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On the geometrical structure of symmetric matrices

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ABSTRACT

The identity ray, αI for $\alpha > 0$, can be seen as the center ray of the cone of symmetric and positive definite (SPD) matrices. In that sense, the angle that any SPD matrix forms with the identity plays a very important role to understand the geometrical structure of the cone. In this work, we extend this relationship, and analyze the geometrical structure of symmetric matrices including the location of all orthogonal matrices, not only the identity matrix. This geometrical understanding leads to new results in the subspace of symmetric matrices. We also extend some of the geometrical results for the case of general (not necessarily symmetric) nonsingular matrices.

1. Introduction

The space of square real $n \times n$ matrices can be equipped with the Frobenius inner product defined by

$$< A, B >_F = tr(A^T B),$$

for which we have the associated norm that satisfies $\|A\|_F^2 =< A, A >_F$. In here, $tr(A) = \sum_i a_{ii}$ is the trace of the matrix A. In this inner product space, the cone of symmetric and positive definite (SPD) matrices has a rich geometrical structure. In that context the angle that any matrix forms with the identity ray, αI for $\alpha > 0$, plays a very important role. Our work has been motivated by the rich geometrical structure of the positive semidefinite cone of $n \times n$ matrices and specially by the discussion presented by Tarazaga [3,4], and more recently by Chehab and Raydan [1].

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In this work, we extend this geometrical point of view, and analyze the geometrical structure of symmetric matrices, including the location of all orthogonal matrices, not only the identity ray.

The rest of this paper is divided into sections as follows. In Section 2 we introduce the required notation, review the previously obtained results for SPD matrices, and we present new results that add understanding to the structure of the subspace of symmetric matrices. In particular we describe the multiple rays in the subspace of symmetric matrices that generalize the role of the identity matrix in the SPD case. In Section 3, we will show properties about the location of orthogonal matrices. As a by product, we present a new lower bound for the Frobenius condition number of symmetric matrices. In Section 4 we present an extension of the obtained results for general matrices.

2. Basic results and structure of symmetric matrices

The Frobenius inner product allow us to define the cosine of the angle between two given real $n \times n$ matrices as

$$\cos(A, B) = \frac{< A, B >_F}{\|A\|_F \|B\|_F}. \tag{1}$$

In particular, for a given symmetric matrix A,

$$\cos(A, I) = \frac{tr(A)}{\|A\|_F \sqrt{n}}. \tag{2}$$

Note that, for any nonsingular symmetric matrix A, using the Cauchy-Schwarz inequality we have

$$n = tr(I) =< A, A^{-1} >_F \leqslant \|A\|_F \|A^{-1}\|_F = \kappa_F(A),$$

and so, n is a lower bound for $\kappa_F(A)$. Moreover, it also follows that

$$\cos(A, A^{-1}) = \frac{< A, A^{-1} >_F}{\|A\|_F \|A^{-1}\|_F} = \frac{n}{\|A\|_F \|A^{-1}\|_F} = \frac{n}{\kappa_F(A)}. \tag{3}$$

In particular, for a given SPD matrix A, it was established in [1] that

$$0 \leqslant \cos(A, A^{-1}) \leqslant \cos(A, I) \cos(A^{-1}, I) \leqslant 1. \tag{4}$$

Let us now analyze the geometrical structure of the subspace S_n of symmetric matrices of order n. Given $A \in S_n$, we can always diagonalize A as follows

$$Q^t A Q = D,$$

where the columns of the orthogonal matrix Q are a set of orthonormal eigenvectors of A. In here, we only consider nonsingular matrices. It is important to recall that the map

$$\phi_Q(X) = Q^t X Q$$

is an isometry and so it preserves the norm of a matrix and the angle between matrices. It also preserves eigenvalues and the trace of a matrix. In particular note that $\phi_Q(I) = I$, i. e., the identity matrix is a fixed point of ϕ_Q for every orthogonal matrix Q.

We are interested in the angles that A, A^{-1}, and any other matrix that shares the same eigenvectors, form between them. Using ϕ_Q we can shift all these matrices to the set of diagonal matrices, since all of them are simultaneously diagonalizable. Let us now consider the matrix Q_A that belongs to the class mentioned above. This is a very interesting matrix that will play a key role throughout this work. Given a matrix $A \in S_n$ with spectral decomposition $A = \sum_{i=1}^n \lambda_i x_i x_i^t$ we define Q_A as follows

$$Q_A = \sum_{i=1}^{n} \text{sign}(\lambda_i) x_i x_i^t.$$

It is worth noticing that $Q_A = \text{sign}(A)$, where $\text{sign}(A) \equiv A(A^2)^{-1/2}$, and $A^{1/2}$ is the principal square root of A; see Higham for details [2]. Clearly, Q_A shares the eigenvectors of A and the sign of the corresponding eigenvalues which implies that they share the inertia. It is also straightforward that Q_A is an orthogonal matrix. Also we have that $Q_A = Q_{A^{-1}}$. It is clear now that given $A = \sum_{i=1}^{n} \lambda_i x_i x_i^t$ and Q, the matrix whose columns are the eigenvectors of A, it follows that $\phi_Q(A) = diag(\lambda_1, \ldots, \lambda_n)$ and $\phi_Q(Q_A) = diag(\text{sign}(\lambda_1), \ldots, \text{sign}(\lambda_n))$.

For example, the diagonal matrices of order two form a two dimensional subspace of S_2 and any matrix in that subspace can be written as

$$D = \lambda_1 e_1 e_1^t + \lambda_2 e_2 e_2^t,$$

where e_1 and e_2 are the canonical vectors in $\mathbb{R}^2$, and λ_1 and λ_2 are the eigenvalues of D. Note that the identity matrix is written as $I = e_1 e_1^t + e_2 e_2^t$. This subspace of diagonal matrices contains four orthogonal matrices: the identity matrix I, $-I$, and the other two diagonal matrices with a 1 and a -1 in the diagonal. As we said, the subspace of diagonal matrices has dimension two and the bisectors of the quadrants are the orthogonal matrices just mentioned. We consider the system of coordinates generated by $e_1 e_1^t,\ e_2 e_2^t$. Notice that, given a matrix A, its inverse A^{-1} and Q_A have the same inertia (and also its transpose in the nonsymmetric case).

We can observe that inversion happens in the same quadrant (orthant in the general case S_n, for $n > 2$). It is worth noticing that, in reference to this 2-dimensional example, the paper by Chehab and Raydan [1] deals with the positive quadrant.

Lemma 2.1. *Given a nonsingular matrix $A \in S_2$, we have that*

$$\cos(A, Q_A) = \cos(A^{-1}, Q_A). \tag{5}$$

Proof. First of all notice that since A and Q_A are simultaneously diagonalizable, it suffices to show that

$$\cos(D, Q_D) = \cos(D^{-1}, Q_D),$$

where D satisfies $A = QDQ^t$. In other words the diagonal elements of D are the eigenvalues of A. Recall that D, D^{-1} and Q_D have the same inertia. Let us now compute the cosines

$$\cos(D, Q_D) = \frac{tr(DQ_D)}{\|D\|_F \sqrt{2}} = \frac{|\lambda_1| + |\lambda_2|}{\sqrt{\lambda_1^2 + \lambda_2^2}\sqrt{2}},$$

$$\cos(D^{-1}, Q_D) = \frac{tr(D^{-1}Q_D)}{\|D^{-1}\|_F \sqrt{2}} = \frac{\frac{1}{|\lambda_1|} + \frac{1}{|\lambda_2|}}{\sqrt{\frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2}}\sqrt{2}}.$$

Then it suffices to prove that

$$\frac{|\lambda_1| + |\lambda_2|}{\sqrt{\lambda_1^2 + \lambda_2^2}} = \frac{\frac{1}{|\lambda_1|} + \frac{1}{|\lambda_2|}}{\sqrt{\frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2}}},$$

which follows by simple algebraic manipulations. □

This implies that if the angle between D and Q_D is θ then the angle between D and D^{-1} is 2θ. Recall that the three matrices are in a two dimensional linear space. Using a well-known trigonometric identity we have that

$$\cos(D, D^{-1}) = 2\cos^2(D, Q_D) - 1. \tag{6}$$

On the other hand, using (3) it follows that

$$\kappa_F(D) = \frac{2}{\cos(D, D^{-1})}.$$

Hence, we have established the following result.

Theorem 2.2. *Given $A \in S_2$, we have that*

$$\kappa_F(A) = \frac{2}{2\cos^2(A, Q_A) - 1}. \tag{7}$$

Determining Q_A requires the spectral decomposition of A, but the angle between A and Q_A is easy to determine in this two dimensional subspace. In the case of positive trace, if $\cos(A, I)$ is larger than $\frac{1}{\sqrt{2}}$ then $Q_A = I$. If $\cos(A, I)$ is smaller than $\frac{1}{\sqrt{2}}$ then the angle between A and Q_A is the complement of the angle between A and I (note that if $\cos(A, I) = \frac{1}{\sqrt{2}}$, then A is singular). If the trace is zero then $\lambda_2 = -\lambda_1$. In this case $A = |\lambda_1| Q_A$ and the angle between the two matrices is zero. The negative trace case follows considering $-A$.

Now we want to point out a particular case where similar results hold. It is clear that if the minimal polynomial of A has degree two (in other words A has only two distinct eigenvalues), then A^{-1} is in the subspace generated by A and the identity matrix. This was the case of the two dimensional case analyzed above. Unfortunately this is not enough to guarantee that (5) holds. However, given a nonsingular matrix $A \in S_n$, if n is even and A has only two distinct eigenvalues both with multiplicity $n/2$ then (5) holds. As in the comments following Lemma 2.1 we also have that (6) holds, or equivalently

$$\cos(A, A^{-1}) = 2\cos^2(A, Q_A) - 1,$$

that, using (3), establishes that if $A \in S_n$, n is even, and A has only two distinct eigenvalues both with multiplicity $n/2$ then (7) holds. A couple of comments are in order. First, the identity matrix plays a relevant geometrical role for positive definite matrices as shown in [1], and for general symmetric matrices the orthogonal matrices seem to play that role. Second, it is clear in this two dimensional example that the closer (angle-wise) to an orthogonal matrix the lower the Frobenius condition number, and a relationship has been established. Hence, the angle to the closest orthogonal matrix is a key measure for estimating the Frobenius condition number.

For $n > 2$ our next result relates the angle between a given symmetric matrix A and Q_A and the angle between A^{-1} and $Q_{A^{-1}} = Q_A$; and extends in a natural way Theorem 3.1 in [1]. First, we need to recall that

$$< A, Q_A >_F = tr(A\, Q_A) = \sum_{i=1}^{n} |\lambda_i|,$$

and

$$< A^{-1}, Q_A >_F = tr(A^{-1}\, Q_A) = \sum_{i=1}^{n} 1/|\lambda_i|,$$

where $\lambda_i \neq 0$ for $1 \leqslant i \leqslant n$ are the eigenvalues of A.

Theorem 2.3. *If A is a symmetric and nonsingular matrix, then*

$$1/\sqrt{n} \leqslant \frac{\cos(A, Q_A)}{\cos(A^{-1}, Q_A)} \leqslant \sqrt{n}. \tag{8}$$

Proof. Using (1) for $\cos(A, Q_A)$ and $\cos(A^{-1}, Q_A)$ and recalling that $\|A\|_F^2 = \sum_{i=1}^n \lambda_i^2$, we have

$$\cos^2(A, Q_A)/\cos^2(A^{-1}, Q_A) = \frac{(\sum_{i=1}^n |\lambda_i|)^2(\sum_{i=1}^n 1/\lambda_i^2)}{(\sum_{i=1}^n 1/|\lambda_i|)^2(\sum_{i=1}^n \lambda_i^2)}.$$

Consider now the vector $\lambda \in \mathbb{R}^n$ with entries $|\lambda_i|$, and consider also the vector $y \in \mathbb{R}^n$ with entries $1/|\lambda_i|$, for $i = 1, \ldots, n$. Using these two vectors, we can write

$$\cos^2(A, Q_A)/\cos^2(A^{-1}, Q_A) = (\lambda^T e)^2\ (y^T y)/(\lambda^T \lambda)\ (y^T e)^2, \tag{9}$$

where e is the vector of all ones. Using the Cauchy-Schwarz inequality and the fact that $\|x\|_2 \leqslant \|x\|_1$ for any vector $x \in \mathbb{R}^n$, it follows that

$$1 \leqslant \|\lambda\|_1^2/\|\lambda\|_2^2 = (\lambda^T e)^2/\|\lambda\|_2^2 \leqslant ((\lambda^T \lambda)\ (e^T e))/\|\lambda\|_2^2 = e^T e = n,$$

and also that

$$1 \geqslant \|y\|_2^2/\|y\|_1^2 = (y^T y)/(y^T e)^2 \geqslant (y^T y)/(\|y\|_2^2\ \|e\|_2^2) = 1/(e^T e) = 1/n.$$

Therefore, substituting the last two inequalities in (9) we obtain that

$$1/n \leqslant \cos^2(A, Q_A)/\cos^2(A^{-1}, Q_A) \leqslant n,$$

and the result is established. □

Moreover, using the well-known harmonic-arithmetic inequality for the collection $\{|\lambda_i|\}$ of positive real numbers, for $i = 1, \ldots, n$, which can be written as follows,

$$n\left(\frac{1}{|\lambda_1|} + \cdots + \frac{1}{|\lambda_n|}\right)^{-1} \leqslant \frac{|\lambda_1| + \cdots + |\lambda_n|}{n},$$

we obtain an extension of Lemma 2.2 in [1], for symmetric and nonsingular matrices:

$$< A, Q_A >_F < A^{-1}, Q_A >_F = tr(A\, Q_A)\ tr(A^{-1}\, Q_A) \geqslant n^2. \tag{10}$$

Notice now that multiplying by $1/\kappa_F(A)$ in both sides of (10) it can also be written in the equivalent form

$$\frac{n}{\kappa_F(A)} \leqslant \frac{tr(A\, Q_A)}{\sqrt{n}\|A\|_F}\ \frac{tr(A^{-1}\, Q_A)}{\sqrt{n}\|A^{-1}\|_F},$$

that combined with (1) gives the following upper bound for $\cos(A, A^{-1})$

$$0 \leqslant \cos(A, A^{-1}) \leqslant \cos(A, Q_A)\ \cos(A^{-1}, Q_A) \leqslant 1, \tag{11}$$

which means, as predicted by the geometrical intuition, that the angle between A and A^{-1} is larger than the angle between A and Q_A or between A^{-1} and Q_A.

Now, since $\cos(A^{-1}, Q_A) \leqslant 1$, from (11) it follows that $\cos(A, A^{-1}) \leqslant \cos(A, Q_A)$, which together with the equality given by (3), yields the following new lower bound for the Frobenius condition number $\kappa_F(A)$ in the symmetric case

$$\kappa_F(A) \geqslant \frac{n}{\cos(A, Q_A)} \geqslant n. \tag{12}$$

It is worth stressing out that, except from the SPD case in which $Q_A = I$, $\cos(A, Q_A)$ cannot be computed without knowing the spectral decomposition of A, and so it is not a practical lower bound. In Section 3 we will make it practical by exploiting some geometrical properties related to the location of orthogonal matrices in the subspace of symmetric matrices.

Before we close this section, we will look into another direction to add some geometrical understanding that explains the difference between the Frobenius condition number and the Euclidean condition number. First we need to point out that singular matrices in S_2, except for the zero matrix, are rank one matrices and they make an angle with the identity whose cosine is $\frac{1}{\sqrt{2}}$ (see [3]). Only for $n = 2$, any matrix that makes this angle with the identity is a rank one matrix.

Now given a matrix $A \in S_2$ with eigenvalues $\lambda_1 > \lambda_2$ and nonnegative trace (for the negative trace works with $-A$), we have that

$$\widehat{A} = A - \lambda_2 I$$

is a rank one matrix and the closest rank one matrix to A. Note that the eigenvalues of $\widehat{A}$ are $\lambda_1 - \lambda_2$ and 0. We now compute the angle between A and $\widehat{A}$, which is the angular distance to the set of singular matrices:

$$\cos(A, \widehat{A}) = \frac{tr(A\widehat{A})}{\|A\|_F \|\widehat{A}\|_F} = \frac{\lambda_1(\lambda_1 - \lambda_2)}{\sqrt{\lambda_1^2 + \lambda_2^2}(\lambda_1 - \lambda_2)} = \frac{\lambda_1}{\sqrt{(\lambda_1^2 + \lambda_2^2)}}.$$

If we denote $\cos(A, \widehat{A})$ by γ and square the last equation we have

$$\gamma^2 = \frac{\lambda_1^2}{\lambda_1^2 + \lambda_2^2} = \frac{\left(\frac{\lambda_1}{\lambda_2}\right)^2}{\left(\frac{\lambda_1}{\lambda_2}\right)^2 + 1}.$$

Solving for $\frac{\lambda_1}{\lambda_2}$ yields

$$\left|\frac{\lambda_1}{\lambda_2}\right| = \frac{\lambda_1}{|\lambda_2|} = \sqrt{\frac{\gamma^2}{1 - \gamma^2}}.$$

Note that under our hypothesis $\frac{\lambda_1}{|\lambda_2|} = \kappa_2(A)$. Therefore, the following result has been established.

Theorem 2.4. *Given $A \in S_2$, we have*

$$\kappa_2(A) = \sqrt{\frac{\cos^2(A, \widehat{A})}{1 - \cos^2(A, \widehat{A})}}.$$

Our first observation is that even when $\cos(A, \widehat{A})$ seems difficult to compute, it is not, since the angle between the two matrices is given by the difference between $\frac{\pi}{2}$ and the angle that A makes with the identity. In Section 4, Theorem 2.4 will be extended to general nonsingular matrices of any dimension (see Theorem 4.1).

Closing up, concerning the difference between the condition numbers $\kappa_F(A)$ and $\kappa_2(A)$, the Frobenius condition number is a function that measures how close A is to an orthogonal matrix, while the condition number associated with the 2-norm is related to how close A is to the set of singular matrices.

3. Orthogonal matrices: location properties

As we saw in the previous section, any matrix that is close to an orthogonal matrix is well-conditioned. In this section we will show properties about the location of orthogonal matrices. We start by observing that the eigenvalues of symmetric orthogonal matrices can only take the values ± 1. Indeed, all the eigenvalues of a symmetric matrix are real and because of the orthogonality they must have absolute values equal to one.

Theorem 3.1. *If Q is a symmetric orthogonal matrix with k negative eigenvalues then*

$$\cos(Q, I) = \frac{n-2k}{n}.$$

Proof. Based on the definition of the cosine between two matrices we have that

$$\cos(Q, I) = \frac{tr(Q)}{\|Q\|_F\|I\|_F} = \frac{(n-k)-k}{\sqrt{n}\sqrt{n}} = \frac{n-2k}{n}. \quad \square$$

Clearly k can be any integer between zero and n. The extreme cases correspond to the identity matrix I, and $-I$. Given k, we can define now the following surface

$$S(I, \frac{n-2k}{n}) = \left\{X \in S_n : \cos(X, I) = \frac{n-2k}{n}\right\}.$$

All these surfaces, for $0 \leqslant k \leqslant n$, are conical shells around I when $n \geqslant 2k$, and around $-I$ otherwise. Every orthogonal matrix is in one of these shells, and the only case when every matrix, in the shells, is orthogonal is again $n = 2$. A consequence of this observations is that the set of orthogonal matrices is in general disconnected, except for orthogonal matrices with the same inertia. It is worth pointing out that several properties of matrices around the identity matrix are a consequence only of the fact that the identity is an orthogonal matrix. Some of these properties can be generalized for arbitrary symmetric orthogonal matrices (see Theorem 4.2 for an extension to general matrices).

Theorem 3.2. *If $A \in S_n$ and the rank of A is k then for any symmetric orthogonal matrix Q we have that*

$$-\frac{\sqrt{k}}{\sqrt{n}} \leqslant \cos(Q, A) \leqslant \frac{\sqrt{k}}{\sqrt{n}}.$$

Proof. Since $A = \sum_{i=1}^{k} \lambda_i x_i x_i^t$, then

$$\cos(Q, A) = \frac{\langle Q, A\rangle_F}{\|Q\|_F\|A\|_F} = \frac{\sum_{i=1}^{k} \lambda_i \langle Q, x_i x_i^t\rangle_F}{\sqrt{n}\|A\|_F} = \frac{\sum_{i=1}^{k} \lambda_i x_i^t Q x_i}{\sqrt{n}\|A\|_F}.$$

Now we have that

$$|\cos(Q, A)| = |\frac{\sum_{i=1}^{k} \lambda_i x_i^t Q x_i}{\sqrt{n}\|A\|_F}| \leqslant \frac{\sum_{i=1}^{k} |\lambda_i||x_i^t Q x_i|}{\sqrt{n}\|A\|_F} \leqslant \frac{\|\lambda\|_1}{\sqrt{n}\|\lambda\|_2} \leqslant \frac{\sqrt{k}}{\sqrt{n}},$$

where λ denotes the vector with the k nonzero eigenvalues of A. In the last inequalities we have used first the fact that the Rayleigh quotient for an orthogonal matrix in absolute value is bounded by one; and second the standard inequality between the 1-norm and the 2-norm, which completes the proof. □

An interesting consequence is the following result.

Corollary 3.3. *Given Q a symmetric orthogonal matrix and x a vector in $\mathbb{R}^n$, then*

$$-\frac{1}{\sqrt{n}} \leqslant \cos(Q, xx^t) \leqslant \frac{1}{\sqrt{n}}.$$

If $Q = I$, the equality holds in the right inequality, and if $Q = -I$, the equality holds in the left inequality.

It is interesting to note how well located are rank one matrices with respect to orthogonal matrices. The angle corresponding to the cosine $\frac{1}{\sqrt{n}}$ is very large as n increases. Similar results were introduced by Tarazaga in [3,4] for the case of the identity matrix, which is obviously orthogonal. An easy consequence of Theorem 3.2 is the following.

Corollary 3.4. *If A is singular and Q is any symmetric orthogonal matrix then*

$$|\cos(A, Q)| \leqslant \frac{\sqrt{n-1}}{\sqrt{n}}.$$

The contrapositive is a more interesting result.

Corollary 3.5. *Given $A \in S_n$ and any symmetric orthogonal matrix Q, if $|\cos(A, Q)| > \frac{\sqrt{n-1}}{\sqrt{n}}$, then A is nonsingular, and A has the same inertia of Q.*

This result guarantees a circular cone around Q of nonsingular matrices similar to the cone introduces by Tarazaga in [4], around the identity.

Now we introduce a characterization of symmetric orthogonal matrices. First of all, for a given unit vector u, we will denote by H_u the Householder matrix

$$H_u = I - 2uu^t.$$

Recall that any symmetric orthogonal matrix Q has eigenvalues ± 1. If Q has k negative eigenvalues then it can be written as

$$Q = \sum_{i=1}^{k} -x_i x_i^t + \sum_{i=k+1}^{n} x_i x_i^t,$$

or modified as follows

$$Q = \sum_{i=1}^{n} x_i x_i^t - 2\sum_{i=1}^{k} x_i x_i^t = I - 2\sum_{i=1}^{k} x_i x_i^t.$$

Let us now multiply a couple of Householder matrices H_u and H_v under the condition that $u^t v = 0$

$$H_u H_v = (I - 2uu^t)(I - 2vv^t) = I - 2vv^t - 2uu^t - 4(uu^t)(vv^t) = I - 2vv^t - 2uu^t.$$

It is straightforward to generalize this property to the product of k Householder matrices to obtain

$$\prod_{i=1}^{k} H_{u_i} = I - 2\sum_{i=1}^{k} u_i u_i^t,$$

which yields the following result.

Theorem 3.6. *If Q is a symmetric orthogonal matrix different from the identity matrix, then*

$$Q = \prod_{i=1}^{k} H_{u_i},$$

where u_i are the eigenvectors corresponding to the negative eigenvalues.

To close this section, as a by product of the previous results, we now develop a new practical bound for the Frobenius condition number, $\mathcal{K}_F(A)$, of symmetric matrices, which is based on the location of orthogonal matrices described above and also on the theoretical bound given by (12). Since $\cos(A, Q_A)$ cannot be computed without knowing the spectral decomposition of A, we will estimate it by exploiting the location of the orthogonal matrices, in particular by using Theorem 3.1, and the fact that Q_A belongs to one of the conical shells $S(I, \frac{n-2k}{n})$ for some k. Notice that there exists a value of $k = 0, \ldots, n-1$ such that

$$\frac{n-2(k+1)}{n} \leqslant \cos(A, I) \leqslant \frac{n-2k}{n}.$$

Once this value of k has been identified, we choose the shell associated with the end point, of the interval above, closest to $\cos(A, I)$. If there is a tie any one of them can be chosen.

As a second step we need to find the matrix in that shell closest to A. For that we move from A along $\pm I$, as a direction, if the selected shell corresponds to the right or the left end point of the interval, respectively. Clearly, the angle between A and Q_A will be greater than or equal to the angle between A and the closest matrix on the identified shell.

In what follows we will assume, without any loss of generality, that $tr(A) \geqslant 0$. The explicit calculations are obtained by forcing only one of the following equalities:

$$\cos(A + \alpha I, I) = \frac{n-2k}{n},$$

or

$$\cos(A - \alpha I, I) = \frac{n-2(k+1)}{n}.$$

In order to compute α, we first expand $\cos^2(A + \alpha I, I)$ as follows

$$\cos^2(A + \alpha I, I) = \frac{< A + \alpha I, I >_F^2}{\|A + \alpha I\|_F^2 \, n} = \frac{(tr(A + \alpha I))^2}{tr((A + \alpha I)^2)n} = \frac{(tr(A))^2 + 2\alpha n \, tr(A) + \alpha^2 n^2}{(tr(A^2) + 2\alpha \, tr(A) + \alpha^2 n)n}.$$

Now, since $\cos^2(A + \alpha I, I) = (\frac{n-2k}{n})^2$, using the expansion above we obtain

$$n((tr(A))^2 + 2\alpha n \, tr(A) + \alpha^2 n^2) = (n-2k)^2 (tr(A^2) + 2\alpha \, tr(A) + \alpha^2 n).$$

This equation generates the following quadratic equation in α

$$n(n^2-(n-2k)^2)\alpha^2+2tr(A)(n^2-(n-2k)^2)\alpha+n\,(tr(A))^2-(n-2k)^2tr(A^2)=0,$$

and after simple manipulations we obtain

$$\alpha^2+\frac{2tr(A)}{n}\alpha+\frac{n\,(tr(A))^2-(n-2k)^2tr(A^2)}{n(n^2-(n-2k)^2)}=0,$$

whose solutions are

$$\alpha=-\frac{tr(A)}{n}\pm\sqrt{\left(\frac{tr(A)}{n}\right)^2-\frac{n\,(tr(A))^2-(n-2k)^2tr(A^2)}{n(n^2-(n-2k)^2)}}, \tag{13}$$

which is valid for $k\geqslant 1$. The extreme case $k=0$ (SPD) will be discussed at the end of this section. Since A forms an angle with the identity larger than the shell whose cosine with the identity is $\frac{n-2k}{n}$, we have that $\frac{tr(A)}{\|A\|_F\sqrt{n}}<\frac{n-2k}{n}$, and as we will now argue, this condition guarantees that α can be obtained as a positive value with the plus (+) sign in (13), recalling that $tr(A)\geqslant 0$. Indeed, from (13), to be able to obtain a positive α, we need

$$-\frac{n\,(tr(A))^2-(n-2k)^2tr(A^2)}{n(n^2-(n-2k)^2)}>0$$

or equivalently

$$(n-2k)^2tr(A^2)-n\,(tr(A))^2>0.$$

After some algebraic manipulations we have that

$$\begin{aligned}
n(tr(A))^2 &< (n-2k)^2tr(A^2)\\
\frac{n(tr(A))^2}{tr(A^2)} &< (n-2k)^2\\
\frac{(tr(A))^2}{tr(A^2)n} &< \frac{(n-2k)^2}{n^2},
\end{aligned}$$

which is precisely our angle condition, $\frac{tr(A)}{\|A\|_F\sqrt{n}}<\frac{n-2k}{n}$, squared. Summing up, for the case where $\cos(A,I)$ is closer to $\frac{n-2k}{n}$ than to $\frac{n-2(k+1)}{n}$, $k\geqslant 1$, and $tr(A)\geqslant 0$, it follows that

$$\cos(A,Q_A)\leqslant\cos(A,A+\alpha I),$$

and α is given by (13) with the plus (+) sign.

For the case where $\cos(A,I)$ is closer to $\frac{n-2(k+1)}{n}$ than to $\frac{n-2k}{n}$ we have that

$$\cos(A,Q_A)\leqslant\cos(A,A-\alpha I)$$

and, after similar algebraic manipulations, we obtain the value of α as

$$\alpha=\frac{tr(A)}{n}\pm\sqrt{\left(\frac{tr(A)}{n}\right)^2-\frac{n\,(tr(A))^2-(n-2(k+1))^2tr(A^2)}{n(n^2-(n-2(k+1))^2)}}, \tag{14}$$

which is valid for $k \leqslant n-2$. The extreme case $k = n-1$ will be discussed at the end of this section. To guarantee that α can be obtained as a positive value with the minus $(-)$ sign, in (14), we need to prove that the radicand of the second term is nonnegative, and also that

$$-\frac{n\,(tr(A))^2 - (n-2(k+1))^2 tr(A^2)}{n(n^2-(n-2(k+1))^2)} < 0$$

or equivalently

$$n\,(tr(A))^2 - (n-2(k+1))^2 tr(A^2) > 0. \tag{15}$$

Since A forms an angle with the identity smaller than the shell whose cosine with the identity is $\frac{n-2(k+1)}{n}$, we have that $\frac{tr(A)}{\|A\|_F\sqrt{n}} > \frac{n-2(k+1)}{n}$, which implies (15) by squaring in both sides. To prove that the radicand in (14) is nonnegative we need

$$\left(\frac{tr(A)}{n}\right)^2 \geqslant \frac{n\,(tr(A))^2 - (n-2(k+1))^2 tr(A^2)}{n(n^2-(n-2(k+1))^2)},$$

that, after algebraic manipulations, is equivalent to

$$(tr(A))^2 \leqslant n\,tr(A^2). \tag{16}$$

To establish (16) we recall that $tr(A) = \sum_{i=1}^n \lambda_i$, and so by Cauchy–Schwarz inequality

$$tr(A) = e^T\hat{\lambda} \leqslant \|e\|_2\,\|\hat{\lambda}\|_2 = \sqrt{n}\|\hat{\lambda}\|_2$$

where $\hat{\lambda} \in \mathbb{R}^n$ is the vector with entries λ_i, and e is the vector of all ones. By squaring both terms in the last inequality we obtain (16). Summing up, for the case where $\cos(A, I)$ is closer to $\frac{n-2(k+1)}{n}$ than to $\frac{n-2k}{n}$, $k \leqslant n-2$, and $tr(A) \geqslant 0$, it follows that α is given by (14) with the minus $(-)$ sign.

Taking all cases into account we obtain the following conclusive theorem.

Theorem 3.7. *Given $A \in S_n$, satisfying $\frac{n-2(k+1)}{n} \leqslant \cos(A, I) \leqslant \frac{n-2k}{n}$, where $1 \leqslant k \leqslant n-2$, and $tr(A) \geqslant 0$, it follows that*

$$\kappa_F(A) \geqslant \frac{n}{\cos(A, A \pm \alpha I)}, \tag{17}$$

where α is given by (13) with the plus $(+)$ sign, and using the plus $(+)$ sign in (17) if $\cos(A, I)$ is closer to $(n-2k)/n$; or α is given by (14) with the minus $(-)$ sign, and using the minus $(-)$ sign in (17), if $\cos(A, I)$ is closer to $(n-2(k+1))/n$.

Notice that the new bound (17) only requires the value of k, n, $tr(A)$, and $\|A\|_F$. Note also that since $\kappa_F(A) = \kappa_F(-A)$, then when $tr(A) < 0$ we can apply Theorem 3.7 on the matrix $-A$ and obtain the same bound for $\kappa_F(A)$.

Two practical comments are in order. The first one is related to matrices that are close to the extreme conical shell that corresponds to I $(k = 0)$ or $-I$ $(k = n-1)$. In these cases we simply compute (trivially) the angle between the matrix A and I or $-I$. Second if the inertia of the matrix A is known then we know exactly the conical shell where Q_A is located, and then we compute the angle between A and the corresponding shell. This bound will be sharper than the one given by the nearest shell, unless they coincide.

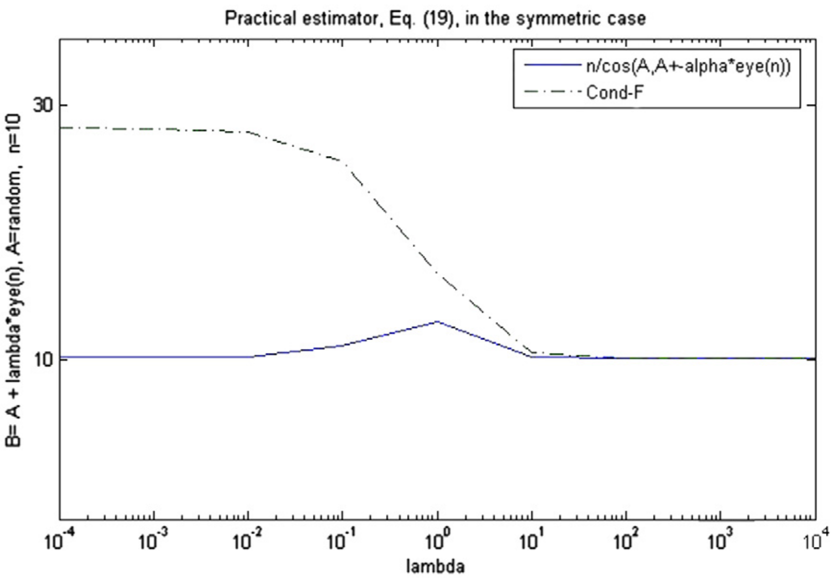

Fig. 1. Behavior of the condition number bound given by (17) for symmetric matrices of the form $B = A + \lambda I$, where A is a 10×10 random symmetric matrix and $10^{-4} \leqslant \lambda \leqslant 10^4$.

We now present a numerical experiment to evaluate the accuracy of the new bound (17) for indefinite symmetric matrices. In Fig. 1 we compare, in a `loglog` plot, the value of $\kappa_F(A)$ with (17) for a family of matrices B: $B = A + \lambda I$ where A is a random symmetric matrix (built with the `rand(n)` function in MATLAB) of dimension 10×10, and $10^{-4} \leqslant \lambda \leqslant 10^4$. This test matrices are chosen to monitor the quality of the bound while moving from a matrix ($\lambda = 10^{-4}$) with approximately half the eigenvalues on the positive side of the real axis, and half on the negative side, towards the identity matrix ($\lambda = 10^4$). We observe, in Fig. 1, that the quality of the bound improves when the condition number is reduced, and tends to the exact condition number when close to the identity matrix. We also note that since (17) uses different shells to approximate $\kappa_F(A)$, as a function of λ, the estimating curve is not smooth. A quite similar behavior, to the one reported in Fig. 1, is observed for different choices of A and different values of n.

4. The general case

Let us now consider the general (not necessarily symmetric) nonsingular case. Some of the basic results described in Sections 2 and 3 for symmetric matrices can be extended. It is straightforward from the definition of $\kappa_F(A)$ that

$$< A^T, A^{-1} >_F = tr(AA^{-1}) = tr(I) = n,$$

and using the Cauchy-Schwarz inequality we obtain

$$n =< A^T, A^{-1} >_F \leqslant \|A^T\|_F \|A^{-1}\|_F = \|A\|_F \|A^{-1}\|_F = \kappa_F(A). \tag{18}$$

Using now the usual definition of cosine of the angle between two matrices, it follows that

$$\cos(A^T, A^{-1}) = \frac{< A^T, A^{-1} >_F}{\|A^T\|_F \|A^{-1}\|_F} = \frac{n}{\|A\|_F \|A^{-1}\|_F} = \frac{n}{\kappa_F(A)}. \tag{19}$$

We observe that $\kappa_F(A)$ is inversely proportional to the cosine of the angle between A^T and A^{-1}, that can be viewed as a measure of orthogonality, since A is orthogonal if and only if $A^T = A^{-1}$, in which case the cosine equals 1. From (19) we also observe that $\cos(A^T, A^{-1}) > 0$, and so

$$0 < \cos(A^T, A^{-1}) \leqslant 1.$$

Moreover, we can also consider the Singular Value Decomposition (SVD) for a general nonsingular matrix A:

$$A = U\Sigma V^T.$$

Using the SVD, we have that $A^{-1} = V\Sigma^{-1}U^T$, and then if we set $\sigma = (\sigma_1, \ldots, \sigma_n)^t$ and $\widehat{\sigma} = (\frac{1}{\sigma_1}, \ldots, \frac{1}{\sigma_n})^t$ we have that

$$n = < A^T, A^{-1} >_F = tr(AA^{-1}) = tr(U\Sigma V^T V\Sigma^{-1}U^T) = tr(\Sigma\Sigma^{-1}) = \sigma^T\widehat{\sigma}.$$

Using, once again, the Cauchy-Schwarz inequality but now with the SVD of A, it follows that

$$n = \sigma^T\widehat{\sigma} \leqslant \|\sigma\|_2\|\widehat{\sigma}\|_2.$$

Equality holds if and only if σ and $\widehat{\sigma}$ share the same direction. Since σ and $\widehat{\sigma}$ have both positive entries, this happens if and only if σ is a constant vector, and that constant must be 1 to be aligned with $\widehat{\sigma}$. This can be summarized in the following well-known result.

Lemma 4.1. *Given a nonsingular matrix A, $\kappa_F(A) = n$ if and only if A is orthogonal or a multiple of an orthogonal matrix.*

This last result justifies the previous claim that $\kappa_F(A)$ can be viewed as a measure of orthogonality. Moreover, similar to the conclusion drawn at the end of Section 3, in the general case the condition number associated with the 2-norm is also related to how close A is to the set of singular matrices.

Theorem 4.1. *Given a nonsingular matrix A, we have*

$$\kappa_2(A) \leqslant \sqrt{\frac{1}{1 - \cos^2(A, \widehat{A})}}.$$

Proof. Since $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_n > 0$, then the closest singular matrix to A is given by

$$\widehat{A} = \sum_{i=1}^{n-1} \sigma_i u_i v_i^t,$$

where u_i and v_i are the columns of U and V respectively. Clearly, $A - \widehat{A}$ is a rank one matrix, and so

$$\sin(A, \widehat{A}) \equiv \frac{\|A - \widehat{A}\|_F}{\|A\|_F} = \frac{\sigma_n}{\|A\|_F} = \frac{1}{\|A^{-1}\|_2 \, \|A\|_F}.$$

Now, using that $\|A\|_2 \leqslant \|A\|_F$, we obtain

$$1 - \cos^2(A, \widehat{A}) = \sin^2(A, \widehat{A}) = \frac{1}{(\|A^{-1}\|_2 \, \|A\|_F)^2} \leqslant \frac{1}{(\|A^{-1}\|_2 \, \|A\|_2)^2},$$

which implies

$$\kappa_2^2(A) \leqslant \frac{1}{1-\cos^2(A,\widehat{A})}. \qquad \square$$

Finally, Theorem 3.2 can also be extended to general rank deficient matrices.

Theorem 4.2. *If the rank of A is k then for any orthogonal matrix Q we have that*

$$-\frac{\sqrt{k}}{\sqrt{n}} \leqslant \cos(Q,A) \leqslant \frac{\sqrt{k}}{\sqrt{n}}.$$

Proof. Since $A = \sum_{i=1}^{k} \sigma_i u_i v_i^t$, then

$$\cos(Q,A) = \frac{\langle Q,A\rangle_F}{\|Q\|_F\|A\|_F} = \frac{\sum_{i=1}^{k} \sigma_i \langle Q, u_i v_i^t\rangle_F}{\sqrt{n}\|A\|_F}.$$

Now we have that

$$|\cos(Q,A)| = \frac{\sum_{i=1}^{k} \sigma_i |u_i^t Q v_i|}{\sqrt{n}\|A\|_F} \leqslant \frac{\sum_{i=1}^{k} \sigma_i}{\sqrt{n}\|A\|_F} \leqslant \frac{\|\sigma\|_1}{\sqrt{n}\|\sigma\|_2} \leqslant \frac{\sqrt{k}}{\sqrt{n}}.$$

In the first inequalities we have used that Q is orthogonal and u_i and v_i are unitary vectors, and hence for all i, $|u_i^t Q v_i| \leqslant \|u_i\|_2\|Qv_i\|_2 = 1$. For the last inequality we have used the standard inequality between the 1-norm and the 2-norm, which completes the proof. $\square$

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