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A SHARP UPPER BOUND FOR DEPARTURE FROM NORMALITY

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Abstract

The departure from normality of a matrix is a real scalar that is impractical to compute if a matrix is large and its eigenvalues are unknown. A simple formula is presented for computing an upper bound for departure from normality in the Frobenius norm. This new upper bound is cheaper to compute than the upper bound derived by Henrici [*Numer. Math.*, 4 (1962), pp. 24 – 40]. Moreover, the new bound is sharp for Hermitian matrices, skew-Hermitian matrices and, in general, any matrix with eigenvalues that are horizontally or vertically aligned in the complex plane. In terms of applications, the new bound can be used in computing bounds for the spectral norm of matrix functions or bounds for the sensitivity of eigenvalues to matrix perturbations.

1. Introduction

The departure from normality of a matrix, like the condition number of a matrix, is a real scalar that can be used to compute bounds for various matrix computations. For example, departure from normality can be used to bound the powers, inverses, spectral variation, and fields of values of nonnormal matrices [5] or bound the spectral norm of matrix functions [1]. Unfortunately, the departure from normality of a matrix is impractical to compute if a matrix is large and its eigenvalues are unknown. The main result of this paper is a simple formula for computing an upper bound for the departure from normality of a matrix in the Frobenius norm. This new upper bound is cheaper to compute than the upper bound derived by Henrici [5], and it is sharp for any matrix with eigenvalues that are horizontally or vertically aligned in the complex plane. The practical significance is that the new upper bound can be used in computing bounds for many of the matrix computations described in [1,5].

The outline of this paper is as follows. In §2, we establish notation, motivate the definition of the departure from normality of a matrix, and give Henrici's upper bound for departure from normality [5]. In §3, we derive a new upper bound for departure from normality and prove that it is sharp for certain classes of matrices. In §4, we conclude with some numerical results that compare the tightness of Henrici's bound and the new bound.

2. Preliminaries

Let $A = (a_{ij})$ denote an $n \times n$ complex matrix and let $A^H = (\bar{a}_{ji})$ denote the conjugate transpose of A . (Herein, all matrices are square matrices of order n with real or complex entries.) Several important classes of matrices are defined in terms of their conjugate transpose: for example, A is a Hermitian matrix if and only if (iff) $A^H = A$, A is a skew-Hermitian matrix iff $A^H = -A$, and A is a unitary matrix iff $A^H A = A A^H = I$. Let M and N denote the Hermitian part of A and the skew-Hermitian part of A , respectively. Indeed, let the functions $\mathcal{H}(\cdot)$ and $\mathcal{S}(\cdot)$ be the Hermitian part and skew-Hermitian part of any square matrix. Then, for

$$\mathcal{H}(A) := \frac{1}{2}(A + A^H) \equiv M \quad (1)$$

and

$$\mathcal{S}(A) := \frac{1}{2}(A^H - A) \equiv N, \quad (2)$$

A has the splitting

$$A = M - N. \quad (3)$$

Let R denote an upper triangular matrix, T denote a strictly upper triangular matrix, and Λ denote a diagonal matrix whose entries are the eigenvalues, λ_i , of A . Let $\text{Re}(\Lambda)$ and $\text{Im}(\Lambda)$ denote diagonal matrices whose entries are the real parts and imaginary parts of the eigenvalues of A , respectively. Finally, recall that the sum of the eigenvalues of a matrix is equal to the trace of the matrix, where

$$\text{trace}(A) = \sum_{i=1}^n a_{ii}. \quad (4)$$

The Schur decomposition states that every square matrix A is unitarily similar to an upper triangular matrix R .

Theorem 2.1 (Schur decomposition). *Given a square matrix A , there is a unitary matrix U such that*

$$U^H A U = R. \quad (5)$$

The matrix U is not unique and may be chosen so that the eigenvalues of A appear on the diagonal of R in any order.

If $U = [u_1, \dots, u_n]$ is a column partitioning of the unitary matrix U in (5), then the u_i are referred to as *Schur vectors* [4]. For concreteness, let U denote a particular unitary matrix whose columns are Schur vectors so that R is unique and has the splitting

$$R = \Lambda + T. \quad (6)$$

We now show the connection between the Schur decomposition of A and certain matrix norms of A .

Definition 2.2. *Let*

$$\|A\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2} \quad (7)$$

and

$$\|A\|_2 = \sqrt{\lambda_{\max}(A^H A)}. \quad (8)$$

The Frobenius norm $\|\cdot\|_F$ and the spectral norm $\|\cdot\|_2$ are invariant under unitary similarity transformations; that is,

$$\|A\|_F = \|U^H A U\|_F = \|R\|_F \quad (9)$$

and

$$\|A\|_2 = \|U^H A U\|_2 = \|R\|_2. \quad (10)$$

The Frobenius norm and the Schur decomposition play an important role in the definition of normal matrices.

Definition 2.3. [6] *The matrix A is normal if and only if any of the following equivalent statements hold:*

- (a) A has a complete, unitary set of eigenvectors,
- (b) $\|A\|_F = \|\Lambda\|_F$, or
- (c) $A^H A = A A^H$.

Normal matrices include Hermitian matrices, skew-Hermitian matrices, unitary matrices and, in general, any matrix that is unitarily similar to a diagonal matrix. Hence, any Schur decomposition of a normal matrix gives

$$U^H A U = R = \Lambda + T \quad (11)$$

where $T = 0$. For a matrix that is not normal, it is convenient to quantify its departure from normality in terms of a norm of T . Any matrix norm can be used; however, the Frobenius norm of T is a natural choice since it is easy to compute and its value is the same for all Schur decompositions.

Definition 2.4 (Departure from Normality). [5] *For any $n \times n$ matrix A ,*

$$\text{dep}_F(A) := \|T\|_F = \left(\|A\|_F^2 - \|\Lambda\|_F^2 \right)^{1/2}. \quad (12)$$

This definition of departure from normality, $\text{dep}_F(A)$, follows from the Schur decomposition of A and equation (9) via

$$\|A\|_F^2 = \|U^H A U\|_F^2 = \|R\|_F^2 = \|\Lambda + T\|_F^2 = \|\Lambda\|_F^2 + \|T\|_F^2 \quad (13)$$

so that

$$\text{dep}_F(A) := \|T\|_F = \left(\|A\|_F^2 - \|\Lambda\|_F^2 \right)^{1/2} \quad (14)$$

is independent of the choice of U . It is also easy to prove that $\text{dep}_F(A)$ is independent of complex shifts and unitary scalings (i.e., rotations). For example, in the Schur decomposition of $A - \alpha I$, where

$$U^H (A - \alpha I) U = R - \alpha I = \Lambda + T - \alpha I, \quad (15)$$

note that the shift only alters the diagonal elements of R and that $\text{dep}_F(A) := \|T\|_F$ is unchanged. Hence,

$$\text{dep}_F(A) = \text{dep}_F(e^{-i\theta} (A - \alpha I)) \quad (16)$$

for the complex scalar α and $0 \leq \theta < 2\pi$. Later, we show the significance of this observation.

For normal matrices, $\text{dep}_F(A) = 0$ via Definition 2.3(b). For nonnormal matrices, $\text{dep}_F(A)$ is the nonzero quantity defined by (12). To be clear, a small example helps to summarize the main ideas up to this point.

Example 1. Consider two different Schur decompositions of

$$A = \begin{pmatrix} 4 & \sqrt{1/2} & -3 \\ \sqrt{2} & 2 & -\sqrt{2} \\ 1 & \sqrt{1/2} & 0 \end{pmatrix}, \quad (17)$$

where U_1 and U_2 are unitary matrices such that

$$U_1^H A U_1 = R_1 = \begin{pmatrix} 1 & 1 & 4 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{pmatrix} \quad \text{and} \quad U_2^H A U_2 = R_2 = \begin{pmatrix} 2 & -1 & 3\sqrt{2} \\ 0 & 1 & \sqrt{2} \\ 0 & 0 & 3 \end{pmatrix}. \quad (18)$$

The Schur decompositions in (18) show that A has eigenvalues $\lambda(A) = \{1, 2, 3\}$ and that A is nonnormal since R_1 and R_2 are not diagonal matrices. Moreover, the strictly upper triangular parts of the decompositions show that $\text{dep}_F(A) := \|T\|_F = \sqrt{21}$.

The value of $\text{dep}_F(A)$ is impractical to compute if A is large and its eigenvalues are unknown. Lower bounds for $\text{dep}_F(A)$ have been derived by Eberlein [3]

$$\text{dep}_F(A) \geq \frac{\|A^H A - A A^H\|_F}{\sqrt{6} \|A\|_F} \quad (19)$$

and Loizou [7, Theorem 2]

$$\text{dep}_F(A) \geq \frac{\|A^H A - A A^H\|_F}{\beta^{1/2} + (\beta + \sqrt{2} \|A^H A - A A^H\|_F)^{1/2}}, \quad (20)$$

where

$$\beta = \|A\|_F^2 - \frac{1}{n} |\text{trace}(A)|^2 \quad \text{and} \quad A \neq 0. \quad (21)$$

The following upper bound has been derived by Henrici.

Theorem 2.5. [5, Theorem 1] For any $n \times n$ matrix A ,

$$\text{dep}_F(A) \leq \left(\frac{n^3 - n}{12} \right)^{1/4} \left(\|A^H A - A A^H\|_F \right)^{1/2}. \quad (22)$$

The bounds (19), (20) and (22) reduce to zero when A is a normal matrix. Unfortunately, such bounds involve the matrix-matrix computation $A^H A - A A^H$, which generally requires $O(n^3)$ multiplications to obtain.

3. A Sharp Upper Bound

In deriving an upper bound for $\text{dep}_F(A)$, a trivial bound comes from its definition:

$$\text{dep}_F(A) = \left(\|A\|_F^2 - \|\Lambda\|_F^2 \right)^{1/2} \leq \|A\|_F. \quad (23)$$

We can obtain better upper bounds for $\text{dep}_F(A)$ by manipulating expressions that arise after splitting A into its Hermitian part M and skew-Hermitian part N .

Lemma 3.1. *If $A = M - N$ has the Schur decomposition $U^H A U = \Lambda + T$, then*

$$\|M\|_F^2 = \|\text{Re}(\Lambda)\|_F^2 + \frac{1}{2}\|T\|_F^2, \quad (24)$$

$$\|N\|_F^2 = \|\text{Im}(\Lambda)\|_F^2 + \frac{1}{2}\|T\|_F^2. \quad (25)$$

Proof: The following chain of equalities follows directly from the definitions of the Frobenius norm, and the functions $\mathcal{H}(\cdot)$ and $\mathcal{S}(\cdot)$:

$$\|M\|_F^2 = \|\mathcal{H}(A)\|_F^2 = \|\mathcal{H}(R)\|_F^2 = \|\mathcal{H}(\Lambda)\|_F^2 + \|\mathcal{H}(T)\|_F^2 = \|\text{Re}(\Lambda)\|_F^2 + \frac{1}{2}\|T\|_F^2, \quad (26)$$

$$\|N\|_F^2 = \|\mathcal{S}(A)\|_F^2 = \|\mathcal{S}(R)\|_F^2 = \|\mathcal{S}(\Lambda)\|_F^2 + \|\mathcal{S}(T)\|_F^2 = \|\text{Im}(\Lambda)\|_F^2 + \frac{1}{2}\|T\|_F^2. \quad (27)$$

These equalities can also be found in [8, pg. 495]. ■

Equations (26) and (27) show that $\text{dep}_F(A)$ can be defined in two different, but equivalent, ways:

$$\text{dep}_F(A) = \sqrt{2} \left(\|M\|_F^2 - \|\text{Re}(\Lambda)\|_F^2 \right)^{1/2} \quad (28)$$

or

$$\text{dep}_F(A) = \sqrt{2} \left(\|N\|_F^2 - \|\text{Im}(\Lambda)\|_F^2 \right)^{1/2}. \quad (29)$$

A simple upper bound for $\text{dep}_F(A)$ follows directly from these equalities.

Lemma 3.2. *If $A = M - N$, where M is the Hermitian part of A and N is the skew-Hermitian part of A , then*

$$\text{dep}_F(A) \leq \sqrt{2} \min \{ \|M\|_F, \|N\|_F \}. \quad (30)$$

Proof: By breaking the equalities (28) and (29), we obtain

$$\text{dep}_F(A) = \sqrt{2} \left(\|M\|_F^2 - \|\text{Re}(\Lambda)\|_F^2 \right)^{1/2} \leq \sqrt{2} \|M\|_F, \quad (31)$$

$$\text{dep}_F(A) = \sqrt{2} \left(\|N\|_F^2 - \|\text{Im}(\Lambda)\|_F^2 \right)^{1/2} \leq \sqrt{2} \|N\|_F, \quad (32)$$

and the upper bound

$$\text{dep}_F(A) \leq \sqrt{2} \min \{ \|M\|_F, \|N\|_F \}. \quad (33)$$

■

We now consider the use of the complex shift αI for improving the bound (30). As in Lemma 3.1, we can split $A - \alpha I$ into its Hermitian part $M - \text{Re}(\alpha)I$ and skew-Hermitian part $N - \text{Im}(\alpha)I$ and rearrange terms to obtain

$$\text{dep}_F(A) = \text{dep}_F(A - \alpha I) = \sqrt{2} \left(\|M - \text{Re}(\alpha)I\|_F^2 - \|\text{Re}(\Lambda) - \text{Re}(\alpha)I\|_F^2 \right)^{1/2} \quad (34)$$

and

$$\text{dep}_F(A) = \text{dep}_F(A - \alpha I) = \sqrt{2} \left(\|N - \text{Im}(\alpha)I\|_F^2 - \|\text{Im}(\Lambda) - \text{Im}(\alpha)I\|_F^2 \right)^{1/2}. \quad (35)$$

A tighter bound can be obtained by minimizing the terms

$$\|\text{Re}(\Lambda) - \text{Re}(\alpha)I\|_F^2 \quad \text{and} \quad \|\text{Im}(\Lambda) - \text{Im}(\alpha)I\|_F^2 \quad (36)$$

before dropping them from equations (34) and (35), respectively. In particular,

$$f_1(\text{Re}(\alpha)) = \|\text{Re}(\Lambda) - \text{Re}(\alpha)I\|_F^2 = \sum (\text{Re}(\lambda_i) - \text{Re}(\alpha))^2 \quad (37)$$

and

$$f_2(\text{Im}(\alpha)) = \|\text{Im}(\Lambda) - \text{Im}(\alpha)I\|_F^2 = \sum (\text{Im}(\lambda_i) - \text{Im}(\alpha))^2 \quad (38)$$

are quadratic functions that can be minimized using standard calculus techniques. By solving $f'_1 = 0$ and $f'_2 = 0$, we find that

$$\operatorname{Re}(\alpha) = \frac{\sum \operatorname{Re}(\lambda_i)}{n} \quad \text{and} \quad \operatorname{Im}(\alpha) = \frac{\sum \operatorname{Im}(\lambda_i)}{n}. \quad (39)$$

These values minimize equations (37) and (38), respectively, since f''_1 and f''_2 are positive. Hence, both terms of equation (36) are minimized by choosing

$$\alpha = \operatorname{Re}(\alpha) + \operatorname{Im}(\alpha) = \frac{\sum \operatorname{Re}(\lambda_i)}{n} + \frac{\sum \operatorname{Im}(\lambda_i)}{n} = \frac{\sum \lambda_i}{n} = \frac{\operatorname{trace}(A)}{n}. \quad (40)$$

Theorem 3.3. *If $A = M - N$, where M is the Hermitian part of A and N is the skew-Hermitian part of A , then*

$$\operatorname{dep}_F(A) \leq \sqrt{2} \min \{ \|M - \operatorname{Re}(\alpha)I\|_F, \|N - \operatorname{Im}(\alpha)I\|_F \} \quad (41)$$

where the upper bound is minimized for

$$\alpha = \frac{\operatorname{trace}(A)}{n}. \quad (42)$$

Moreover, the bound is sharp (i.e., equality holds) if and only if the eigenvalues of A are horizontally or vertically aligned in the complex plane.

Proof: The upper bound is obtained from equations (34) and (35) by dropping the terms $\|\operatorname{Re}(\Lambda) - \operatorname{Re}(\alpha)I\|_F^2$ and $\|\operatorname{Im}(\Lambda) - \operatorname{Im}(\alpha)I\|_F^2$, respectively. The bound is sharp iff

$$\|\operatorname{Re}(\Lambda) - \operatorname{Re}(\alpha)I\|_F^2 = 0 \quad \text{or} \quad (43)$$

$$\|\operatorname{Im}(\Lambda) - \operatorname{Im}(\alpha)I\|_F^2 = 0. \quad (44)$$

The first condition (43) says that the real parts of the eigenvalues of A are constant (i.e., vertically aligned). The second condition (44) says that the imaginary parts of the eigenvalues of A are constant (i.e., horizontally aligned). ■

Equations (34) and (35) also show that

$$\operatorname{dep}_F(A) \approx \sqrt{2} \min \{ \|M - \operatorname{Re}(\alpha)I\|_F, \|N - \operatorname{Im}(\alpha)I\|_F \} \quad (45)$$

iff

$$\|\operatorname{Re}(\Lambda) - \operatorname{Re}(\alpha)I\|_F^2 \ll \|M - \operatorname{Re}(\alpha)I\|_F^2 \quad \text{or} \quad (46)$$

$$\|\operatorname{Im}(\Lambda) - \operatorname{Im}(\alpha)I\|_F^2 \ll \|N - \operatorname{Im}(\alpha)I\|_F^2. \quad (47)$$

Hence, the new bound (41) is a good approximation when the eigenvalues of A are relatively close to being horizontally or vertically aligned; otherwise, the bound is weak.

Example 2. Let's compare the Henrici bound (22) and the new bound (41) for the matrix A in Example 1, in which $\text{dep}_F(A) = \sqrt{21}$. Using the intermediate quantities

$$\|A^H A - A A^H\|_F = \sqrt{996}, \quad \alpha = 2, \quad \|M - 2I\|_F = \sqrt{25/2} \quad \text{and} \quad \|N\|_F = \sqrt{21/2}, \quad (48)$$

the Henrici bound gives

$$\text{dep}_F(A) \leq (2)^{1/4} (\sqrt{996})^{1/2} = (\sqrt{1992})^{1/2} \approx \sqrt{44.6318} \quad (49)$$

and the new bound gives

$$\text{dep}_F(A) \leq \sqrt{2} \min \left\{ \sqrt{25/2}, \sqrt{21/2} \right\} = \sqrt{21}. \quad (50)$$

In this example, the new bound is tighter than the Henrici bound. The new bound is sharp since the eigenvalues of A are strictly real.¹

Numerous examples can be contrived for which the new bound is tighter than the Henrici bound or vice versa. In general, the new bound is preferable since the Henrici bound is an $O(n^3)$ computation and the new bound is an $O(n^2)$ computation. It is sometimes possible to further improve the new bound by rotating $A - \alpha I$. For complex matrices, the eigenvalues of $A - \alpha I$ can be arbitrarily distributed and the best rotation θ can not be determined *a priori*. For real matrices, the eigenvalues of $A - \alpha I$ occur in complex-conjugate pairs and the new bound is minimized for $\theta \in \{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\}$. Note that the implicit use of $\theta = 0$ has the advantage that the new bound reduces to zero for Hermitian and skew-Hermitian matrices. Unfortunately, for normal matrices whose eigenvalues are not horizontally or vertically aligned, the new bound does not reduce to zero.

In contrast to the improvements for the new bound, the Henrici bound is unaffected by complex shifts and rotations of A . This is so because, for complex shifts of A ,

$$\|(A - \alpha I)^H (A - \alpha I) - (A - \alpha I)(A - \alpha I)^H\|_F \quad (51)$$

$$= \|(A^H A - \alpha^H A - \alpha A^H + \alpha^H \alpha I) - (A A^H - \alpha^H A - \alpha A^H + \alpha \alpha^H I)\|_F \quad (52)$$

$$= \|A^H A - A A^H\|_F. \quad (53)$$

The same simplification (51)–(53) also occurs for the more general case of $e^{-i\theta}(A - \alpha I)$.

¹For completeness, the Eberlein (19) and Loizou (20) lower bounds are 2.1778 and 2.4240, respectively.

4. Numerical Results

Table 1 compares the upper bounds (22) and (41) for the nonnormal test matrices given by Eberlein in [2]. Loizou in [7] used this set of matrices to compare the two lower bound formulas (19) and (20). Table 1 shows the new upper bound is tighter than the Henrici upper bound for all 17 examples. Moreover, the new bound is sharp for test matrix 4, 6, 7, 9, 11 and 17.

Table 2 compares the upper bounds for some of the 32×32 nonnormal test matrices studied by Trefethen in [9]. In each case, the new upper bound is tighter than the Henrici upper bound. Moreover, the new bound is sharp for the matrices entitled: Jordan block, Limaçon, Wilkinson, Frank, Kahan, Demmel, Lenferink-Spijker, Companion, and Gauss-Seidel. Such good results are predicted by Theorem 3.3 since the aforementioned matrices have strictly real eigenvalues and the other matrices (Grcar, Chebyshev spectral) have eigenvalues that are almost vertically aligned.

Test matrix	Henrici bound (22)	new bound (41)	$\text{dep}_F(A)$ (12)	ratio	
				(22)/(12)	(41)/(12)
1	1.411	1.005	0.99	1.43	1.02
2	0.141	0.100	0.100	1.41	1.00
3	7.416	3.423	2.449	3.03	1.40
4	5.214	1.610	1.610	3.24	1.
5	93.325	40.623	33.086	2.82	1.23
6	1.778	1.732	1.732	1.03	1.
7	3.310	2.828	2.828	1.17	1.
8	21.644	10.955	10.895	1.99	1.01
9	15.477	10.010	10.010	1.55	1.
10	95.933	46.033	45.924	2.09	1.00
11	128.24	34.785	34.785	3.69	1.
12	1.584e+3	361.994	357.659	4.43	1.01
13	7.524e+3	924.661	917.796	8.20	1.01
14	86.759	75.974	58.481	1.48	1.30
15	250.249	188.149	94.184	2.66	2.00
16	95.933	46.033	45.924	2.09	1.00
17	2.115	1.414	1.414	1.50	1.

Table 1: Departure from normality results for Eberlein [2] nonnormal test matrices.

Test matrix	Henrici bound (22)	new bound (41)	$\text{dep}_F(A)$ (12)	ratio	
				(22)/(12)	(41)/(12)
Jordan block	8.594	5.568	5.568	1.54	1.
Limaçon	13.980	7.810	7.810	1.79	1.
Grcar	18.398	7.681	6.007	3.06	1.28
Wilkinson	8.659	5.568	5.568	1.56	1.
Frank	1.821e+3	2.772e+2	2.772e+2	6.57	1.
Kahan	38.092	4.982	4.982	7.65	1.
Demmel	1.236e+9	1.438e+8	1.438e+8	8.59	1.
Lenferink-Spijker	2.384e+2	1.067e+2	1.067e+2	2.23	1.
Companion	5.281e+5	6.145e+4	6.145e+4	8.59	1.
Gauss-Seidel	4.555	2.149	2.149	2.12	1.
Chebyshev spectral	4.392	0.572	0.570	7.71	1.00

Table 2: Departure from normality results for Trefethen [9] nonnormal test matrices.

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