Structure of almost diagonal matrices

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Abstract. *Classical and recent results on almost diagonal matrices are presented. These results measure the absolute and the relative distance between diagonal elements and the appropriate eigenvalues or singular values, and in case of multiple eigenvalues or singular values, reveal special structure in matrices. Simple MATLAB programs serve to illustrate how good the theoretical estimates are.*

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Introduction

In this overview paper we present classical and recent results concerning special properties of almost diagonal matrices. Almost diagonal matrices play an important role in the asymptotic convergence analysis of different matrix algorithms for eigenvalue and singular value problems. Our intention is to extract the most important or the characteristic information from the papers that appeared in this area. We shall not prove theorems, except in one instance to show the tools and reasonings. Instead, we shall illustrate the results by observing the quantities they deal with. To this end we use MATLAB.

The paper is divided into two sections. The first one deals with "older" or classical results, while the second one deals with more recent results.

1. Classical results

This section is divided into three subsections. In the first one, we provide examples of almost diagonal matrices with simple eigenvalues or singular values and observe how closely they are approximated by diagonal elements. In the second one, we deal with matrices having multiple eigenvalues or singular values. We observe interesting structures associated with certain matrix block partitions. Finally, in the third subsection we provide theoretical results which explain these observations. We note that in the classical results one uses absolute gaps in the spectrum or in the set of singular values and norms of certain submatrices.

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1.1. Simple eigenvalues and singular values

Let us consider the following symmetric matrix of order 6,

$$A = \begin{bmatrix} 1 & 0.01 & -0.01 & -0.001 & 0.002 & 0 \\ 0.01 & -2 & 0.01 & -0.003 & -0.001 & 0.002 \\ -0.01 & 0.01 & 3 & 0.001 & -0.001 & -0.0001 \\ -0.001 & -0.003 & 0.001 & -4 & 0.003 & 0.001 \\ 0.002 & -0.001 & -0.001 & 0.003 & 5 & 0.003 \\ 0 & 0.002 & -0.0001 & 0.001 & 0.003 & -6 \end{bmatrix}$$

Using the spectral norm, we find out

$$\|A - \mathrm{diag}(A)\|_2 \approx 2.029490 \cdot 10^{-2},$$

while absolute values of the diagonal elements are not smaller than 1. Thus, it can be considered as almost diagonal. To estimate how close the diagonal elements are from the eigenvalues, we can use the classical perturbation result for Hermitian matrices: if A and B are symmetric, then (see [35])

$$|\ \lambda_i(A) - \lambda_i(B)\ | \leq \|A - B\|_2, \quad 1 \leq i \leq n\,, \tag{1}$$

where $\lambda_i(A)$ and $\lambda_i(B)$ are the eigenvalues of A and B, respectively. Assuming $B = \mathrm{diag}(A)$, where $\mathrm{diag}(A)$ is the diagonal of A, we obtain

$$|\ \lambda_i - a_{ii}\ | \leq \|A - \mathrm{diag}(A)\|_2, \quad 1 \leq i \leq n.$$

Computing the eigenvalues of A by MATLAB, one can find

i	a_{ii}	λ_i	$(a_{ii} - \lambda_i)/\lambda_i$
1	-6	-6.00000232037038	$-3.8673 \cdot 10^{-7}$
2	-4	-4.00000533797954	$-1.3345 \cdot 10^{-6}$
3	-2	-2.00004811652753	$-2.4058 \cdot 10^{-5}$
4	1	0.99998287851289	$1.7122 \cdot 10^{-5}$
5	3	3.00006943063431	$-2.3143 \cdot 10^{-5}$
6	5	5.00000346573025	$-6.9315 \cdot 10^{-7}$

Denoting $\|A - \mathrm{diag}(A)\|_2$ by ϵ, we see that $|\ a_{ii} - \lambda_i\ | \,/\, |\ \lambda_i\ |$ is actually of order ϵ^2. Later, we shall see that this holds because the condition

$$\|A - \mathrm{diag}(A)\|_2 < \min_{i \neq j} |\ \lambda_i - \lambda_j\ |$$

is fulfilled.

Next, we consider how close the singular values of an almost diagonal triangular matrix are to (the moduli of) diagonal elements. For general $m \times n$ matrices A and B, we have the known perturbation result, which can be deduced from (1) (cf. [7, Corollary 8.3.2]),

$$|\ \sigma_i(A) - \sigma_i(B)\ | \leq \|A - B\|_2, \quad 1 \leq i \leq n\,.$$

Here $\sigma_i(A)$ and $\sigma_i(B)$ are the singular values of A and B, respectively, and $n \leq m$. If one takes $B = \mathrm{diag}(A)$, this result reduces to

$$| \sigma_i - | a_{ii} || \leq \|A - \mathrm{diag}(A)\|_2, \quad 1 \leq i \leq n,$$

where $\sigma_i = \sigma_i(A)$ for all i and $\mathrm{diag}(A)$ is $m \times n$. The usual preprocessing step for singular value computations is the QR factorization (often with column pivoting), which transforms A to the upper-triangular form. For this reason, we first consider upper-triangular matrices.

Consider the following example. Let A be the matrix of order 6 from the first example, and let it be split into lower-triangular, diagonal and upper-triangular part, $A = L + D + U = L + T$ (in MATLAB notation, $T = \mathrm{triu}(A)$),

$$T = \begin{bmatrix} 1 & 0.01 & -0.01 & -0.001 & 0.002 & 0 \\ & -2 & 0.01 & 0.003 & -0.001 & 0.002 \\ & & 3 & 0.001 & -0.001 & -0.0001 \\ & & & -4 & 0.003 & 0.001 \\ & & & & 5 & 0.003 \\ & & & & & -6 \end{bmatrix}.$$

Since

$$\|T - \mathrm{diag}(T)\|_2 \approx 1.638970 \cdot 10^{-2} \ll \min_i | t_{ii} | = 1, \qquad T = (t_{ij}),$$

T can be considered as almost diagonal. Computing the singular values of T, we obtain

i	$\mid t_{ii} \mid$	σ_i	$(\mid t_{ii} \mid - \sigma_i)/\sigma_i$
1	1	0.99997705061184	$2.2950 \cdot 10^{-5}$
2	2	2.00001214305070	$-6.0715 \cdot 10^{-5}$
3	3	3.00004859484805	$-1.6198 \cdot 10^{-5}$
4	4	3.99999981504819	$4.6238 \cdot 10^{-8}$
5	5	5.00000114649816	$-2.2930 \cdot 10^{-7}$
6	6	6.00000298158935	$-4.9693 \cdot 10^{-7}$

Denoting $\epsilon = \|T - \mathrm{diag}(T)\|_2$, we see that $| \, | t_{ii} | - \sigma_i \, | = \mathcal{O}(\epsilon^2)$. Later, we shall see that this is true because

$$\|T - \mathrm{diag}(T)\|_2 < \min_{i \neq j} | \sigma_i - \sigma_j |$$

holds.

The same property holds for a full square matrix. For example, let

$$\begin{aligned} C &= D + N, \ D = \mathrm{diag}(1, -2, 3, -4, 5, -6) \\ N &= (n_{ij}), \ n_{ij} = 10^{-2} \cdot r_{ij} \cdot \delta_{ij}, \end{aligned}$$

where δ_{ij} is the Kronecker symbol and each r_{ij} is a random number (generated by the MATLAB rand function) in the interval $(0,1)$. The matrix reads

$$C = \frac{1}{1000}\begin{bmatrix} 1000 & 6.5502 & 4.8063 & 3.5191 & 3.1944 & 9.1158 \\ 9.1029 & -2000 & 5.3722 & 2.6872 & 0.7282 & 6.4122 \\ 7.7302 & 0.3600 & 3000 & 6.9243 & 9.7534 & 8.3867 \\ 1.6254 & 7.9346 & 9.9191 & -4000 & 8.6082 & 4.0731 \\ 1.6525 & 9.0016 & 0.4876 & 7.2894 & 5000 & 5.0003 \\ 4.9974 & 6.2425 & 2.5143 & 8.3743 & 3.7282 & -6000 \end{bmatrix},$$

where only four decimals are displayed. We have

$$\|N\|_2 \approx 2.739199 \cdot 10^{-2} \ll \min_i \mid c_{ii} \mid = 1$$

and the SVD computation reveals

i	$\mid c_{ii} \mid$	σ_i	$(\mid c_{ii} \mid - \sigma_i)/\sigma_i$
1	1	1.00000556168780	$-5.5617 \cdot 10^{-6}$
2	2	1.99999209161829	$3.9542 \cdot 10^{-6}$
3	3	3.00002608164948	$-8.6938 \cdot 10^{-6}$
4	4	4.00001696355321	$-4.2409 \cdot 10^{-6}$
5	5	5.00003095907297	$-6.1918 \cdot 10^{-6}$
6	6	6.00004753371360	$-7.9222 \cdot 10^{-6}$

.

Later, we shall understand that this result holds whenever

$$\|C - \mathrm{diag}(C)\|_2 < \min_{i \neq j} \mid \sigma_i - \sigma_j \mid .$$

Next, we construct a pair of Hermitian almost diagonal matrices (A, B), such that B is positive definite. Let A be as in the first example, while

$$B = \mathrm{diag}(1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \frac{1}{6}) + 10^{-3} \cdot N_B,$$

where N_B is symmetric with $(N_B)_{ij} = \delta_{ij} r_{ij}$, $i \leq j$ and r_{ij} are as above. We have

$$A = 10^{-4} \cdot \begin{bmatrix} 10000 & 100 & -100 & -10 & 20 & 0 \\ 100 & -20000 & 100 & -30 & -10 & 20 \\ -100 & 100 & 30000 & 10 & -10 & -1 \\ -10 & -30 & 10 & -40000 & 30 & 10 \\ 20 & -10 & -10 & 30 & 50000 & 30 \\ 0 & 20 & -1 & 10 & 30 & -60000 \end{bmatrix},$$

$$B = 10^{-4} \cdot \begin{bmatrix} 10000 & 2.64 & 4.39 & 2.03 & 6.63 & 8.47 \\ 2.64 & 5000 & 5.28 & 5.36 & 4.09 & 4.87 \\ 4.39 & 5.28 & 10000/3 & 8.67 & 3.78 & 4.92 \\ 2.03 & 5.36 & 8.67 & 2500 & 4.35 & 5.22 \\ 6.63 & 4.09 & 3.78 & 4.35 & 2000 & 4.95 \\ 8.47 & 4.87 & 4.92 & 5.22 & 4.95 & 10000/6 \end{bmatrix}$$

where only four decimals are displayed for the elements of B. Since

$$\|A - \mathrm{diag}(A)\|_2 \approx 2.02949 \cdot 10^{-2} \ll \min_i \mid a_{ii} \mid = 1$$

and

$$\|B - \mathrm{diag}(B)\|_2 \approx 2.57188 \cdot 10^{-3} \ll \min_i \mid b_{ii} \mid = \frac{1}{6},$$

both matrices can be considered as almost diagonal. From the perturbation theory for Hermitian matrices we know that quotients a_{ii}/b_{ii} approximate the eigenvalues of the pair (A, B) by quantities bouned by $\epsilon = \|B^{-\frac{1}{2}}AB^{-\frac{1}{2}} - \mathrm{diag}(B^{-\frac{1}{2}}AB^{-\frac{1}{2}})\|_2$, which is of order 10^{-2}. Computing the eigenvalues of (A, B), we find

i	$\frac{a_{ii}}{b_{ii}}$	$\lambda_i(A, B)$	$\frac{a_{ii}/b_{ii} - \lambda_i}{\lambda_i}$
1	-36	-36.000995971169	$-2.7665 \cdot 10^{-5}$
2	-16	-16.000058846852	$-3.6779 \cdot 10^{-6}$
3	-4	-4.0001082947362	$-2.7073 \cdot 10^{-5}$
4	1	0.9999951457235	$4.8543 \cdot 10^{-6}$
5	9	9.0000580297349	$-6.4477 \cdot 10^{-6}$
6	25	25.000634216742	$-2.5368 \cdot 10^{-5}$

Again, we see that a_{ii}/b_{ii} approximate the eigenvalues by $\mathcal{O}(\epsilon^2)$.

We can notice that in all examples presented so far, the eigenvalues and the singular values were simple. What happens if they are multiple?

1.2. Multiple eigenvalues and singular values

In order to construct matrices with multiple eigenvalues and/or singular values we shall use the following MATLAB function.

```
function q=rado2(n,m)
% rado2: Generates random, almost diagonal, orthogonal matrix
% of order n whose off-diagonal elements are of order 10^(-m)
% Usage: Q=rado2(n,m)
% Standard precision (double).
C=rand(n); D=diag(diag(C)); C=D+(C-D)*10^(-m); [Q,R]=qr(C);
```

For example, the command Q =rado2(6,5) generates the following orthogonal 6×6 matrix whose off-diagonal elements are of order 10^{-5},

$$\begin{bmatrix} -1.0000e+00 & 7.4136e-05 & 3.8998e-05 & 7.7435e-05 & 2.5064e-05 & -4.7130e-05 \\ -7.4134e-05 & -1.0000e+00 & 5.2260e-06 & 4.3292e-06 & 1.4150e-05 & -1.0449e-05 \\ -3.8995e-05 & -5.2225e-06 & -1.0000e+00 & 2.6712e-05 & 2.1571e-05 & -1.5348e-05 \\ -7.7435e-05 & -4.3233e-06 & -2.6709e-05 & -1.0000e+00 & 1.3510e-05 & -9.0622e-06 \\ -2.5067e-05 & -1.4149e-05 & -2.1570e-05 & -1.3507e-05 & -1.0000e+00 & -2.7418e-06 \\ -4.7132e-05 & -1.0445e-05 & -1.5347e-05 & -9.0582e-06 & -2.7400e-06 & 1.0000e+00 \end{bmatrix}.$$

Using this tool, we can easily generate almost diagonal matrices that have (up to the finite arithmetic accuracy) multiple eigenvalues or singular values.

Almost diagonal symmetric matrices

The following MATLAB code generates a symmetric matrix with prescribed eigenvalues and displays its diagonal elements, its eigenvalues and their relative distances.

```
format short e; S=diag([1,1,1,2,3,3]'); Q=rado2(6,6); H=Q'*S*Q;
H=(H+H')/2; D=sort(diag(H)); EV=sort(eig(H)); H format long e;
disp('  diagonals          eigenvalues        relative error');
disp([D,EV,(D-EV)./EV])
```

Here is the matrix

$$\left[\begin{array}{ccc|c|cc} 1.0000e+00 & 1.8923e-11 & 2.8546e-11 & 1.6529e-05 & 5.0062e-06 & -6.3360e-07 \\ 1.8923e-11 & 1.0000e+00 & 8.2134e-12 & 8.4769e-07 & 1.6709e-06 & -2.3022e-06 \\ 2.8546e-11 & 8.2134e-12 & 1.0000e+00 & 1.1456e-06 & 3.3511e-06 & -3.8594e-06 \\ \hline 1.6529e-05 & 8.4769e-07 & 1.1456e-06 & 2.0000e+00 & 1.5423e-06 & -1.9950e-06 \\ \hline 5.0062e-06 & 1.6709e-06 & 3.3511e-06 & 1.5423e-06 & 3.0000e+00 & 1.3053e-11 \\ -6.3360e-07 & -2.3022e-06 & -3.8594e-06 & -1.9950e-06 & 1.3053e-11 & 3.0000e+00 \end{array}\right].$$

We have partitioned the matrix according to the multiplicities of the eigenvalues. The relative distances between the diagonals and the corresponding eigenvalues are given in the following table:

i	diagonals	eigenvalues	relative error
1	1.000000000001434	0.999999999999999	1.4343e-12
2	1.000000000031410	1.000000000000000	3.1410e-11
3	1.000000000041638	1.000000000000001	4.1637e-11
4	2.000000000002086	2.000000000000000	1.0432e-12
5	2.999999999953910	3.000000000000000	-1.5363e-11
6	2.999999999969522	3.000000000000004	-1.0160e-11

.

Again, we see that diagonal elements approximate the eigenavalues, in the relative sense, by quantities which are of order ϵ^2. From the displayed matrix we can notice another interesting property: all off-diagonal elements within diagonal blocks are of order ϵ^2.

Almost diagonal square matrices

To generate a square matrix with multiple singular values one can first define a diagonal matrix with prescribed singular values and then multiply it (from both sides) with almost diagonal orthogonal matrices. Here is the MATLAB code

```
format short e;
S=diag([1,1,1,2,3,3]'); Q1=rado2(6,6); Q2=rado2(6,6);
C=Q1'*S*Q2
D=sort(abs(diag(C))); SV=sort(svd(C)); format long e;
disp('c(i,i)    s(i)   (c(i,i)-s(i))/s(i)');
disp([D,SV,(D-SV)./SV])
```

here the generated matrix,

$$\left[\begin{array}{ccc|c|cc} 1.0000e+00 & -5.2059e-07 & 2.3338e-06 & 5.5417e-06 & 1.2732e-05 & -4.6115e-06 \\ 5.2064e-07 & 1.0000e+00 & -1.5587e-06 & -2.6820e-06 & 1.6057e-07 & -1.5511e-06 \\ -2.3337e-06 & 1.5588e-06 & 1.0000e+00 & 9.5698e-06 & 2.5433e-05 & -2.0974e-05 \\ \hline -1.7762e-06 & 5.5570e-06 & -4.0199e-07 & 2.0000e+00 & 2.0095e-05 & -9.7478e-06 \\ \hline -4.0468e-06 & 4.6179e-06 & 5.8989e-06 & -1.2367e-05 & 3.0000e+00 & -2.6155e-05 \\ -1.7717e-07 & -1.8079e-06 & -7.5699e-06 & 3.3136e-06 & 2.6156e-05 & 3.0000e+00 \end{array}\right],$$

and finally, the diagonals, the singular values and their relative distances

i	diagonals	singular values	relative error
1	0.999999999989694	1.000000000000000	-1.0306e-011
2	0.999999999998078	1.000000000000000	-1.9216e-012
3	1.000000000198260	1.000000000000000	1.9826e-010
4	1.999999999919032	2.000000000000001	-4.0484e-011
5	2.999999999640680	2.999999999999999	-1.1977e-010
6	2.999999999748523	2.999999999999999	-8.3826e-011

.

Beside the expected result seen in the last column of the table, we can see a peculiar behavior of the off-diagonal elements within diagonal blocks. In particular, we see that for these elements there holds

$$a_{ij} + a_{ji} = \mathcal{O}(\epsilon^2), \quad a_{ij} = \mathcal{O}(\epsilon) = a_{ji}. \tag{2}$$

Almost diagonal triangular matrices

Let us make the QR factorization of the last matrix. Using MATLAB, we obtain the triangular matrix

$$\left[\begin{array}{ccc|c|cc}
-1.0000e+00 & -1.1112e-11 & -3.7085e-11 & -1.9893e-06 & -5.9185e-07 & 5.1428e-06 \\
0 & -1.0000e+00 & -1.3828e-10 & -8.4320e-06 & -1.4014e-05 & 6.9750e-06 \\
0 & 0 & -1.0000e+00 & -8.7658e-06 & -4.3129e-05 & 4.3683e-05 \\
\hline
0 & 0 & 0 & -2.0000e+00 & -1.5445e-06 & 4.7772e-06 \\
\hline
0 & 0 & 0 & 0 & -3.0000e+00 & -7.4873e-10 \\
0 & 0 & 0 & 0 & 0 & 3.0000e+000
\end{array}\right]$$

and we compute the quantities for the next table

i	diagonals	singular values	relative error
1	1.000000000002334	1.000000000000000	2.3346e-012
2	1.000000000027166	1.000000000000000	2.7166e-011
3	1.000000000248329	1.000000000000000	2.4833e-010
4	1.999999999954411	2.000000000000001	-2.2794e-011
5	2.999999999613621	2.999999999999999	-1.2879e-010
6	2.999999999621276	2.999999999999999	-1.2624e-010

.

As expected, the relative distances displayed in the last column of the table are ϵ^2 small. More interesting, all off-diagonal elements from the diagonal blocks are ϵ^2 small, just like in the symmetric case.

Positive definite pair of almost diagonal symmetric matrices

Let us generate a pair of almost diagonal symmetric matrices (A, B), such that B is positive definite, and such that the pair has prescribed multiple eigenvalues. This can be accomplished by defining a diagonal matrix D with prescribed eigenvalues, and then making $A = F^T DF$, $B = F^T F$. We can control the condition of F by premultiplying and postmultiplying an almost diagonal orthogonal matrix Q with appropriate diagonal scaling matrices. Here is the code that generates A and B.

```
format short e; Q=rado2(6,6); D1=diag(diag(rand(6)));
D2=diag(diag(rand(6))); F=D1*Q*D2; cond(F)
A=F'*diag([1,1,1,2,3,3]')*F; A=(A+A')/2
B=F'*F; B=(B+B')/2
DAB=diag(A)./diag(B); C=A-diag(DAB)*B
EV=sort(qzval(A,B)); format long e; disp([DAB,EV,(DAB-EV)./EV])
```

Here are the results,

$$cond(F) = 5.95e+01$$

$$A = \left[\begin{array}{ccc|c|cc} 1.71e\text{-}4 & 0.15e\text{-}9 & 9.49e\text{-}9 & -0.58e\text{-}9 & 4.36e\text{-}8 & -2.66e\text{-}9 \\ 0.15e\text{-}9 & 9.61e\text{-}3 & 5.36e\text{-}7 & -8.21e\text{-}8 & 2.19e\text{-}5 & -8.43e\text{-}7 \\ 9.49e\text{-}9 & 5.36e\text{-}7 & 1.69e\text{-}1 & -4.06e\text{-}8 & 2.36e\text{-}6 & -5.25e\text{-}8 \\ \hline -0.58e\text{-}9 & -8.21e\text{-}8 & -4.06e\text{-}8 & -3.10e\text{-}4 & 2.63e\text{-}8 & -3.73e\text{-}9 \\ \hline 4.36e\text{-}8 & 2.19e\text{-}5 & 2.36e\text{-}6 & 2.63e\text{-}8 & 1.64e+0 & 1.07e\text{-}7 \\ -2.66e\text{-}9 & -8.43e\text{-}7 & -5.25e\text{-}8 & -3.73e\text{-}9 & 1.07e\text{-}7 & 7.10e\text{-}3 \end{array}\right]$$

$$B = \left[\begin{array}{ccc|c|cc} 1.71e\text{-}4 & 0.15e\text{-}9 & 9.49e\text{-}9 & 0.09e\text{-}9 & 1.42e\text{-}8 & -0.81e\text{-}9 \\ 0.15e\text{-}9 & 9.61e\text{-}3 & 5.36e\text{-}7 & 1.02e\text{-}8 & 7.15e\text{-}6 & -2.54e\text{-}7 \\ 9.49e\text{-}9 & 5.36e\text{-}7 & 1.69e\text{-}1 & -2.53e\text{-}8 & 6.14e\text{-}7 & 6.31e\text{-}9 \\ \hline 0.09e\text{-}9 & 1.02e\text{-}8 & -2.53e\text{-}8 & 1.55e\text{-}4 & 8.05e\text{-}9 & -0.87e\text{-}9 \\ \hline 1.42e\text{-}8 & 7.15e\text{-}6 & 6.14e\text{-}7 & 8.05e\text{-}9 & 5.47e\text{-}1 & 3.58e\text{-}8 \\ -0.81e\text{-}9 & -2.54e\text{-}7 & 6.31e\text{-}9 & -0.87e\text{-}9 & 3.58e\text{-}8 & 2.37e\text{-}3 \end{array}\right].$$

Note the relative distance between the quantities a_{ii}/b_{ii} and the eigenvalues of the pair (A,B),

i	a_{ii}/b_{ii}	$\lambda_i(A,B)$	$(a_{ii}/b_{ii} - \lambda_i)/\lambda_i$
1	1.00000000000323	1	3.2334e-12
2	1.00000002650055	1	2.6501e-08
3	1.00000000001790	1	1.7902e-11
4	-1.99999999901644	-2	-4.9178e-10
5	2.99999999997519	3	-8.2688e-12
6	2.99999999985046	3	-4.9846e-11

.

The special structure in the pair (A,B) is revealed from the matrix $A - \text{diag}(\lambda_i)\cdot B$, or from the matrix

$$C = A - diag(a_{ii}/b_{ii}) \cdot B$$

$$= \left[\begin{array}{ccc|c|cc} 0 & 4.94e\text{-}13 & 4.79e\text{-}14 & -6.65e\text{-}10 & 2.94e\text{-}08 & -1.85e\text{-}09 \\ 4.94e\text{-}13 & 0 & 2.79e\text{-}11 & -9.23e\text{-}08 & 1.48e\text{-}05 & -5.89e\text{-}07 \\ 4.79e\text{-}14 & 2.79e\text{-}11 & 0 & -1.53e\text{-}08 & 1.75e\text{-}06 & -5.88e\text{-}08 \\ \hline -3.91e\text{-}10 & -6.18e\text{-}08 & -9.11e\text{-}08 & 0 & 4.24e\text{-}08 & -5.48e\text{-}09 \\ \hline 8.64e\text{-}10 & 4.95e\text{-}07 & 5.21e\text{-}07 & 2.13e\text{-}09 & 0 & 2.19e\text{-}12 \\ -2.21e\text{-}10 & -8.05e\text{-}08 & -7.14e\text{-}08 & -1.12e\text{-}09 & 2.19e\text{-}12 & 0 \end{array}\right].$$

We see that actually each diagonal block in A is an ϵ^2 good approximation of the corresponding diagonal block in B premultiplied by the appropriate eigenvalue.

1.3. Theoretical results

After providing examples of almost diagonal matrices, we present the known theoretical results. First, we introduce notation and basic assumptions.

The eigenvalues of the underlying matrices (or matrix pairs) are assumed to be ordered nonincreasingly,

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n .$$

The same will hold for the singular values,

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0.$$

To avoid usage of permutation matrices we assume the same ordering of the diagonal elements. In particular, we assume that for a

(a) single Hermitian matrix $H = (h_{ij})$ there holds

$$h_{11} \geq h_{22} \geq \cdots \geq h_{nn}\,;$$

(b) pair of Hermitian matrices $A = (a_{ij}),\ B = (b_{ij})$, with positive definite B, there holds

$$\frac{a_{11}}{b_{11}} \geq \frac{a_{22}}{b_{22}} \geq \cdots \geq \frac{a_{nn}}{b_{nn}}\,;$$

(c) single non-Hermitian matrix $C = (c_{ij})$ (if its singular values are considered), there holds

$$|\, c_{11} \,|\geq|\, c_{22} \,|\geq \cdots \geq|\, c_{nn} \,|\,.$$

In the case of multiple eigenvalues and singular values we assume

$$\lambda_1 = \cdots = \lambda_{s_1} > \lambda_{s_1+1} = \cdots = \lambda_{s_2} > \cdots > \lambda_{s_{p-1}+1} = \cdots = \lambda_{s_p}\,,$$
$$\sigma_1 = \cdots = \sigma_{s_1} > \cdots > \sigma_{s_{p-1}+1} = \cdots = \sigma_{s_p},$$

where $s_p = n$. Note that for each $1 \leq i \leq p$,

$$n_i = s_i - s_{i-1}, \qquad (s_0 \stackrel{\text{def}}{=} 0)$$

is the multiplicity of λ_{s_i} and σ_{s_i}. Closely connected with multiplicities $n_1, \ldots, n_p$ and with the ordering of diagonal elements, is the following matrix block partition,

$$X = \begin{bmatrix} X_{11} & \cdots & X_{1p} \\ \vdots & \ddots & \vdots \\ X_{p1} & \cdots & X_{pp} \end{bmatrix}, \quad X_{ij} \in \mathbb{C}^{n_i \times n_j},\ 1 \leq i\,,\, j \leq p\,,$$

where X stands for the considered matrix. In connection with the block partition $X = (X_{ij})$, we introduce measures $\pi(X)$ and $\tau(X)$,

$$\begin{cases} X = \pi(X) + \tau(X) \\ \pi(X) = \operatorname{diag}(X_{11}, \ldots, X_{pp}) \\ \tau(X) = X - \pi(X) \end{cases}$$

Thus, $\pi(X)$ is the block-diagonal part of X and $\tau(X)$ is the block off-diagonal part of X. We shall also use the notation

$$\begin{aligned} \pi_i(X) &= X_{ii}, \\ \tau_i(X) &= [X_{i1} \ldots X_{i,i-1}\; X_{i,i+1} \ldots X_{ip}]\,. \end{aligned}$$

Note that in case $n_1 = \cdots = n_p = 1$, $\pi(X) = \operatorname{diag}(X)$ and $\tau(X) = \Omega(X)$, where generally,

$$\Omega(X) = X - \operatorname{diag}(X)$$

is the off-diagonal part of X.

As for the norms, we shall mostly use the Frobenius and the spectral (operator) matrix norm,

$$\|X\|_F = \sqrt{\mathrm{trace}(X^*X)}, \qquad \|X\|_2 = \sqrt{\mathrm{spr}(X^*X)}\,.$$

Note that $\|\Omega(X)\|_F$ (or $\|\Omega(X)\|_2$) can be considered as departure from the diagonal form. Then $\|\tau(X)\|_F$ (or $\|\tau(X)\|_2$) is departure from the block diagonal form. More frequently, we shall use the quantities

$$\begin{aligned} \|\Omega(\pi_i(X))\|_F &= \|\Omega(X_{ii})\|_F = \|X_{ii} - \mathrm{diag}(X_{ii})\|_F \quad \text{and} \\ \|\tau_i(X)\|_F^2 &= \sum_{\substack{j=1 \\ j\neq i}} \|X_{ij}\|_F^2. \end{aligned}$$

The absolute value of the matrix $X = (x_{ij})$ is $|X| = (|x_{ij}|)$.

As we may have noticed from the displayed almost diagonal matrices, the minimum distance between two distinct eigenvalues (singular values) matters. Therefore, for each $1 \leq i \leq p$, we define the absolute gap (or separation) of λ_{s_i} from other eigenvalues as

$$\delta_i = \min_{\substack{1\leq j\leq p \\ j\neq i}} \mid \lambda_{s_i} - \lambda_{s_j} \mid .$$

Similarly, in case of singular values, absolute gap of σ_{s_i} is (we use the same notation)

$$\delta_i = \min_{\substack{1\leq j\leq p \\ j\neq i}} \mid \sigma_{s_i} - \sigma_{s_j} \mid .$$

The minimum absolute gap is then

$$\delta = \min_{1\leq i\leq p} \delta_i.$$

In the following we present the sharpest known estimates for almost diagonal matrices based on absolute gaps.

Estimates for a positive definite pair

We start with a simple proof of the result for a positive definite pair of almost diagonal Hermitian matrices. We assume that diagonal elements and eigenvalues are ordered as indicated above.

Theorem 1. *[12, 16] Let A be a Hermitian and B a Hermitian positive definite matrix, both of order n. Let $B_S = \Delta_B^{-1} B \Delta_B^{-1}$, $\Delta_B = [\mathrm{diag}\,(B)]^{1/2}$. If*

$$\|\Omega\left(\Delta_B^{-1} A \Delta_B^{-1} - \lambda_{s_i} B_S\right)\|_2 < \frac{1}{3}\delta_i\,,$$

holds for all $1 \leq i \leq p$, then

$$\left\|\pi_i\left(\Delta_B^{-1} A \Delta_B^{-1} - \lambda_{s_i} B_S\right)\right\|_F \leq \frac{3}{\delta_i} \left\|\tau_i\left(\Delta_B^{-1} A \Delta_B^{-1} - \lambda_{s_i} B_S\right)\right\|_F^2,\ 1 \leq i \leq p.$$

Proof. Note that (A, B) and $(\Delta_B^{-1} A \Delta_B^{-1}, B_S)$ have the same eigenvalues. Therefore, in the proof we shall assume that the diagonal elements of B are ones, so that $\Delta_B = I_n$.

Let $i \in \{1, 2, \ldots, p\}$ and let $\gamma_j^{(i)}$, $1 \leq j \leq n$ be the eigenvalues of the Hermitian matrix $C_i = A - \lambda_{s_i} B$. Using the perturbation theorem (c.f. [38, Section 2.44]) for the eigenvalues of Hermitian matrices (that is the relation (1) here) in connection with C_i and $D_i = \mathrm{diag}(C_i)$, and using the assumption, we conclude that

$$\mid \gamma_j^{(i)} - (a_{jj} - \lambda_{s_i} b_{jj}) \mid \leq \|C_i - D_i\|_2 < \frac{1}{3}\delta_i, \quad 1 \leq j \leq n, \tag{3}$$

holds for an ordering $\gamma_1^{(i)}, \ldots, \gamma_n^{(i)}$. Since C_i has rank $n - n_i$, there are exactly n_i eigenvalues $\gamma_j^{(i)}$ which are zeroes. Hence, from the relation (3), we see that

$$\mid a_{jj} - \lambda_{s_i} \cdot 1 \mid \leq \frac{1}{3}\delta_i \tag{4}$$

holds for at least n_i values of j. Let $\mathcal{S}_i$ be the set of all indices j $(1 \leq j \leq n)$ for which the inequality (4) holds. Then $\mathcal{S}_i \subseteq \mathcal{S}$, where $\mathcal{S} = \{1, \ldots, n\}$. This conclusion holds for all i; hence $\cup_i \mathcal{S}_i \subseteq \mathcal{S}$. Since for $j \in \mathcal{S}_i$, $i \neq k$ there holds

$$\begin{aligned} \mid a_{jj} - \lambda_{s_k} \mid &\geq \mid \lambda_{s_i} - \lambda_{s_k} \mid - \mid a_{jj} - \lambda_{s_i} \mid \\ &> \max\{\delta_i, \delta_k\} - \frac{1}{3}\delta_i \\ &\geq \frac{2}{3}\max\{\delta_i, \delta_k\} \\ &\geq \frac{2}{3}\delta_k\,, \end{aligned}$$

we conclude that $\mathcal{S}_i \cap \mathcal{S}_k = \emptyset$ whenever $i \neq k$. Note that each $\mathcal{S}_i$ contains at least n_i elements and that $n_1 + \cdots + n_p = n$. So, we can conclude that $\mathcal{S}_1, \ldots, \mathcal{S}_p$ make a partition of $\mathcal{S}$ and that each $\mathcal{S}_i$ contains exactly n_i indices. Now the orderings of eigenvalues and of diagonal elements imply that

$$\mathcal{S}_i = \{s_{i-1} + 1, \ldots, s_p\}, \quad 1 \leq i \leq p.$$

Let $C_i = (C_{jk}^{(i)})$ be the block partition of C_i. By an appropriate permutation matrix P_i, we can write

$$P_i^* C_i P_i = \begin{bmatrix} C_{ii}^{(i)} & G_i \\ G_i^* & K_i \end{bmatrix}, \quad 1 \leq i \leq p.$$

Let $\kappa_j^{(i)}$, $j \in \mathcal{S} \backslash \mathcal{S}_i$ denote the eigenvalues of K_i. Applying the perturbation theorem to K_i and $\mathrm{diag}(K_i)$ we obtain

$$\mid (a_{jj} - \lambda_{s_i}) - \kappa_j^{(i)} \mid \leq \|K_i - \mathrm{diag}(K_i)\|_2, \quad j \in \mathcal{S} \setminus \mathcal{S}_i. \tag{5}$$

Since the spectral norm of a principal submatrix is not larger than the spectral norm of the whole matrix, we have

$$\|K_i - \mathrm{diag}(K_i)\|_2 \leq \|P_i^*(C_i - D_i)P_i\|_2 < \frac{1}{3}\delta_i. \tag{6}$$

Combining (5) and (6), we have

$$| \kappa_j^{(i)} | \geq | a_{jj} - \lambda_{s_i} | - \frac{1}{3}\delta_i > \frac{2}{3}\delta_i - \frac{1}{3}\delta_i = \frac{1}{3}\delta_i, \quad j \in \mathcal{S} \setminus \mathcal{S}_i.$$

Thus K_i is invertible and

$$\|K_i^{-1}\|_2 = \frac{1}{\min_{j\in\mathcal{S}\setminus\mathcal{S}_i} | \kappa_j^{(i)} |} \leq \|P_i^*(C_i - D_i)P_i\|_2 < \frac{3}{\delta_i}, \quad 1 \leq i \leq p.$$

Since the rank of C_i is equal to the order of K_i, which is invertible, we can conclude that the Schur complement $C_{ii}(i) - G_i K_i^{-1} G_i^*$ is the null matrix. Now, we have

$$\begin{aligned} \|C_{ii}^{(i)}\|_F &= \|G_i K_i^{-1} G_i^*\|_F \leq \|G_i K_i^{-1}\|_2 \|G_i^*\|_F \\ &\leq \|K_i^{-1}\|_2 \|G_i\|_F^2 \leq \frac{3}{\delta_i}\|G_i\|_F^2, \quad 1 \leq i \leq p. \end{aligned}$$

The assertion now follows by recognizing that

$$\|G_i\|_F^2 = \|\tau_i(A - \lambda_{s_i} B)\|_F.$$

□

If neither A nor B is positive definite, but there exists a real linear combination $\alpha A + \beta B$, $\alpha, \beta \in \mathbb{R}$, which is positive definite (such pairs are called *definite*), one can generalize the above result by using projective lines and the chordal metrics (see [16]).

The above result is used in the quadratic convergence proof of diagonalization methods for solving the positive definite generalized eigenproblem (see [12, 16]) and the definite generalized eigenproblem (using the Falk-Langemeyer method, see [33]).

Estimates for a single Hermitian matrix

Assuming $B = I_n$ and therefore $\Delta_B = I_n$ in *Theorem 1*, we obtain

Corollary 1. *Let* $H = H^*$. *If*

$$\|\Omega(H)\|_F < \frac{\delta}{3}, \qquad \textit{then} \qquad \|H_{ii} - \lambda_{s_i} I_{n_i}\|_F \leq \frac{3}{\delta_i} \sum_{\substack{j=1 \\ j\neq i}} \|H_{ij}\|_F^2 \,.$$

In [17] it has been shown that under the same assumptions, the constant 3 in the numerator can be replaced by 1.32. Note however, that for tiny δ_i, the bound becomes large and often useless.

Example 1. *Let*

$$H = \begin{bmatrix} 1 & 10^{-8} & 10^{-8} \\ 10^{-8} & 10^{-6} & 10^{-11} \\ 10^{-8} & 10^{-11} & 10^{-8} \end{bmatrix}, \quad H' = \begin{bmatrix} 1 & 10^{-8} & 10^{-8} \\ 10^{-8} & 10^{-8} & 10^{-11} \\ 10^{-8} & 10^{-11} & 10^{-8} \end{bmatrix}.$$

We have

$$\left.\begin{array}{l} \lambda_1(H) \approx 1.00000000000000e{+}00 \\ \lambda_2(H) \approx 9.99999979899192e{-}09 \\ \lambda_3(H) \approx 1.00000000000101e{-}06 \end{array}\right\} \quad \begin{array}{l} \delta_1 \approx 0.999999 \\ \delta_2 \approx 9.9e-07 \\ \delta_3 \approx 9.9e-07 \end{array}.$$

Since

$$\|\Omega(H)\|_F \approx 2e-08 < \delta \approx 9.9e-07\,,$$

we can apply Corollary 1. *From the table below*

i	$\mid h_{ii}-\lambda_i \mid$	$\frac{1.32}{\delta_i}\|\tau_i(A)\|_F^2$
1	*2.000001e-16*	*2.64e-16*
2	*1.007981e-18*	*1.33e-10*
3	*-2.010081e-16*	*1.33e-10*

we see that the bounds for $\mid h_{22}-\lambda_2 \mid$ *and* $\mid h_{33}-\lambda_3 \mid$ *are* 6 *and* 8 *orders of magnitude larger than the true values.*

The matrix H' *is obtained from* H *by replacing the central element* 10^{-6} *with* 10^{-8}. *For* H' *we have*

$$\left.\begin{array}{l} \lambda_1(H') \approx 1.000000000e+00 \\ \lambda_2(H') \approx 1.000999980e-08 \\ \lambda_3(H') \approx 9.990000000e-09 \end{array}\right\} \begin{array}{l} \delta_1' \approx 0.99999999 \\ \delta_2' \approx 1.99998e-11 \\ \delta_3' \approx 1.99998e-11 \end{array}\;.$$

Since

$$\|\Omega(H')\|_F \approx 2e-08 \gg 1.99998e-11 \approx \delta(H')$$

no estimate can be obtained from Corollary 1.

Corollary 1 is used for proving the quadratic (cubic) convergence of the standard row-cyclic (quasi-cyclic) Jacobi method for the symmetric or Hermitian eigenvalue problem (see [39, 22, 17, 27]).

Estimates for a J-symmetric matrix

Let $H \in \mathbb{C}^{n\times n}$ be Hermitian and $J = I_k \oplus (-I_{n-k})$. If there is a real scalar μ, such that $H-\mu J$ is positive definite, then the pair (H,J) is called positive definite. Such pairs have real eigenvalues. The matrix $\tilde{H} = JH$ which is referred to as J-Hermitian (J-symmetric if H is real symmetric) has the same eigenvalues as the pair (H,J).

Using the same assumptions on the orderings of eigenvalues and diagonals of $\tilde{H}$, and using a similar technique as in the proof of *Theorem 1*, one can prove (see [5])

Theorem 2. *If*

$$\|\Omega(H)\|_F < \frac{1}{\eta}\cdot\frac{\delta}{3}, \quad \eta \geq 1,$$

then

$$\|\tilde{H}_{ii}-\lambda_{s_i} I_{n_i}\|_F = \|\pi_i(\tilde{H}-\lambda_{s_i} I_n)\|_F \leq \frac{3\eta}{3\eta-2}\cdot\frac{1}{\delta_i}\sum_{\substack{j=1\\ j\neq i}}\|H_{ij}\|_F^2\,.$$

This result is used in [5] for proving the quadratic convergence of the $J-$*symmetric* Jacobi method, introduced by Veselić in [36]). A positive definite pair (H,J) is illustrated in the example below.

Example 2. *Let*

$$H = \left[\begin{array}{rrr|r|rr} 2.00 & -6.44e\text{-}14 & -4.82e\text{-}13 & 6.16e\text{-}07 & 6.13e\text{-}07 & 2.09e\text{-}07 \\ -6.44e\text{-}14 & 2.00 & -3.78e\text{-}13 & -8.65e\text{-}09 & -5.73e\text{-}07 & 1.26e\text{-}08 \\ -4.82e\text{-}13 & -3.78e\text{-}13 & 2.00 & 1.48e\text{-}06 & 3.38e\text{-}06 & 3.73e\text{-}07 \\ \hline 6.16e\text{-}07 & -8.65e\text{-}09 & 1.48e\text{-}06 & 1.00 & -6.02e\text{-}07 & 1.08e\text{-}05 \\ \hline 6.13e\text{-}07 & -5.73e\text{-}07 & 3.38e\text{-}06 & -6.02e\text{-}07 & 3.00 & -1.35e\text{-}12 \\ 2.09e\text{-}07 & 1.26e\text{-}08 & 3.73e\text{-}07 & 1.08e\text{-}05 & -1.35e\text{-}12 & 3.00 \end{array}\right]$$

and $J = diag(1,1,1,1,-1,-1)$.

From the table below, one can see that the pair (H, J) *has multiple eigenvalues. Hence, one can recognize the block partition in the displayed matrix, and see how well the estimates of* Theorem 2 *describe the inherent structure in the matrix.*

i	h_{ii}/j_{ii}	$\lambda(H,J) = \lambda(JH)$	$(h_{ii}/j_{ii} - \lambda_i)\lambda_j$
1	*-3.00000000002922*	*-3.00000000000000*	*9.7393e-12*
2	*-3.00000000000252*	*-3.00000000000000*	*8.3918e-13*
3	*1.00000000003184*	*1.00000000000000*	*3.1845e-11*
4	*1.99999999999970*	*2.00000000000000*	*-1.4599e-13*
5	*2.00000000000007*	*2.00000000000000*	*3.2862e-14*
6	*2.00000000000012*	*2.00000000000000*	*5.9064e-14*

,

where $H = (h_{rs})$ *and* $J = (j_{rs})$.

Estimates for a general square matrix

If $C \in \mathbb{C}^{m \times n}$, $m \geq n$, has singular values $\sigma_1 \geq \cdots \geq \sigma_n$, then the Hermitian matrix (see [7, Sec.8.3])

$$H = \begin{bmatrix} 0 & C \\ C^* & 0 \end{bmatrix} \tag{7}$$

has eigenvalues $\sigma_1 \geq \cdots \geq \sigma_n \geq 0 = \cdots = 0 \geq -\sigma_n \geq \cdots \geq -\sigma_1$ with exactly $2(m-n)$ zeros between σ_n and $-\sigma_n$. To avoid singularity of H we further assume $m = n$. Also, to avoid multiplying C by an appropriate diagonal unitary matrix, we assume that the diagonal elements of C are nonnegative (and ordered nonincreasingly). Now, let

$$\tilde{H} = Q^* H Q = \frac{1}{2} \begin{bmatrix} C + C^* & C - C^* \\ -(C - C^*) & -(C + C^*) \end{bmatrix}, \quad Q = \frac{\sqrt{2}}{2} \begin{bmatrix} I_n & -I_n \\ I_n & I_n \end{bmatrix}.$$

The Hermitian matrix $\tilde{H}$ has the diagonals $c_{11},\ldots,c_{nn}$, $-c_{11}, \ldots, -c_{nn}$, and the eigenvalues $\sigma_1, \ldots, \sigma_n, -\sigma_1, \ldots, -\sigma_n$. Since

$$\Omega(\tilde{H}) = Q^* \begin{bmatrix} 0 & \Omega(C) \\ \Omega(C)^* & 0 \end{bmatrix},$$

we have $\|\Omega(\tilde{H})\|_F = \sqrt{2}\|\Omega(C)\|_F$ and $\|\Omega(\tilde{H})\|_2 = \|\Omega(C)\|_2$. These facts make it possible to apply *Corollary 1* to $\tilde{H}$ in order to obtain appropriate estimates for the matrix C. Note however, that this approach takes into account a gap between eigenvalues σ_n and $-\sigma_n$ provided that $\sigma_n \neq 0$. Although such a gap does not exist among the singular values of C, it appears in the result. For the complete formulation of the result, one defines the additional (we can call it "artificial") local gap $\tilde{\delta}_p$,

$$\tilde{\delta}_p = \begin{cases} \sigma_{s_{p-1}} - \sigma_{s_p} & \text{if } \sigma_{s_p} = 0 \text{ or } \sigma_{s_{p-1}} - \sigma_{s_p} \le 2\sigma_{s_p} \\ 2\sigma_{s_p} & \text{if } 0 < 2\sigma_{s_p} < \sigma_{s_{p-1}} - \sigma_{s_p} \end{cases},$$

and the additional minimum gap, $\tilde{\delta} = \min\{\delta\ ,\ \tilde{\delta}_p\}$.

Theorem 3. *[14] Let $C \in \mathbf{C}^{n\times n}$ have diagonal elements $c_{11} \ge \cdots \ge c_{nn} \ge 0$. If*

$$\|\Omega(C)\|_2 < \frac{\delta}{3}\,, \tag{8}$$

then for $1 \le i \le p-1$ there holds

$$\|(C_{ii} + C_{ii}^*)/2 - \sigma_{s_i} I_{n_i}\|_F \le \frac{3}{8\delta_i}\left[\|C_{ii} - C_{ii}^*\|_F^2 + 2\sum_{\substack{j=1\\ j\neq i}}(\|C_{ij}\|_F^2 + \|C_{ji}\|_F^2)\right],$$

where (C_{ij}) is the block partition of C. The estimate holds for $i = p$ provided that any of the following conditions is met:
(i) C is singular;
(ii) C is nonsingular and $2\sigma_{s_p} \ge \delta$;
(iii) C is nonsingular and in the assumption (8) δ is replaced by $\tilde{\delta}$.

This result explains the peculiar relation (2). *Theorem 3* has been used in proving the failure of the quadratic convergence of the SVD Jacobi methods for general square matrices (see [14]). Note that it has been proved earlier in [13] and [3], that these methods are quadratically convergent provided the singular values were distinct or at most double.

Estimates for a triangular matrix

If $T = (t_{rs})$ is triangular, or more generally, essentially triangular (meaning that $t_{rs}t_{sr} = 0$ for all $r \neq s$), *Theorem 3* implies

Corollary 2. *[14] Let $T \in \mathbf{C}^{n\times n}$. If*

$$\|\Omega(T)\|_2 < \frac{\delta}{3}\,,$$

then for $1 \le i \le p-1$ there holds

$$\begin{aligned} \|\Omega(T_{ii})\|_F &\le \sqrt{2}\|(T_{ii} + T_{ii}^*)/2 - \sigma_{s_i} I_{n_i}\|_F \\ &\le \frac{3\sqrt{2}}{4\delta_i}\left[\|\Omega(T_{ii})\|_F^2 + \sum_{\substack{j=1\\ j\neq i}}(\|T_{ij}\|_F^2 + \|T_{ji}\|_F^2)\right], \end{aligned}$$

where (T_{ij}) is the block partition of T. The estimate holds for $i = p$ provided that any of the three corresponding conditions from Theorem 3 *are met.*

Corollary 2 has been slightly improved in [15] and [17], mostly in connection with obtaining sharp quadratic convergence bounds for the Kogbetliantz method for triangular matrices.

Other similar results

Here we note some other results concerning the structure of almost diagonal matrices. Since they do not seem so important in applications, we shall not explicitly state the theorems. Instead, we shall very briefly explain the topics and give the proper references.

In [29, 30] Ruhe gives estimate for almost diagonal normal and diagonazible square matrices having multiple eigenvalues. These results are used for proving the quadratic and also global [11] convergence of the appropriate diagonalization methods.

In [9, 10] an "almost diagonal"[1] skew-symmetric matrix is described and a very special structure estimated, when multiple eigenvalues are present. These estimates are used in connection with the quadratic and cubic convergence of the Paardekooper method for reducing a skew-symmetric matrix to Murnaghan form (see [10, 19, 28, 8]). A more complicated structure is connected with the pair (A, B) of an almost diagonal positive definite matrix B and a skew-symmetric A which is almost in Murnaghan form (see [20]).

2. Scaled almost diagonal matrices

Let us consider the following symmetric matrix of order four,

$$H = \begin{bmatrix} 1 & 10^{-5} & 10^{-8} & 10^{-8} \\ 10^{-5} & 10^{-6} & 10^{-10} & -10^{-12} \\ 10^{-8} & 10^{-10} & -10^{-10} & 10^{-14} \\ 10^{-8} & -10^{-12} & 10^{-14} & -10^{-12} \end{bmatrix}.$$

Since

$$\left.\begin{array}{l} \lambda_1 \approx 1.0000e+00 \\ \lambda_2 \approx 9.9990e-07 \\ \lambda_3 \approx -1.0001e-10 \\ \lambda_4 \approx -1.0001e-12 \end{array}\right\} \quad \begin{array}{l} \delta_1 \approx 0.999999e+00 \\ \delta_2 \approx 9.999010e-07 \\ \delta_3 \approx 9.900998e-11 \\ \delta_4 \approx 9.900998e-11 \end{array}$$

we have $\delta = \delta_3 = \delta_4 \approx 9.900998e-11$ and therefore

$$\|H - \mathrm{diag}(H)\|_F \approx 1.41e-05 \gg \delta\,.$$

Thus, almost no information concerning the relative distances between the eigenvalues and the diagonal elements of H can be deduced from earlier results. Still, from the displayed data, one can see that these distances are very small. Even more, if we "normalize" H by diagonal congruency transformation, so that diagonals become ones,

$$H_S = \Delta_H^{-\frac{1}{2}} H \Delta_H^{-\frac{1}{2}},\ \Delta_H = \mid \mathrm{diag}(H) \mid$$

we can see that the obtained matrix

$$H_S = \begin{bmatrix} 1 & 10^{-2} & 10^{-3} & 10^{-2} \\ 10^{-2} & 1 & 10^{-2} & -10^{-3} \\ 10^{-3} & 10^{-3} & -1 & 10^{-3} \\ 10^{-2} & -10^{-3} & 10^{-3} & -1 \end{bmatrix},$$

[1] Meaning almost in the Murnaghan form.

is in some way almost diagonal. For example, we have

$$\|\Omega(H_S)\|_F \leq 2.4618 \cdot 10^{-2}.$$

Such matrices recently became important for several reasons. First, the new theory of the so-called relative perturbations of eigenvalues, singular values and the corresponding eigenvectors, frequently uses such diagonal scaling (see [1, 2, 37, 34, 21]). Second, in [2], [32] and elsewhere, it has been proved that diagonalization methods can compute the eigendecomposition and SVD with high relative accuracy. This precious property is not shared with other algorithms. In connection with this, it has been found that the proper measure for advancing of the process by such algorithms is not the off-norm of the matrix itself, but of the scaled matrix which is obtained by diagonal scaling.

This is the reason why several papers appeared recently (see [1, 5, 24]), that deal with almost diagonal matrices in the scaled sense. We propose a common name for such matrices: "scaled almost diagonal matrices". The main class of such matrices is the class of

2.1. Scaled diagonally dominant matrices

In [1] Barlow and Demmel introduced *scaled diagonally dominant matrices* and matrix pairs. Later, Drmač [4], and Hari and Drmač [18] slightly generalized the notion of scaled diagonally dominant matrix pairs. Scaled diagonally dominant matrices with special (symplectic) structure are considered in [26]. Finally, scaled diagonally dominant matrices with multiple singular values are considered in [24].

Suppose $A = D + N$, where D is diagonal and N has zero diagonal. Then $A = (a_{ij})$ is referred to as α–*diagonally dominant* with respect to a norm $\|\cdot\|$ if $\|N\| \leq \alpha \min_{1\leq i\leq n} |a_{ii}|$, with $0 \leq \alpha < 1$. If $A = D+N$ with $|a_{ii}| = 1$, $1 \leq i \leq n$ and Δ_1, Δ_2 are arbitrary nonsingular diagonal matrices, then $\tilde{A} = \Delta_1 A \Delta_2$ is α–*scaled diagonally dominant* (α–s.d.d.) with respect to a given norm, provided that A is α–diagonally dominant with respect to that norm. Note that an α–s.d.d matrix has nonzero diagonal elements. If A is Hermitian, it is presumed that $\Delta_1 = \Delta_2$ and Δ_1 is real. Such scaling, which is a congruence transformation, will be called symmetric.

The pair (A, B) of Hermitian matrices is (α, β)–*scaled diagonally dominant definite* ((α, β)–s.d.d.d.) with respect to a given norm if A is α–s.d.d., B is β–s.d.d., both with respect to that norm, and B is positive definite. If A is positive definite as well, (A, B) is (α, β)–*scaled diagonally dominant positive definite* ((α, β)–s.d.d.p.d.). If $\alpha = \beta$, (α, α)–s.d.d.d. ((α, α)–s.d.d.p.d.) is abbreviated to α–s.d.d.d. (α–s.d.d.p.d.) matrix pair.

In the classical results, described in *Section 1*, special role is played by the absolute gap(s) in the spectrum or in the set of singular values. The so-called *relative gaps* are closely connected With s.d.d. matrices.

Relative gaps

Although there are several definitions of relative gaps (cf. [34, 21]), here we use the following one. For each $1 \leq i \leq p$, the relative gap of the eigenvalue λ_{s_i}, is given by

$$\gamma_i = \min_{\substack{1\leq j\leq p \\ j\neq i}} \frac{|\ \lambda_{s_i} - \lambda_{s_j}\ |}{|\ \lambda_{s_i}\ | + |\ \lambda_{s_j}\ |}\,.$$

The relative gap of σ_{s_i} is defined by

$$\gamma_i = \min_{\substack{1\leq j\leq p \\ j\neq i}} \frac{|\ \sigma_{s_i} - \sigma_{s_j}\ |}{\sigma_{s_i} + \sigma_{s_j}}\,.$$

The minimum relative gap is therefore

$$\gamma = \min_{1\leq i\leq p} \gamma_i\,.$$

Note that all γ_i and therefore γ lie in the interval $[0, 1]$.

Example 3. *Let H be as above. From the given eigenvalues, and the above definition, one easily computes the relative gaps,*

$$\left.\begin{array}{r} \lambda_1 \approx 1.0000e+00 \\ \lambda_2 \approx 9.9990e-07 \\ \lambda_3 \approx -1.0001e-10 \\ \lambda_4 \approx -1.0001e-12 \end{array}\right\} \quad \begin{array}{l} \gamma_1 \approx 0.9999980 \\ \gamma_2 \approx 0.9999980 \\ \gamma_2 \approx 0.9801980 \\ \gamma_3 \approx 0.9801980 \end{array}\,.$$

We see that $\gamma \approx 0.9801980$, hence all the relative gaps are very close to one.

2.2. Results for a single Hermitian matrix

We start with the case of a scaled diagonally dominant Hermitian matrix. The following result is deduced from the corresponding result for s.d.d.d. matrix pairs. We note that the assumptions and notation proposed in *Section 1.3* hold throughout the paper.

Theorem 4. *[18] (i) Let $H = H^*$ be α-s.d.d. and $H = \Delta_H H_S \Delta_H$, where $\Delta_H = [\ |diag(H)|\ ]^{\frac{1}{2}}$. If $\alpha < \gamma/(\gamma+3)$, then*

$$\sum_{j=s_{i-1}+1}^{s_i} |1 - \frac{\lambda_{s_i}}{h_{jj}}|^2 + \|\Omega\,(\pi_i(H_S))\,\|_F^2 \leq \frac{16}{\gamma_i^2}\|\tau_i(H_S)\|_F^4,\ 1 \leq i \leq p.$$

(ii) Let $H = H^*$ be α-s.d.d. and positive definite. Let $H = \Delta_H H_S \Delta_H$ with $\Delta_H = [diag(H)]^{\frac{1}{2}}$. If $\alpha < \gamma/3$, then

$$\sum_{j=s_{i-1}+1}^{s_i} |1 - \frac{\lambda_{s_i}}{h_{jj}}|^2 + \|\Omega\,(\pi_i(H_S))\,\|_F^2 \leq \frac{4}{\gamma_i^2}\|\tau_i(H_S)\|_F^4,\ 1 \leq i \leq p.$$

Example 4. *Let H be as above. An easy computation yields*

$$\alpha = \|\Omega(H_S)\|_F \approx 2.4618 \cdot 10^{-2},$$

and since $\gamma \approx 0.9801980$, we have

$$\alpha < \frac{\gamma}{\gamma + 3} \approx 2.4627 \cdot 10^{-1}.$$

By the first assertion of Theorem 4*,*

$$r_i = \left|1 - \frac{\lambda_{s_i}}{h_{jj}}\right| \leq \frac{4}{\gamma_i}\|\tau_i(H_S)\|_F^2 < 8.205 \cdot 10^{-4}$$

and therefore,

$$\left|\frac{\lambda_{s_i} - h_{jj}}{\lambda_{s_i}}\right| \leq \frac{r_i}{1 - r_i} < 8.22 \cdot 10^{-4}.$$

Except for $i = 1$, this is an overestimate by a factor less than 8.

Theorem 4 has several applications. First, it can be used to obtain appropriate estimates for scaled almost diagonal square matrices with multiple singular values (see [24]). Second, it is essential in proving the asymptotic convergence of scaled iterates by the Jacobi method for Hermitian matrices (see [23]).

2.3. Results for (A, B)

A generalization of *Theorem 4* is proved in [18].

Theorem 5. *Let (A, B) be a (α, β)–s.d.d.d. pair, $A = \Delta_A A_S \Delta_A$, $B = \Delta_B B_S \Delta_B$ with $\Delta_A = [|\mathrm{diag}\ (A)|]^{1/2}$, $\Delta_B = [\mathrm{diag}\ (B)]^{1/2}$. If*

$$\frac{\alpha + \beta}{1 - \alpha} < \frac{1}{3}\gamma, \tag{1}$$

then for each $1 \leq i \leq p$ there holds

(i) $$\|\pi_i\left(A_S - \lambda_{s_i}\Delta_A^{-1}B\Delta_A^{-1}\right)\|_F \leq \frac{4}{\gamma_i}\|\tau_i\left(A_S - \lambda_{s_i}\Delta_A^{-1}B\Delta_A^{-1}\right)\|_F^2,$$

(ii) $$\|\pi_i\left(A - \lambda_{s_i}B\right)\|_F \leq \frac{4}{\gamma_i}\|\tau_i\left(A\Delta_A^{-1} - \lambda_{s_i}B\Delta_A^{-1}\right)\|_F^2,$$

(iii) $$\|\pi_i\left(\lambda_{s_i}^{-1}\Delta_B^{-1}A\Delta_B^{-1} - B_S\right)\|_F \leq \frac{2}{\gamma_i}\|\tau_i\left(\lambda_{s_i}^{-1}\Delta_B^{-1}A\Delta_B^{-1} - B_S\right)\|_F^2,$$

(iv) $$\|\pi_i\left(\lambda_{s_i}^{-1}A - B\right)\|_F \leq \frac{2}{\gamma_i}\|\tau_i\left(\lambda_{s_i}^{-1}A\Delta_B^{-1} - B\Delta_B^{-1}\right)\|_F^2.$$

If both matrices A and B are positive definite, one can further improve the latest result.

Corollary 3. *Suppose the pair (A, B) is (α, β)-s.d.d.p.d. and let A_S, Δ_A, B_S and Δ_B be as in* Theorem 5.

(a) *If in (1) the denumerator* $1-\alpha$ *is replaced by* $1-\beta$*, then the constants* 4 *and* 2 *in the assertions (i), (ii) and (iii), (iv), respectively, interchange their places.*

(b) *If in (1) the denumerator* $1-\alpha$ *is replaced by* $1-\max\{\alpha,\beta\}$*, then all the assertions of* Theorem 5 *hold with the same constant* 2 *on the right-hand sides.*

The results expressed in *Theorem 5* and *Corollary 3* can be used for estimating eigenvalues (or Ritz values) by diagonal elements. This is important for stopping of eigenvalue routines for the simultaneous diagonalization of a positive definite matrix pair (e.g. in the subspace iteration method combined with the Falk-Langemeyer method [33, 6]).

2.4. Results for a square matrix C

By techniques similar to those used in *Subsection 1.3*, one can deduce from *Theorem 4* results that deal with square matrices and singular values. Let C be a square matrix with (possibly multiple) singular values $\sigma_{s_1} > \cdots > \sigma_{s_p} > 0$. Then the Hermitian matrix H from (7) has eigenvalues $\sigma_{s_1} > \cdots > \sigma_{s_p} > 0 > -\sigma_{s_p} > \cdots > -\sigma_{s_1}$. When we deal with absolute gaps we have to introduce $\tilde{\delta}_p = 2\sigma_{s_p}$, the artificial gap between σ_{s_p} and $-\sigma_{s_p}$. However, if relative gaps are used, the problem with artificial gaps is avoided in the very natural way. Since

$$\frac{|\lambda_{s_i} - \lambda_{s_j}|}{|\lambda_{s_i}| + |\lambda_{s_j}|} = \frac{|\sigma_{s_i} - (-\sigma_{s_j})|}{\sigma_{s_i} + \sigma_{s_j}} = 1\,,$$

whenever $\lambda_{s_i} = \sigma_{s_i}$ and $\lambda_{s_j} = -\sigma_{s_j}$, we see that the relative gap between eigenvalues of different sign is one. Hence in this measure, σ_{s_p} and $-\sigma_{s_p}$ as eigenvalues of H are "as far as possible", and the relative gaps between the eigenvalues of H reduce to the relative gaps between the singular values of C. This favourable situation results in the following theorem from [24].

Theorem 6. *Let* $C \in \mathbb{C}^{n\times n}$ *be an* α*-s.d.d. matrix whose diagonal elements satisfy the condition* $c_{11} \geq \cdots \geq c_{11} \geq 0$*, and let* $C = \Delta_C^{1/2} C_S \Delta_C^{1/2}$, $\Delta_C = diag(C)$*. Let* C *and* C_S *be partitioned according to the multiplicities of the singular values. If* $\alpha < \gamma/(\gamma+3)$*, then*

(i) $$\|\pi_i(\frac{C_S + C_S{}^*}{2} - \sigma_{s_i}\Delta_C^{-1})\|_F \leq \frac{1}{\gamma_i}\left[\|\pi_i(C_S - C_S{}^*)\|_F^2 + 2\|\tau_i(C_S)\|_F^2 + \right.$$
$$\left. + 2\|\tau_i(C_S{}^*)\|_F^2\right], \quad 1 \leq i \leq p.$$

(ii) $$\|\pi_i(\frac{C + C^*}{2} - \sigma_{s_i}I)\|_F \leq \frac{1}{\gamma_i}\min\Big\{\|\pi_i((C - C^*)\Delta_C^{-1/2})\|_F^2$$
$$+2\|\tau_i(C\Delta_C^{-1/2})\|_F^2 + 2\|\tau_i(C^*\Delta_C^{-1/2})\|_F^2\,,$$
$$\frac{1}{2\sigma_{s_i}}\left[2\|\tau_i(C)\|_F^2 + 2\|\tau_i(\tilde{C}^*)\|_F^2 + \|\pi_i(C - C^*)\|_F^2\right]\Big\}, \quad 1 \leq i \leq p.$$

2.5. Results for an essentially triangular matrix T

If the matrix is triangular, or more generally, essentially triangular, the last theorem reduces to (cf. [24])

Corollary 4. *Let T be as in* Theorem 6. *If in addition, T is essentially triangular, then*

(i) $$\sum_{j=s_{i-1}+1}^{s_i} |1-\frac{\sigma_{s_i}}{b_{jj}}|^2 + \frac{\|\Omega(\pi_i(T_S))\|_F^2}{2} \le \frac{4}{\gamma_i^2}\left[\|\Omega(\pi_i(T_S))\|_F^2 + \|\tau_i(T_S)\|_F^2 + \|\tau_i({T_S}^*)\|_F^2\right]^2, \; 1 \le i \le p.$$

(ii) $$\sum_{j=1}^{n} |1-\frac{\sigma_j}{b_{jj}}|^2 + \frac{\|\Omega(\pi_i(T_S))\|_F^2}{2} \le \frac{4\|\Omega(T_S)\|_F^2}{\gamma^2}\left[\|\Omega(T_S)\|_F^2 + \|\tau(T_S)\|_F^2\right].$$

In particular, if $T = (t_{ij})$ is triangular and some singular value σ_i is simple, the assertion (i) of *Corollary 4* implies the following simple and useful estimate

$$| 1 - \frac{\sigma_i}{t_{kk}} | \le \frac{2}{\gamma}\left[\sum_{j=1}^{k-1} \frac{|\, t_{jk}\,|^2}{|\, t_{kk}t_{jj}\,|} + \sum_{j=k+1}^{n} \frac{|\, t_{kj}\,|^2}{|\, t_{kk}t_{jj}\,|}\right]. \tag{2}$$

Here, we assumed that σ_i is affiliated with t_{kk}. As has been proved in [24, Corollary 7], in the last estimate the diagonal elements can be complex, and no special ordering of diagonals has to be assumed. These and similar results from [24] have been used in proving the quadratic convergence of scaled iterates by the Kogbetliantz method for triangular matrices (see [25]).

Example 5. *Let*

$$T = \begin{bmatrix} 1 & \sqrt{2}\cdot 10^{-7} & 10^{-8} \\ 0 & 2\cdot 10^{-6} & \sqrt{2}\cdot 10^{-10} \\ 0 & 0 & 10^{-10} \end{bmatrix}, \quad \textit{then} \quad T_S = \begin{bmatrix} 1 & 10^{-4} & 10^{-5} \\ 0 & 1 & 10^{-4} \\ 0 & 0 & 1 \end{bmatrix}.$$

By MATLAB one finds out that

$$\left.\begin{array}{l} \sigma_1 = 1.000000000000010 \\ \sigma_2 = 2.000000004999980\cdot 10^{-6} \\ \sigma_3 = 9.999999975000000\cdot 10^{-11} \end{array}\right\} \begin{array}{l} \gamma_1 = 9.999960000079900\cdot 10^{-1} \\ \gamma_2 = 9.999000050002500\cdot 10^{-1} \\ \gamma_3 = 9.999000050002500\cdot 10^{-1} \end{array}.$$

The left- and right-hand sides of the inequality (2), as well as the appopriate quotients are displayed in the following table

left	right	right / left
$-1.0214\cdot 10^{-14}$	$2.0200\cdot 10^{-8}$	$-1.9777\cdot 10^{6}$
$-2.5000\cdot 10^{-09}$	$2.0002\cdot 10^{-8}$	$-8.0008\cdot 10^{0}$
$2.5000\cdot 10^{-09}$	$2.0002\cdot 10^{-8}$	$8.0008\cdot 10^{0}$

We see that the the bounds for the smallest singular values overestimate the true values only by the factor $\approx$ 8.

The true relative error of t_{ii} as an approximation of σ_i is given by $\rho_i = 1 - \frac{|t_{ii}|}{\sigma_i}$. Note that ρ_i is linked with $r_i = 1 - \frac{\sigma_i}{|t_{ii}|}$ by $\rho_i = r_i/(1-r_i)$, hence for tiny r_i, $\rho_i \approx r_i$.

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