# Forward stable eigenvalue decomposition of rank-one modifications of diagonal matrices

N. Jakovčević Stor<sup>a,1,\*</sup>, I. Slapničar<sup>a,1</sup>, J. L. Barlow<sup>b,2</sup>

<sup>a</sup>Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture,
 University of Split, Rudjera Boškovića 32, 21000 Split, Croatia
 <sup>b</sup>Department of Computer Science and Engineering, The Pennsylvania State University,
 University Park, PA 16802-6822, USA

#### Abstract

We present a new algorithm for solving an eigenvalue problem for a real symmetric matrix which is a rank-one modification of a diagonal matrix. The algorithm computes each eigenvalue and all components of the corresponding eigenvector with high relative accuracy in O(n) operations. The algorithm is based on a shift-and-invert approach. Only a single element of the inverse of the shifted matrix eventually needs to be computed with double the working precision. Each eigenvalue and the corresponding eigenvector can be computed separately, which makes the algorithm adaptable for parallel computing. Our results extend to the complex Hermitian case. The algorithm is similar to the algorithm for solving the eigenvalue problem for real symmetric arrowhead matrices from: N. Jakovčević Stor, I. Slapničar and J. L. Barlow, Accurate eigenvalue decomposition of real symmetric arrowhead matrices and applications, Lin. Alg. Appl., 464 (2015).

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## 1. Introduction and Preliminaries

In this paper we consider the eigenvalue problem for an  $n \times n$  real symmetric matrix A of the form

$$A = D + \rho z z^T, \tag{1}$$

<sup>\*</sup>Corresponding author

Email addresses: nevena@fesb.hr (N. Jakovčević Stor), ivan.slapnicar@fesb.hr (I. Slapničar), barlow@cse.psu.edu (J. L. Barlow)

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where

$$D = \operatorname{diag}(d_1, d_2, \dots, d_n)$$

is a diagonal matrix of order n,

$$z = \begin{bmatrix} \zeta_1 & \zeta_2 & \cdots & \zeta_n \end{bmatrix}^T$$

is a vector and  $\rho \neq 0$  is a scalar. Notice that A is a rank-one modification of a diagonal matrix. Subsequently, we shall refer to such matrices as "diagonal-plus-rank-one" (DPR1) matrices. DPR1 matrices arise, for example, in solving symmetric real tridiagonal eigenvalue problems with the divide-and-conquer method [6], [9], [13], [26, Sections 3.2.1 and 3.2.2], [27, Section III.10].

Without loss of generality, we make the following assumptions:

- $\rho > 0$  (otherwise we consider the matrix  $A = -D \rho z z^T$ ),
- A is irreducible, that is,  $\zeta_i \neq 0, i = 1, \ldots, n$ , and  $d_i \neq d_j$ , for all  $i \neq j$ ,  $i, j = 1, \ldots, n$ , and
- the diagonal elements of D are decreasingly ordered,

$$d_1 > d_2 > \dots > d_n. \tag{2}$$

Indeed, if  $\zeta_i = 0$  for some i, then the diagonal element  $d_i$  is an eigenvalue whose corresponding eigenvector is the i-th unit vector, and if  $d_i = d_j$ , then  $d_i$  is an eigenvalue of the matrix A (we can reduce the size of the problem by annihilating  $\zeta_j$  with a Givens rotation in the (i,j)-plane). Ordering of the diagonal elements of D is attained by symmetric row and column pivoting.

Let

$$A = V\Lambda V^T$$

be the eigenvalue decomposition of A, where

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$$

is a diagonal matrix whose diagonal elements are the eigenvalues of A, and

$$V = [v_1 \quad \cdots \quad v_n]$$

is an orthonormal matrix whose columns are the corresponding eigenvectors.

The eigenvalue problem for a DPR1 matrix A can be solved by any of the standard methods for the symmetric eigenvalue problem (see, for example [28, 25]). However, because of the special structure of diagonal-plus-rank-one matrices, we can use the following approach. The eigenvalues of A are the zeros of the secular function (see, for example, [6] and [11, Section 8.5.3]):

$$f(\lambda) = 1 + \rho \sum_{i=1}^{n} \frac{\zeta_i^2}{d_i - \lambda} = 1 + \rho z^T (D - \lambda I)^{-1} z,$$
 (3)

and the corresponding eigenvectors are given by

$$v_i = \frac{x_i}{\|x_i\|_2}, \quad x_i = (D - \lambda_i I)^{-1} z, \quad i = 1, \dots, n.$$
 (4)

Diagonal elements of the matrix D,  $d_i$ , are called poles of the function f. It is easy to see that, for  $\rho > 0$ , f is strictly increasing between the poles, implying the strict interlacing property

$$\lambda_1 > d_1 > \lambda_2 > d_2 > \dots > \lambda_n > d_n. \tag{5}$$

The formulae (3) and (4) are simple, and have been used to solve similar eigenvalue problems [2, 5, 6, 9]. but maintaining orthogonality among the eigenvectors  $v_i$  requires all of the eigenvalues  $\lambda_i$  to be computed with high accuracy [13]. In other words, if the computed eigenvalues are not accurate enough, then the computed eigenvectors may not be sufficiently orthogonal (see Example 3). The existing algorithms for DPR1 matrices [6, 9, 13] obtain orthogonal eigenvectors with the following procedure:

- compute the eigenvalues  $\tilde{\lambda}_i$  of A by solving (3),
- construct a new matrix

$$\tilde{A} = D + \rho \tilde{z} \tilde{z}^T$$

by solving an inverse problem with the prescribed eigenvalues,

- compute the eigenvectors of  $\tilde{A}$  by (4) but using  $\tilde{z}$  instead of z.

The eigenvectors computed by this algorithm are orthogonal to machine precision (for details see [13, 6, 9, 2]). This results in an algorithm which requires only  $O(n^2)$  computations and O(n) storage for eigenvalues and O(n) storage for each eigenvector. This algorithm is implemented in the LAPACK subroutine DLAED9 and its subroutines [1].

Our algorithm uses a different approach and is forward stable, that is, it computes all eigenvalues and all individual components of the corresponding eigenvectors of a given arrowhead matrix of floating-point numbers to almost full accuracy, a feature which no other method has. The accuracy of the eigenvectors and their numerical orthogonality follows from the high relative accuracy of the computed eigenvalues. Each eigenvalue and the corresponding eigenvector is computed independently of the others in O(n) operations, making our algorithm suitable for parallel computing.

The algorithm is based on a shift-and-invert technique. Basically, an eigenvalue  $\lambda$  is computed from the largest or the smallest eigenvalue of the inverse of the matrix shifted to the pole  $d_i$  which is nearest to  $\lambda$ , that is,

$$\lambda = \frac{1}{\nu} + d_i,\tag{6}$$

where  $\nu$  is either largest or smallest eigenvalue of the matrix

$$A_i^{-1} \equiv (A - d_i I)^{-1}.$$

The algorithm and its error analysis are similar to the algorithm for arrow-head matrices from [17], thus, the present paper can be viewed as a note related to [17].

The organization of the paper is the following. In Section 2, we describe our algorithm named dpr1eig and give error bounds. We also discuss fast secular equation solvers and three implementations of the double the working precision. In Section 3, we illustrate our algorithm with few examples.

## 2. The algorithm

Let A be an irreducible DPR1 matrix of the form (1), with the diagonal elements of D ordered as in (2), and  $\rho > 0$ . Let  $\lambda$  be an eigenvalue of A, let v be its eigenvector, and let x be the unnormalized version of v from (4). Let  $d_i$  be a pole which is closest to  $\lambda$ . Clearly, from (5) it follows that either  $\lambda = \lambda_i$  or  $\lambda = \lambda_{i+1}$ . Let  $A_i$  be the shifted matrix

$$A_i = A - d_i I = \begin{bmatrix} D_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D_2 \end{bmatrix} + \rho \begin{bmatrix} z_1 \\ \zeta_i \\ z_2 \end{bmatrix} \begin{bmatrix} z_1^T & \zeta_i & z_2^T \end{bmatrix},$$

where

$$D_1 = \operatorname{diag}(d_1 - d_i, \dots, d_{i-1} - d_i),$$

$$D_2 = \operatorname{diag}(d_{i+1} - d_i, \dots, d_n - d_i),$$

$$z_1 = \begin{bmatrix} \zeta_1 & \zeta_2 & \cdots & \zeta_{i-1} \end{bmatrix}^T,$$

$$z_2 = \begin{bmatrix} \zeta_{i+1} & \zeta_{i+2} & \cdots & \zeta_n \end{bmatrix}^T.$$

Notice that  $D_1$  ( $D_2$ ) is positive (negative) definite. Obviously,  $\lambda$  is an eigenvalue of A if and only if

$$\mu = \lambda - d_i$$

is an eigenvalue of  $A_i$ , and they share the same eigenvector.

The inverse of  $A_i$  is a permuted arrowhead matrix

$$A_i^{-1} = \begin{bmatrix} D_1^{-1} & w_1 & 0 \\ w_1^T & b & w_2^T \\ 0 & w_2 & D_2^{-1} \end{bmatrix},$$
 (7)

where

$$w_{1} = -D_{1}^{-1} z_{1} \frac{1}{\zeta_{i}},$$

$$w_{2} = -D_{2}^{-1} z_{2} \frac{1}{\zeta_{i}},$$

$$b = \frac{1}{\zeta_{i}^{2}} \left( \frac{1}{\rho} + z_{1}^{T} D_{1}^{-1} z_{1} + z_{2}^{T} D_{2}^{-1} z_{2} \right).$$
(8)

The above formulas for the inverse, which can be verified directly, can also be deduced from [3, Fact 2.16.4], [8, pp. 225] or [10, Theorem 1]. The computation of the scalar b in (8), is critical to how well we are able to compute  $\lambda$ .

The eigenvalue  $\nu$  of a real symmetric arrowhead matrix  $A_i^{-1}$  from (7) is a zero of the secular equation (see, for example [24, 17])

$$g(\nu) = b - \nu - w^{T} (\Delta - \nu I)^{-1} w = 0, \tag{9}$$

where

$$\Delta = \begin{bmatrix} D_1 & \\ & D_2 \end{bmatrix}, \qquad w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}.$$

Once  $\nu$  is computed, we compute  $\mu = 1/\nu$ . The normalized and unnormalized eigenvectors v and x are computed by applying (4) to the matrix  $A_i$ , that is,

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} (D_1 - \mu I)^{-1} z_1 \\ -\frac{\zeta_i}{\mu} \\ (D_2 - \mu I)^{-1} z_2 \end{bmatrix}, \quad v = \frac{x}{\|x\|_2}.$$
 (10)

If  $\lambda$  is an eigenvalue of A which is closest to the pole  $d_i$ , then  $\mu$  is the eigenvalue of matrix  $A_i$  which is closest to zero and

$$\nu = \frac{1}{\mu} = \pm \|A_i^{-1}\|_2$$
.

We say that  $\nu$  is the *largest absolute eigenvalue* of  $A_i^{-1}$ . In this case, if all entries of  $A_i^{-1}$  are computed with high relative accuracy, then, according to standard perturbation theory, any reasonable algorithm can compute  $\nu$  to high relative accuracy (see Section 2.2).

Throughout the paper, we assume that the computations are carried out in the standard floating-point arithmetic with the machine precision  $\varepsilon_M = 2^{-52} \approx 2.2204 \cdot 10^{-16}$  (see [14, Chapter 2] for details). Thus, the floating-point numbers have approximately 16 significant decimal digits. The term "double the working precision" means that the computations are performed with numbers having approximately 32 significant decimal digits, or with the machine precision  $\varepsilon_M^2$  or smaller.

Notice that all entries of  $A_i^{-1}$  are computed to high relative accuracy using standard precision, except possibly b in (8). For example, using the standard model from [14, Section 2.2], the error analysis for the respective indices k gives

$$fl([D_1]_k) = \frac{1}{d_k - d_1} (1 + \varepsilon_1), \quad |\varepsilon_1| \le 2\varepsilon_M,$$
  
$$fl([w_1]_k) = \frac{\zeta_k}{\zeta_i (d_k - d_i)} (1 + \varepsilon_2), \quad |\varepsilon_2| \le 3\varepsilon_M,$$

If b is not computed to high relative accuracy and it influences  $||A_i^{-1}||_2$ , it is sufficient to compute it with double the working precision. Whether double

the working precision is needed is determined as follows: set

$$K_{b} = \frac{1 + \rho z_{1}^{T} D_{1}^{-1} z_{1} - \rho z_{2}^{T} D_{2}^{-1} z_{2}}{\left|1 + \rho z_{1}^{T} D_{1}^{-1} z_{1} + \rho z_{2}^{T} D_{2}^{-1} z_{2}\right|},$$

$$K_{z} = \frac{1}{\left|\zeta_{i}\right|} \sum_{\substack{j=1\\j \neq i}}^{n} \left|\zeta_{j}\right|,$$

$$\kappa_{\nu} \leq \min\left\{(n+4)\sqrt{n} K_{b}, 3\sqrt{n} + (n+4)\left(1 + 2K_{z}\right)\right\}. \tag{11}$$

Here  $K_b$  measures whether b is computed with high relative accuracy,  $K_z$  measures whether b influences  $||A_i^{-1}||_2$ , and  $\kappa_{\nu}$  measures the accuracy of the exact eigenvalue  $\hat{\nu}$  of the computed matrix  $fl(A_i^{-1})$ ,

$$\widehat{\nu} = \nu (1 + \kappa_{\nu} \varepsilon_{M}),$$

similarly as in [17, Theorem 5].

If  $\kappa_{\nu} \gg O(n)$ , then b needs to be computed in double the working precision (see section 2.3). The details of the proofs of the above facts are similar to the proofs of [17, Theorems 5 and 7].

If  $\lambda$  is an eigenvalue of A which is not closest to the pole  $d_i$ , then  $\mu$  is not the eigenvalue of  $A_i$  which is closest to zero. Further,  $|\nu| < ||A_i^{-1}||_2$ , and the quantity

$$K_{\nu} = \frac{\|A_i^{-1}\|_2}{|\nu|} \tag{12}$$

tells us how far  $\nu$  is from the largest absolute eigenvalue of  $A_i^{-1}$ . If  $K_{\nu} \gg 1$ , then the standard perturbation theory does not guarantee that the eigenvalue  $\mu$  will be computed with high relative accuracy. One remedy to this situation is to use non-standard shifting as follows:

- (R1) we can compute  $\lambda$  by shifting to the neighboring pole on the other side if that gives a smaller value of  $K_{\nu}$ ,
- (R2) if shifting to another neighboring pole is not possible, we can invert  $A \sigma I$ , where the shift  $\sigma$  is chosen near but not equal to  $\lambda$ , and not equal to the neighboring poles. This results in a DPR1 matrix whose largest absolute eigenvalue is computed accurately. If no floating-point numbers  $\sigma$  lie between  $\lambda$  and the neighboring poles,  $\sigma$  and the corresponding DPR1 matrix must be computed in double the working precision.

We need to address one more special situation. If  $\lambda$  is much closer to zero than to the neighboring pole or poles<sup>3</sup>,  $|\lambda| \ll \min\{|\lambda - d_k|, |\lambda - d_{k-1}|\}$ , then the formula (6) may involve large cancellation, and  $\lambda$  may be inaccurate in spite of the accurately computed  $\nu$  and  $\nu$ . In this case,  $\lambda$  can be computed accurately

<sup>&</sup>lt;sup>3</sup>There can be at most one such eigenvalue.

as  $\lambda = 1/\nu$ , where  $\nu$  is the largest absolute eigenvalue of  $A^{-1}$ . If all poles are non-zero, the inverse of A is again an unreduced DPR1 matrix of the form

$$A^{-1} = D^{-1} + \gamma D^{-1} z z^T D^{-1}, \quad \gamma = -\frac{\rho}{1 + \rho z^T D^{-1} z}.$$
 (13)

If the denominator in  $\gamma$  is computed as zero, the matrix A is numerically singular and we can set  $\lambda = 0$ .

The described procedure is implemented in algorithm dpr1eiq.

The algorithm dpr1eig extends naturally to the Hermitian case (c.f. [17,  $\S6.1$ ]).

# 2.1. Accuracy of the algorithm

Let  $(\lambda, \widetilde{v})$  denote the eigenpair computed by Algorithm 1 in the standard floating-point arithmetic. Let  $\widetilde{\nu}$  denote the computed eigenvalue of  $A_i^{-1}$ . If  $\widetilde{\nu}$  is the absolutely largest eigenvalue of  $A_i^{-1}$  and if it is computed by bisection, then the error bound from [24, §3.1] immediately implies that<sup>4</sup>

$$\widetilde{\nu} = \nu (1 + \kappa_{bis} \varepsilon_M), \quad \kappa_{bis} \le 1.06 n \left( \sqrt{n} + 1 \right).$$
(14)

The computed eigenpair satisfies

$$\widetilde{\lambda} = fl(\lambda) = \lambda(1 + \kappa_{\lambda} \varepsilon_{M}),$$

$$\widetilde{v}_{i} = fl(v_{i}) = v_{i}(1 + \kappa_{v_{i}} \varepsilon_{M}), \quad i = 1, \dots, n,$$

where

$$|\kappa_{\lambda}|, |\kappa_{v_i}| \leq O(\kappa_{\nu} + \kappa_{bis}),$$

and  $\kappa_{\nu}$  is defined by (11).

If  $1 \ll K_b \leq O(1/\varepsilon_M)$ , then, after evaluating b with double the working precision,  $\kappa_{\nu}$  is given by (11) with  $K_b$  replaced by  $K_b\varepsilon_M$ .<sup>5</sup> With our approach componentwise high relative accuracy of the computed normalized eigenvectors implies, in turn, their numerical orthogonality.

The proofs of the above error bounds are similar to the error analysis in [17].

## 2.2. Fast secular equation solvers

Instead of using bisection to compute zeros of secular equation (9) in Algorithm 1, we can use some fast zero finder with quadratic or even cubic convergence like those from [23, 4, 20]. Such zero finders compute zeros to machine accuracy using a small number of direct evaluations of the Pick function and

<sup>&</sup>lt;sup>4</sup>Notice that a similar error bound holds for all eigenvalues which are of the same order of magnitude as  $\nu$ .

<sup>&</sup>lt;sup>5</sup>If  $K_b \geq O(1/\varepsilon_M)$ , that is, if  $K_b = 1/\varepsilon_E$  for some  $\varepsilon_E < \varepsilon_M$ , then b needs to be computed with extended precision  $\varepsilon_E$ . Usage of higher precision in conjunction with the eigenvalue computation for DPR1 matrices is analyzed in [2], but there the higher precision computation is potentially needed in the iterative part. This is less convenient than our approach where the higher precision computation is used only to compute one element.

# Algorithm 1

```
[\lambda, v] = \mathbf{dpr1eig}(D, z, \rho, k)
\% Computes the k-th eigenpair of an ordered irreducible DPR1 matrix
\% A = \operatorname{diag}(D) + \rho z z', \ \rho > 0
% Find the shift \sigma = d_i such that d_i is the pole nearest to \lambda
% Exterior eigenvalue k=1:
if k == 1
  \sigma = d_1
else
  % Interior eigenvalues k \in \{2, ..., n\}:
  \bar{D} = D - d_k
 \begin{array}{l} \tau = \bar{D}_{k-1}/2 \\ F = 1 + \rho \sum (z.*z./(\bar{D} - \tau)) \end{array}
  if F > 0
    \sigma = d_k
  else
    \sigma = d_{k-1}
  end
end
compute the arrowhead matrix A_i^{-1} \equiv (A - \sigma I)^{-1} according to (7) and (8)
compute \kappa_{\nu} from (11)
if \kappa_{\nu} \gg O(n)
  recompute b from (8) by using double the working precision (c.f. section 2.3)
if \sigma = d_{k-1}
 compute the leftmost eigenvalue \nu of A_i^{-1} by bisection (c.f. section 2.2)
{f else}
  compute the rightmost eigenvalue \nu of A_i^{-1} by bisection
compute v by (10), where \mu = 1/\nu
compute \lambda = \mu + \sigma
compute K_{\nu} from (12)
if K_{\nu} \gg 1
  apply one of the remedies (R1) or (R2)
if |\lambda| \ll \min\{|\lambda - d_k|, |\lambda - d_{k-1}|\}
  recompute \lambda from A^{-1}
end
```

its its derivative, where  $O(\log(\log(1/\varepsilon)))$  iterations are needed to obtain an  $\varepsilon$ -accuracy [21].

In particular, we tested the implementation of the cubically convergent zero finder by Borges and Gragg from [4, §3.3], with the stopping criterion defined by [4, p. 15]. From [4, (21)], it follows that the accuracy of the computed solution satisfies a similar backward error bound as (14). This was indeed, true in all our tests. The number of iterations never exceeded 7.

Similarly, for the solution of the secular equation (3), which may be needed in the last two "if" statements in Algorithm 1, one can use the fast secular equation solver by Li [20]. This solver is implemented in the LAPACK routine DLAED4. The accuracy of the computed solution satisfied a similar backward error bound as (14) and the number of iterations behaved as predicted.

Although the operation count of both fast zero finders is approximately half of the operations needed for bisection, we observed no speed-up in Matlab implementation.

## 2.3. Implementation of the double the working precision

We tried three different implementations of the double the working precision:

- by converting all quantities in the formulas (8) or (13) to variable precision by Matlab [22] command sym with parameter 'f', and then performing the computations;
- by evaluating all parts of the formulas (8) or (13) using extended precision routines add2, sub2, mul2, and div2 from [7]; and
- by converting all quantities in the formulas (8) or (13) from standard 64 bit double precision numbers, declared by REAL(8), to 128 quadruple precision numbers, declared by REAL(16), in Intel FORTRAN compiler ifort [15], and then performing the computations.

Having to invoke higher precision clearly slows the computation down. In Matlab, when using variable precision sym command, the computation may be slowed down by a factor of three hundred or more for each eigenvalue that requires formulas (8) or (13) to be evaluated in higher precision. This makes use of sym prohibitive for higher dimensions. Extended precision routines by Dekker [7] require on average ten floating-point operations. The fastest implementation is the one in ifort which is only about three times slower. Thus, the algorithm benefits from a good implementation of higher precision.

## 3. Numerical Examples

We have used the following implementations of Algorithm 1:

• dpr1eig(M) - Matlab implementation, with double the working precision implemented using extended precision routines from [7].

dpr1eig(J) - Julia [18] implementation, with double the working precision implemented using Julia package DoubleDouble.jl [19] - this implementation is publicly available in the Julia package Arrowhead.jl [19], and is our preferred implementation.

We compared Algorithm 1 with the following routines:

- eig Matlab's standard eigenvalues routine.
- dlaed9 LAPACK routine DLAED9 compiled with ifort Fortran compiler.
- *Math* Mathematica [29] eigenvalue routine with 100 digits of precision (properly rounded to 16 decimal digits).

We illustrate our algorithm with four numerically demanding examples. Examples 1 and 2 illustrate Algorithm 1, Example 3 illustrates the use of double precision arithmetic, Example 4 illustrates an application to higher dimension, and Example 5 shows the effect of using double the working precision on overall timing. Since dpr1eig(M) and dpr1eig(J) give numerical identical results, we denote these results by dpr1eig.

**Example 1.** In this example quantities  $K_b$  from (11) are approximately 1 for all eigenvalues, so we guarantee that all eigenvalues and all components of their corresponding eigenvectors are computed with high relative accuracy by Algorithm 1, using only standard machine precision. Let  $A = D + zz^T$ , where

$$\begin{split} D &= \mathrm{diag}\,(10^{10}, 5, 4\cdot 10^{-3}, 0, -4\cdot 10^{-3}, -5), \\ z &= \begin{bmatrix} 10^{10} & 1 & 1 & 10^{-7} & 1 & 1 \end{bmatrix}^T. \end{split}$$

The computed eigenvalues are:<sup>6</sup>

$\lambda^{(eig)}$	$\lambda^{(dlaed9)}$	$\lambda^{(dpr1eig,Math)}$
$1.000000000100000 \cdot 10^{20}$	$1.000000000100000 \cdot 10^{20}$	$1.000000000100000 \cdot 10^{20}$
5.000000000099998	5.000000000100000	5.000000000100000
$4.000000099999499 \cdot 10^{-3}$	$4.000000100000001 \cdot 10^{-3}$	$4.000000100000001 \cdot 10^{-3}$
$1.665334536937735 \cdot 10^{-16}$	$1.000000023272195 \cdot 10^{-24}$	9.99999999999999999999999999999999999
0	$-3.999999900000001 \cdot 10^{-3}$	$-3.999999900000001 \cdot 10^{-3}$
-25.00000000150000	-4.999999999900000	-4.999999999900000

We see that all eigenvalues computed by dpr1eig (including the tiniest ones), are exact to the machine precision. The eigenvalues computed by dlaed9 are all accurate, except  $\lambda_4$ . The eigenvalues computed by eig are accurate according to the standard perturbation theory, but they have almost no relative accuracy<sup>7</sup>.

 $<sup>^6</sup>$ If, in the last column, the last digits computed by dpr1eig and Mathematica, respectively, differ, they are displayed in parentheses.

<sup>&</sup>lt;sup>7</sup>The displayed eigenvalues are the ones obtained by the Matlab command [V,Lambda]=eig(A). The command Lambda=eig(A) produces slightly different eigenvalues. The reason is that Matlab uses LAPACK routine dsyev.f, which, in turn, uses different algorithms depending whether eigenvectors are required or not.

Due to the the accuracy of the computed eigenvalues, the eigenvectors computed by dpr1eig are componentwise accurate up to machine precision, and therefore, orthogonal up to machine precision. The eigenvectors computed by dlaed9 are also componentwise accurate, except for  $v_4$ :

```
\begin{array}{lll} v_4^{(dlaed9)} & v_4^{(dpr1eig,Math)} \\ 1.000000011586098 \cdot 10^{-17} & 9.9999999899999(6,9) \cdot 10^{-18} \\ 2.000000023172195 \cdot 10^{-18} & 1.99999999800000 \cdot 10^{-18} \\ 2.500000028965244 \cdot 10^{-15} & 2.49999999749999 \cdot 10^{-15} \\ -1.0000000000000000 & -2.500000028965244 \cdot 10^{-15} \\ -2.000000023172195 \cdot 10^{-18} & -1.999999999800000 \cdot 10^{-18} \end{array}
```

**Example 2.** In this example, despite very close diagonal elements, we again guarantee that all eigenvalues and all components of their corresponding eigenvectors are computed with high relative accuracy. Let  $A = D + zz^T$ , where

$$\begin{split} D &= \mathrm{diag} \left( 1 + 40\varepsilon, 1 + 30\varepsilon, 1 + 20\varepsilon, 1 + 10\varepsilon \right), \\ z &= \begin{bmatrix} 1 & 2 & 2 & 1 \end{bmatrix}. \end{split}$$

and  $\varepsilon = 2^{-52} = 2\varepsilon_M$ . For this matrix, the quantities  $K_b$  are again of order one for all eigenvalues, so Algorithm 1 uses only standard working precision. The computed eigenvalues are:

$$\begin{array}{llll} \lambda^{(eig)} & \lambda^{(dlaed9)} & \lambda^{(dpr1eig)} \\ 11 + 32\varepsilon & 11 + 48\varepsilon & 11 + 32\varepsilon \\ 1 + 38\varepsilon & 1 + 41\varepsilon & 1 + 39\varepsilon \\ 1 + 31\varepsilon & 1 + 27\varepsilon & 1 + 25\varepsilon \\ 1 + 8\varepsilon & 1 + 9\varepsilon & 1 + 11\varepsilon \end{array}$$

Notice that all computed eigenvalues are accurate according to standard perturbation theory. However, only the eigenvalues computed by dpr1eig satisfy the interlacing property. The eigenvalues computed by Math, properly rounded to 32 decimal digits are:

```
\begin{array}{l} \lambda^{(Math)} \\ 11.0000000000000005551115123125783 \\ 1.000000000000000085712482686374087 \\ 1.00000000000000055511151231257826 \\ 1.000000000000000025309819776141565 \end{array}
```

If Algorithm 1 is modified to return  $\sigma$  and  $\mu$  (both in standard precision), then for the eigenvalues  $\lambda_2$ ,  $\lambda_3$  and  $\lambda_4$  the corresponding pairs  $(\sigma,\mu)$  give representations of those eigenvalues to 32 decimal digits. In our case, the exact values  $\sigma + \mu$  properly rounded to 32 decimal digits are equal to the corresponding eigenvalues computed by Mathematica displayed above.

The eigenvectors  $v_2$ ,  $v_3$  and  $v_4$  computed by eig span an invariant subspace of  $\lambda_2$ ,  $\lambda_3$  and  $\lambda_4$ , but their components are not accurate. Due to the accuracy of the computed eigenvalues, the eigenvectors computed by dpr1eig are componentwise accurate up to the machine precision (they coincide with the

eigenvectors computed by Math, and are therefore orthogonal. Interestingly, in this example the eigenvectors computed by dlaed9 are also componentwise accurate, but there is no underlying theory for such high accuracy.

**Example 3.** In this example (see [12]) we can guarantee that all eigenvalues and eigenvectors will be computed with componentwise high relative accuracy only if b from (8) is for  $k \in \{2, 3, 4\}$  computed in double of the working precision. Let  $A = D + zz^T$ , where

$$D = \text{diag} (10/3, 2 + \beta, 2 - \beta, 1),$$
  

$$z = \begin{bmatrix} 2 & \beta & \beta & 2 \end{bmatrix}, \quad \beta = 10^{-7}.$$

For  $k \in \{2,3,4\}$  the quantities  $\kappa_{\nu}$  from (11) are of order  $O(10^7)$ , so the element b in each of the matrices needs to be computed in double of the working precision. For example, for k=2, the element  $b=\left[A_2^{-1}\right]_{22}$  computed by Algorithm 1 in standard precision is equal to  $b=5.749999751891721 \cdot 10^7$ , while Matlab routine inv gives  $b=5.749999746046776 \cdot 10^7$ . Computing b in double of the working precision in Algorithm 1 gives the correct value  $b=5.749999754927588 \cdot 10^7$ .

The eigenvalues computed by eig, dlaed9, dpr1eig and Math, respectively, are all highly relatively accurate – they differ in the last or last two digits. However, the eigenvectors  $v_2$ ,  $v_3$  and  $v_4$  computed by dpr1eig (with double precision computation of b's), are componentwise accurate to machine precision and therefore orthogonal. The eigenvectors computed by eig and dlaed9 are, of course, orthogonal, but are not componentwise accurate. For example,

**Example 4.** In this example we extend Example 3 to higher dimension, as in TEST 3 from [12, §6]. Here  $A = D + zz^T \in \mathbb{R}^{202 \times 202}$ , where

$$D = \operatorname{diag}(1, 2 + \beta, 2 - \beta, 2 + 2\beta, 2 - 2\beta, \dots, 2 + 100\beta, 2 - 100\beta, 10/3),$$
  

$$z = \begin{bmatrix} 2 & \beta & \beta & \dots & \beta & 2 \end{bmatrix}, \quad \beta \in \{10^{-3}, 10^{-8}, 10^{-15}\}.$$

For each  $\beta$ , we solved the eigenvalue problem with Algorithm 1 without using double the working precision  $(dpr1eig\_nd)$ , dpr1eig, and dlaed9. For  $\beta=10^{-3}$ , Algorithm 1 used double the working precision for computing 25 eigenvalues, and for  $\beta=10^{-8}$  and  $\beta=10^{-15}$  double the working precision was needed for all but the largest eigenvalue. As in [12, §6], for each algorithm we computed orthogonality and residual measures,

$$\mathcal{O} = \max_{1 \le i \le n} \frac{\|V^T v_i - e_i\|_2}{n\varepsilon_M}, \qquad \mathcal{R} = \max_{1 \le i \le n} \frac{\|A v_i - \lambda_i v_i\|_2}{n\varepsilon_M \|A\|_2},$$

respectively. Here  $V = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix}$  is the computed matrix of eigenvectors, and  $e_i$  is the *i*-th column of the identity matrix.

Since we proved the componentwise accuracy of eigenvectors computed by dpr1eig, we take those as the ones of reference. Table 1 displays orthogonality measures, residual measures, relative errors in the computed eigenvalues and componentwise relative errors in the computed eigenvectors, superscripted by the name of the respective algorithm. From table 1, we see that all algorithms

β	$10^{-3}$	$10^{-8}$	$10^{-15}$
$\mathcal{O}^{(dpr1eig\_nd)}$	1.47	$5.8 \cdot 10^4$	$2.1 \cdot 10^{11}$
$\mathcal{O}^{(dpr1eig)}$	0.059	0.039	0.045
$\mathcal{O}^{(dlaed9)}$	0.049	0.064	0.045
$\mathcal{R}^{(dpr1eig\_nd)}$	0.0086	0.033	0.0043
$\mathcal{R}^{(dpr1eig)}$	0.0086	0.039	0.0043
$\mathcal{R}^{(dlaed9)}$	0.029	0.03	0.013
$\max_{1 \le i \le n} \frac{ \lambda_i^{(dpr1eig \bullet nd)} - \lambda_i^{(dpr1eig)} }{ \lambda_i^{(dpr1eig)} }$	$2.2 \cdot 10^{-16}$	0	$2.2 \cdot 10^{-16}$
$\max_{1 \le i \le n} \frac{ \lambda_i^{(dlaed9)} - \lambda_i^{(dpr1eig)} }{ \lambda_i^{(dpr1eig)} }$	$1.5\cdot10^{-15}$	$2.2\cdot10^{-16}$	0
$\max_{1 \le i,j \le n} \frac{ [v_i^{(dpr1eig\_nd)}]_j - [v_i^{(dpr1eig)}]_j }{ [v_i^{(dpr1eig)}]_j }$	$2.7\cdot10^{-13}$	$2.8\cdot10^{-8}$	0.518
$\max_{1 \le i, j \le n} \frac{ [v_i^{(dlaed9)}]_j - [v_i^{(dpr1eig)}]_j }{ [v_i^{(dpr1eig)}]_j }$	$2.2\cdot10^{-12}$	$1.9\cdot 10^{-8}$	0.043

Table 1: Orthogonality measures, residue measures, relative errors in computed eigenvalues, and componentwise relative errors in computed eigenvectors.

behave exactly as predicted by the theoretical analysis. All algorithms compute all eigenvalues to high relative accuracy because it is the same as normwise accuracy for this case.  $dpr1eig\_nd$  loses orthogonality as predicted by the respective condition numbers. The number of correct digits in the computed eigenvectors is approximately the same for  $dpr1eig\_nd$  and dlaed9, but there is no proof of such componentwise accuracy of the eigenvectors computed by dlaed9. As a consequence of their componentwise accuracy, the eigenvectors computed by dpr1eig are fully orthogonal.

**Example 5.** To illustrate the effect of using double the working precision, in Table 2 we give timings for the matrix  $A \in \mathbb{R}^{202 \times 202}$  of the same form as in Example 4.

	$\beta = 10^{-3}$	$\beta=10^{-8}$	$\beta=10^{-15}$
dpr1eig(M)	11	17	17
$\frac{dpr1eig(M)}{dpr1eig(J)}$	1.2	2.2	2.2
dlaed9	0.13	0.13	0.13

Table 2: Running time (in seconds) for the computation of eigenvalues and eigenvectors of DPR1 matrix A of order n=2002.

We see that the Julia version of Algorithm 1 is almost 10 times faster than the Matlab version, which makes Julia version an implementation of preference. As in Example 4, for  $\beta=10^{-3}$ , dpr1eig used double the working precision to compute respective b when computing 25 eigenvalues, and for  $\beta=10^{-8}$  and  $\beta=10^{-15}$  double the working precision was needed for all but the largest eigenvalue. We see that the overhead of using double the working precision is approximately 55% in both, Julia and Matlab.

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