ldots < d_n < \tilde{\lambda}_n \quad ,$$

[2] Since the exact eigenvalues satisfy the same interlacing property (see Lemma 1), this is only an accuracy requirement on the computed eigenvalues and is not an additional restriction on A.

then the expression on the right-hand side of (3.2) is positive and

$$\tilde{z}_i = \sqrt{\prod_{j=1}^{i-1} \frac{(\tilde{\lambda}_j - d_i)}{(d_j - d_i)} \cdot \prod_{j=i}^{n-1} \frac{(\tilde{\lambda}_j - d_i)}{(d_{j+1} - d_i)} \cdot (\tilde{\lambda}_n - d_i)} \quad . \tag{3.3}$$

Working backward, if $\tilde{z}$ is given by (3.3), then the eigenvalues of $D + \tilde{z}\tilde{z}^T$ are $\{\tilde{\lambda}_i\}_{i=1}^n$.

Each difference, each ratio, and each product in (3.3) can be computed to high relative accuracy. As a result, $\tilde{z}$ can be computed to component-wise high relative accuracy. Substituting the computed $\tilde{z}$ into (3.1), $\tilde{q}_i^{II}$ can also be computed to component-wise high relative accuracy. Consequently, when all the eigenvectors are computed, the resulting eigenvector matrix $\tilde{Q} = (\tilde{q}_1^{II}, \ldots, \tilde{q}_n^{II})$ will be numerically orthogonal.

To show that $\tilde{Q}\tilde{\Lambda}\tilde{Q}^T$ is a numerical eigendecomposition of A, we must show that $\tilde{z}$ is close to z. We do so in Section 4.

3.2. Computing the Eigenvalues

In order to guarantee that $\tilde{z}$ is close to z, we must ensure that the approximations $\{\tilde{\lambda}_i\}_{i=1}^n$ to the eigenvalues are sufficiently accurate. The key is the stopping criterion for the root-finder, which requires a slight reformulation of the secular equation (cf. [7]).

Consider the eigenvalue $\lambda_i \in (d_i, d_{i+1})$, where $1 \le i \le n-1$; the case $i = n$ is considered later. λ_i is a root of the secular equation

$$f(\lambda) \equiv 1 + \sum_{j=1}^{n} \frac{z_j^2}{d_j - \lambda} = 0 \quad .$$

We first assume that[3] $\lambda_i \in (d_i, \frac{d_i + d_{i+1}}{2})$. Let $\delta_j = d_j - d_i$ and let

$$\psi(\mu) \equiv \sum_{j=1}^{i} \frac{z_j^2}{\delta_j - \mu} \quad \text{and} \quad \phi(\mu) \equiv \sum_{j=i+1}^{n} \frac{z_j^2}{\delta_j - \mu} \quad .$$

Since

$$f(\mu + d_i) = 1 + \psi(\mu) + \phi(\mu) \equiv g(\mu) \quad ,$$

we seek the root $\mu_i = \lambda_i - d_i \in (0, \delta_{i+1}/2)$ of $g(\mu) = 0$.

An important property of $g(\mu)$ is that each difference $\delta_j - \mu$ can be evaluated to high relative accuracy for any $\mu \in (0, \delta_{i+1}/2)$. Indeed, since $\delta_i = 0$, we have $fl(\delta_i - \mu) = -fl(\mu)$; since $fl(\delta_{i+1}) = fl(d_{i+1} - d_i)$ and $0 < \mu < (d_{i+1} - d_i)/2$, we can compute $fl(\delta_{i+1} - \mu)$ as $fl(fl(d_{i+1} - d_i) - fl(\mu))$; and in a similar fashion, we can compute $\delta_j - \mu$ to high relative accuracy for any $j \neq i, i+1$.

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[3] This can easily be checked by computing $f(\frac{d_i + d_{i+1}}{2})$. If $f(\frac{d_i + d_{i+1}}{2}) > 0$, then $\lambda_i \in (d_i, \frac{d_i + d_{i+1}}{2})$, otherwise $\lambda_i \in [\frac{d_i + d_{i+1}}{2}, d_{i+1})$.

Because of this property, each ratio $z_j^2/(\delta_j - \mu)$ in $g(\mu)$ can be evaluated to high relative accuracy for any $\mu \in (0, \delta_{i+1}/2)$. And, since both $\psi(\mu)$ and $\phi(\mu)$ are sums of terms of the same sign, we can bound the error in computing $g(\mu)$ by

$$\eta n(1 + |\psi(\mu)| + |\phi(\mu)|) \quad ,$$

where η is a small multiple of ϵ that is independent of n and μ.

We now assume that $\lambda_i \in [\frac{d_i + d_{i+1}}{2}, d_{i+1})$. Let $\delta_j = d_j - d_{i+1}$ and let

$$\psi(\mu) \equiv \sum_{j=1}^{i} \frac{z_j^2}{\delta_j - \mu} \quad \text{and} \quad \phi(\mu) \equiv \sum_{j=i+1}^{n} \frac{z_j^2}{\delta_j - \mu} \quad .$$

We seek the root $\mu_i = \lambda_i - d_{i+1} \in [\delta_i/2, 0)$ of the equation

$$g(\mu) \equiv f(\mu + d_{i+1}) = 1 + \psi(\mu) + \phi(\mu) = 0 \quad .$$

For any $\mu \in [\delta_i/2, 0)$, each difference $\delta_j - \mu$ can again be computed to high relative accuracy, as can each ratio $z_j^2/(\delta_j - \mu)$; and we can bound the error in computing $g(\mu)$ as before.

Finally we consider the case $i = n$. Let $\delta_j = d_j - d_n$ and let

$$\psi(\mu) \equiv \sum_{j=1}^{n} \frac{z_j^2}{\delta_j - \mu} \quad \text{and} \quad \phi(\mu) \equiv 0 \quad .$$

We seek the root $\mu_n = \lambda_n - d_n \in (0, \|z\|_2^2)$ of the equation

$$g(\mu) \equiv f(\mu + d_n) = 1 + \psi(\mu) + \phi(\mu) = 0 \quad .$$

Again, for any $\mu \in (0, \|z\|_2^2)$, each ratio $z_j^2/(\delta_j - \mu)$ can be computed to high relative accuracy, and we can bound the error in computing $g(\mu)$ as before.

In practice the root-finder cannot make any progress at a point μ where it is impossible to determine the sign of $g(\mu)$ numerically. Thus we propose the stopping criterion

$$|g(\mu)| \leq \eta n \, (1 + |\psi(\mu)| + |\phi(\mu)|) \quad , \tag{3.4}$$

where, as before, $\eta n(1+|\psi(\mu)|+|\phi(\mu)|)$ is an upper bound on the round-off error in computing $g(\mu)$. Note that for each i, there is at least one floating point number that satisfies this stopping criterion numerically, namely $fl(\mu_i)$.

We have not specified the scheme used to find the root of $g(\mu)$. We used the rational interpolation strategy in [7] for the numerical experiments, but bisection or the improved rational interpolation strategy given by Kahan and Li [21] would also work. What is most important is the stopping criterion and the fact that, with the reformulation of the secular equation given above, we can find a μ that satisfies it.

4. Numerical Stability of Algorithm II

In this section we show that Algorithm II computes the eigenvalues to high absolute accuracy and that $\tilde{z}$ is indeed close to z.

Since $f(\lambda_i) = 0$, we have

$$1 = -\sum_{j=1}^{n} \frac{z_j^2}{d_j - \lambda_i} \leq \sum_{j=1}^{n} \frac{z_j^2}{|d_j - \lambda_i|} \quad ,$$

and the stopping criterion (3.4) implies that the computed eigenvalue $\tilde{\lambda}_i$ satisfies

$$|f(\tilde{\lambda}_i)| \leq \eta n \left(\sum_{j=1}^{n} \frac{z_j^2}{|d_j - \lambda_i|} + \sum_{j=1}^{n} \frac{z_j^2}{|d_j - \tilde{\lambda}_i|} \right) \quad .$$

Since

$$f(\tilde{\lambda}_i) = f(\tilde{\lambda}_i) - f(\lambda_i) = (\tilde{\lambda}_i - \lambda_i) \sum_{j=1}^{n} \frac{z_j^2}{(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)} \quad ,$$

it follows that

$$|\tilde{\lambda}_i - \lambda_i| \sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|} \leq \eta n \left(\sum_{j=1}^{n} \frac{z_j^2}{|d_j - \tilde{\lambda}_i|} + \sum_{j=1}^{n} \frac{z_j^2}{|d_j - \lambda_i|} \right) \quad . \tag{4.1}$$

Thus

$$|\tilde{\lambda}_i - \lambda_i| \sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|} \leq \eta n \max_{1 \leq k \leq n} \left(|d_k - \tilde{\lambda}_i| + |d_k - \lambda_i| \right) \sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|}$$

or

$$|\tilde{\lambda}_i - \lambda_i| \leq \eta n \max_{1 \leq k \leq n} \left(|d_k - \tilde{\lambda}_i| + |d_k - \lambda_i| \right) \leq \frac{2\eta n}{1 - \eta n} \max_{1 \leq k \leq n} |d_k - \lambda_i| \quad ;$$

i.e., all the eigenvalues are computed to high absolute accuracy.

To show that $\tilde{z}$ is close to z, we note that for any j,

$$\frac{1}{|d_j - \tilde{\lambda}_i|} + \frac{1}{|d_j - \lambda_i|} \leq \frac{2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|^{\frac{1}{2}}} + \frac{|\tilde{\lambda}_i - \lambda_i|}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|} \quad .$$

Substituting this into (4.1), we get

$$\begin{aligned} |\tilde{\lambda}_i - \lambda_i| \sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|} &\leq \frac{2\eta n}{1 - \eta n} \sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|^{\frac{1}{2}}} \\ &\leq \frac{2\eta n}{1 - \eta n} \|z\|_2 \sqrt{\sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|}} \end{aligned}$$

or

$$
\begin{aligned}
|\tilde{\lambda}_i - \lambda_i| &\leq \frac{2\eta n}{1-\eta n}\|z\|_2 \Bigg/ \sqrt{\sum_{j=1}^{n} \frac{z_j^2}{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|}} \\
&\leq \frac{2\eta n \|z\|_2}{(1-\eta n) z_j} \sqrt{|(d_j - \tilde{\lambda}_i)(d_j - \lambda_i)|} \\
&\leq \frac{2\eta n \|z\|_2}{(1-\eta n) z_j} \left(|d_j - \lambda_i| + \frac{1}{2}|\tilde{\lambda}_i - \lambda_i| \right) \quad .
\end{aligned}
$$

Letting $\beta_j = 2\eta n \|z\|_2 / ((1-\eta n) z_j)$, this implies that

$$
|\tilde{\lambda}_i - \lambda_i| \leq \frac{\beta_j}{1 - \frac{1}{2}\beta_j} |d_j - \lambda_i| \tag{4.2}
$$

for every $1 \leq j \leq n$, provided that $\beta_j < 2$.

Let $\tilde{\lambda}_i - \lambda_i = \alpha_{ij}(d_j - \lambda_i)/z_j$ for all i and j. Suppose that we pick $\tau = 2\eta n^2$ in the deflation procedure of Section 1. Then $z_j \geq 2\eta n^2 \|z\|_2$. Assume further that $\eta n < 1/100$. Then $\beta_j \leq 2/3$, and (4.2) implies that $|\alpha_{ij}| \leq \alpha \equiv 4\eta n \|z\|_2$ for all i and j. Thus

$$
\tilde{z}_i = \sqrt{\frac{\prod_j (\tilde{\lambda}_j - d_i)}{\prod_{j \neq i}(d_j - d_i)}} = \sqrt{\frac{\prod_j (\lambda_j - d_i)(1 + \alpha_{ji}/z_i)}{\prod_{j \neq i}(d_j - d_i)}} = z_i \sqrt{\prod_{j=1}^{n} \left(1 + \frac{\alpha_{ji}}{z_i}\right)}
$$

and

$$
\begin{aligned}
|\tilde{z}_i - z_i| &= z_i \left| \sqrt{\prod_{j=1}^{n} \left(1 + \frac{\alpha_{ji}}{z_i}\right)} - 1 \right| \leq z_i \left(\left(1 + \frac{\alpha}{z_i}\right)^{\frac{n}{2}} - 1 \right) \\
&\leq z_i (e^{\frac{\alpha n}{2 z_i}} - 1) \leq (e-1)\alpha n/2 \\
&\leq 4\eta n^2 \|z\|_2 \quad , \qquad (4.3)
\end{aligned}
$$

where we have used the fact that $\alpha n/(2z_i) \leq 1$ and that $(e^x - 1)/x \leq e - 1$ for $0 < x \leq 1$.

One factor of n in τ and (4.3) comes from the stopping criterion (3.4). This is quite conservative and could be reduced to $\log_2 n$ by using a binary tree structure for summing up the terms in $\psi(\mu)$ and $\phi(\mu)$. The other factor of n comes from the upper bound for $\prod_j (1 + \alpha_{ji}/z_i)$. This also seems quite conservative. Thus we might expect the factor of n^2 in τ and (4.3) to be more like $O(n)$ in practice.

5. Another View of Numerical Stability

In this section we review previous results on the numerical stability of the eigenvector computation and show why they impose unnecessary requirements on the accuracy to which the eigenvalues are computed.

The following lemma bounds the lack of numerical orthogonality in the eigenvectors computed by Algorithm I.

LEMMA 2 (DONGARRA AND SORENSEN [9]). *Let λ_k and λ_ℓ be distinct eigenvalues of $D + zz^T$. Let $\hat{q}_k = \hat{u}_k / \|\hat{u}_k\|_2$ and $\hat{q}_\ell = \hat{u}_\ell / \|\hat{u}_\ell\|_2$, where*

$$\hat{u}_k = \left(\frac{z_1}{\tilde{\delta}_{k1}}, \frac{z_2}{\tilde{\delta}_{k2}}, \ldots, \frac{z_n}{\tilde{\delta}_{kn}} \right)^T$$

and

$$\hat{u}_\ell = \left(\frac{z_1}{\tilde{\delta}_{\ell 1}}, \frac{z_2}{\tilde{\delta}_{\ell 2}}, \ldots, \frac{z_n}{\tilde{\delta}_{\ell n}} \right)^T \quad ,$$

be the computed eigenvectors corresponding to the exact eigenvectors q_k and q_ℓ. If

$$\tilde{\delta}_{ij} = (d_j - \lambda_i)(1 + \eta_{ij}) \quad .$$

where $|\eta_{ij}| \leq \gamma \ll 1$ for all i and j, then

$$\hat{q}_k^T \hat{q}_\ell \leq \gamma(2 + \gamma) \left(\frac{1 + \gamma}{1 - \gamma} \right)^2 \quad .$$

Thus numerical orthogonality can be assured for Algorithm I whenever it is possible to compute all of the differences $d_j - \lambda_i$ to high relative accuracy. Sorensen and Tang [24] show that in pathological cases one encounters enormous difficulties meeting this condition, and thus advocate the use of extended precision arithmetic.

But what does this condition imply about Algorithm II? Recall that

$$z_i = \sqrt{\prod_{j=1}^{i-1} \frac{(\lambda_j - d_i)}{(d_j - d_i)} \cdot \prod_{j=i}^{n-1} \frac{(\lambda_j - d_i)}{(d_{j+1} - d_i)} \cdot (\lambda_n - d_i)}$$

and

$$\tilde{z}_i = \sqrt{\prod_{j=1}^{i-1} \frac{(\tilde{\lambda}_j - d_i)}{(d_j - d_i)} \cdot \prod_{j=i}^{n-1} \frac{(\tilde{\lambda}_j - d_i)}{(d_{j+1} - d_i)} \cdot (\tilde{\lambda}_n - d_i)} \quad .$$

Thus if we compute all of the differences $\lambda_j - d_i$ to high relative accuracy, then $\tilde{z}_i$ will be close to z_i to high *relative* accuracy. In contrast we have shown only that the stopping criterion guarantees that $\tilde{z}_i$ is close to z_i to high *absolute* accuracy, but this is enough for Algorithm II to be backward stable.

6. Numerical Results

In this section we present some numerical results for Algorithms I and II. The tests were run on a SPARCstation 1 in double precision arithmetic. The machine precision is $\epsilon \approx 2.2 \times 10^{-16}$. τ was taken small enough that no deflation occurs.

We define the scaled orthogonality and residue measures

$$\mathcal{O} = \max_{1\le i\le n} \frac{\|\tilde{Q}^T\tilde{q}_i - e_i\|_2}{n\epsilon} \quad \text{and} \quad \mathcal{R} = \max_{1\le i\le n} \frac{\|A\tilde{q}_i - \tilde{\lambda}_i\tilde{q}_i\|_2}{n\epsilon\|A\|_2} \quad .$$

$\mathcal{O}_I$ and $\mathcal{O}_{II}$ are the orthogonality measures for Algorithms I and II, respectively; $\mathcal{R}_I$ and $\mathcal{R}_{II}$ are the residue measures for Algorithms I and II, respectively. We also define

$$Z = \max_{1\le i\le n} \frac{|\tilde{z}_i - z_i|}{n\epsilon\|z\|_2} \quad ,$$

which measures the scaled absolute error in replacing z by $\tilde{z}$.

We use three sets of test problems:

- TEST 1 [24]: These problems arise in applying Cuppen's divide-and-conquer algorithm [8, 9] to the matrix

$$T = \begin{pmatrix} W_{21} & \beta & & & & \\ \beta & W_{21} & \beta & & & \\ & \beta & W_{21} & & & \\ & & & \ddots & & \\ & & & & \beta & \\ & & & & \beta & W_{21} \end{pmatrix} ,$$

  where W_{21} is the symmetric tridiagonal matrix of order 21 with diagonal elements $10, 9, \ldots, 1, 0, 1, 2, \ldots, 10$ and off-diagonal elements all 1. As β becomes smaller and the number of copies of W_{21} becomes larger, more and more difficult rank-1 modification problems arise.

- TEST 2 [24]: $D = diag(1, 2-\beta, 2+\beta, 10/3)$ and $z = (2, \beta, \beta, 2)^T$. This example illustrates how badly Algorithm I can fail in computing the eigenvectors.

- TEST 3: $n = 202; d_1 = 1, d_n = 10/3$, and the rest of the d_i's are of the form $2 \pm j\beta$, for $j = 1, 2, \ldots, 100$; and $z = (2, \beta, \ldots, \beta, 2)^T$. As $\beta > 0$ becomes very small, this matrix has $10\frac{1}{3}$ as an isolated eigenvalue; the remaining eigenvalues are clustered around 2. This generalization of TEST 2 is designed to show the stability of Algorithm II in the presence of an extremely large and tight cluster.

Tables 1, 2, and 3 summarize the results. For Algorithm II, the orthogonality and residue are small, and the vectors z and $\tilde{z}$ agree to machine precision. For Algorithm I, the residue is small, but the orthogonality can be very poor.

7. Some Extensions

In this paper we have presented a novel, backward stable algorithm for solving the rank-one modification of the symmetric eigenproblem. The techniques developed have also been

n	20	20	20	48	36
$-\log_{10}\beta$	7	7	7	7	7
$\mathcal{O}_I$	1.1×10^{4}	1.9×10^{6}	3.2×10^{2}	2.0×10^{7}	8.3×10^{9}
$\mathcal{R}_I$	4.2×10^{-2}	3.8×10^{-2}	3.8×10^{-2}	1.8×10^{-2}	1.6×10^{-2}
Z	8.8×10^{-4}	1.8×10^{-3}	1.8×10^{-3}	1.5×10^{-4}	5.5×10^{-4}
$\mathcal{O}_{II}$	1.1×10^{-1}	1.3×10^{-1}	9.3×10^{-2}	8.1×10^{-2}	6.9×10^{-2}
$\mathcal{R}_{II}$	7.5×10^{-2}	4.0×10^{-2}	4.8×10^{-2}	2.1×10^{-2}	5.2×10^{-2}

Table 1: Results for TEST 1

n	4	4	4	4	4
$-\log_{10}\beta$	1	4	7	10	13
$\mathcal{O}_I$	1.0×10^{0}	1.7×10^{3}	1.4×10^{5}	9.6×10^{8}	1.7×10^{12}
$\mathcal{R}_I$	3.5×10^{-2}	2.2×10^{-1}	8.9×10^{-2}	2.0×10^{-1}	2.0×10^{-1}
Z	1.2×10^{-2}	4.4×10^{-2}	4.4×10^{-2}	4.4×10^{-2}	4.4×10^{-2}
$\mathcal{O}_{II}$	2.6×10^{-1}	5.2×10^{-1}	4.2×10^{-1}	4.2×10^{-1}	3.2×10^{-1}
$\mathcal{R}_{II}$	1.0×10^{-1}	2.3×10^{-1}	2.0×10^{-1}	1.6×10^{-1}	2.2×10^{-1}

Table 2: Results for TEST 2

n	202	202	202
$-\log_{10}\beta$	3	8	15
Z	6.9×10^{-5}	6.1×10^{-5}	1.6×10^{-4}
$\mathcal{O}_{II}$	3.7×10^{-2}	2.5×10^{-2}	4.5×10^{-2}
$\mathcal{R}_{II}$	1.4×10^{-2}	3.6×10^{-3}	1.7×10^{-2}

Table 3: Results for TEST 3

extended to the following:

- Cuppen's method for the symmetric tridiagonal eigenproblem [8, 9, 14];
- an algorithm for the eigendecomposition of symmetric arrowhead matrices [22]; this is in turn the basic tool in the arrowhead divide-and-conquer algorithm for the symmetric tridiagonal eigenproblem [3, 14, 17];
- algorithms for updating the *SVD* [6, 16];
- a divide-and-conquer algorithm for computing the bidiagonal *SVD* [2, 4, 13, 19];
- algorithms for downdating the *SVD* [6, 15].

Moreover it should be easy to apply these techniques to the divide-and-conquer algorithms for the unitary and orthogonal eigenproblems developed in [1, 4, 12].

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