Bounds on the Diagonal Elements of a Unitary Matrix

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ABSTRACT

It was shown by A. Horn that the diagonal elements of a unitary $n \times n$ matrix satisfy a set of linear inequalities (Theorem I). We give a simple proof of this result, and we show that the diagonal elements satisfy additional linear inequalities (Theorem II) if the matrix is also symmetric.

DEFINITIONS AND NOTATION

Let $A$ be a complex $n \times n$ matrix. By $A^T$ and $A^\dagger$ we mean the transpose and conjugate-transpose of $A$. A matrix $A$ is unitary if $A^\dagger A = AA^\dagger = I$, and it is symmetric if $A^T = A$. The set of all unitary $n \times n$ matrices is denoted by $\mathcal{U}_n$, and the subset of $\mathcal{U}_n$ of symmetric matrices is denoted by $S_n$. The real Euclidean space of dimension $n$ is denoted by $E_n$.

UNITARY MATRICES

The elements of a unitary $n \times n$ matrix $U = (U_{ij})$ all have norm less than or equal to 1. This means that the $n$-vector $\eta \equiv (|U_{11}|, |U_{22}|, \ldots, |U_{nn}|)$ formed from the diagonal elements of $U$ lies inside or on the unit cube

$$K_n \equiv \{ r \in E_n | 0 \leq r_i \leq 1, i = 1, \ldots, n \}.$$
We shall consider $\eta(U)$ as a mapping of the set $\mathcal{U}_n$ into $K_n$. The range of $\eta(U)$ was first determined by A. Horn [1], who obtained the following result:

**Theorem I.** For $n \geq 2$ a complex vector $(d_1, \ldots, d_n)$ is the diagonal of a unitary matrix if and only if the vector $\eta = (|d_1|, \ldots, |d_n|)$ satisfies the conditions:

1. $\eta \in K_n$,
2. $\sum_{i=1}^{n} \eta_i - 2 \eta_l \leq n - 2 \ (l = 1, \ldots, n)$.

It follows from this theorem that the range of $\eta(U)$ is a convex polyhedron. (A convex polyhedron [2] is the convex hull of a finite number of points in $E_n$. In our case the polyhedron appears as the intersection of a finite number of closed half spaces.) For $n = 2$ the conditions (a) and (b) give $0 < \eta_1 = \eta_2 < 1$. For $n = 3$ we obtain the polyhedron by chopping off three of the corners of the cube $K_3$ (see Fig. 2 of Ref. [3]).

We shall now give a simple proof of the necessity of the conditions (a) and (b) of Theorem I. We refer to Ref. [1] for the proof of the sufficiency (see also Ref. [4]).

**Proof.** Let $U$ be a given element in $\mathcal{U}_n$. Since $\eta(U) \in K_n$ we need only show that $\eta(U)$ satisfies the conditions (b). We write the diagonal elements of $U$ as $U_{kk} = \eta_k \exp(2i\delta_k)$. Let $l$ be a given integer such that $1 \leq l \leq n$. By multiplying the $l$th column in $U$ by $- \exp(\delta_l)$ and the $i$th column by $\exp(-2i\delta_i)$ for all $i$ different from $l$ we obtain a unitary matrix $\hat{U}$ with diagonal elements $\hat{U}_{ii} = \eta_i$ for $i \neq l$ and $\hat{U}_{ll} = -\eta_l$.

The eigenvalues of $\hat{U}$ lie on the unit circle. We denote the eigenvalues by $\exp(i\omega_k), \ (k = 1, \ldots, n)$ and order them such that $0 < \omega_1 \leq \cdots \leq \omega_n < 2\pi$. The convex hull of the eigenvalues is the so-called numerical range $W(\hat{U})$ of $\hat{U}$. By using the eigenvector basis it follows [5] that

$$W(\hat{U}) = \{(x, \hat{U}x) | \|x\| = 1\},$$

so $W(\hat{U})$ contains the diagonal elements of $\hat{U}$. Let $\beta$ be the smallest real number in $W(\hat{U})$. It is less than or equal to $-\eta_l$ and it lies on a boundary line of $W(\hat{U})$ joining two adjacent eigenvalues $\exp(i\omega_p)$ and $\exp(i\omega_{p+1})$. Thus there exists an $\alpha (0 < \alpha \leq 1)$ such that

$$\beta = \alpha \exp(i\omega_p) + (1-\alpha)\exp(i\omega_{p+1}).$$

By multiplying Eq. (2) by $\exp(-i\omega_p) + \exp(-i\omega_{p+1})$ and taking the real part we find

$$\beta (\cos \omega_p + \cos \omega_{p+1}) = 1 + \cos(\omega_{p+1} - \omega_p).$$
Thus since $\beta \leq -\eta \leq 0$, we have $\cos \omega_p + \cos \omega_{p+1} \leq 0$ and therefore

$$\text{tr} \hat{U} = \sum_{i=1}^{n} \eta_i - 2\eta_l = \sum_{i=1}^{n} \cos \omega_i$$

$$\leq \sum_{i=1}^{n} \cos \omega_i \leq n - 2,$$

which is condition (b) of Theorem I. This completes the proof.

UNITARY, SYMMETRIC MATRICES

If we restrict $\eta(U)$ to the set $S_n$ of symmetric unitary matrices, the range of $\eta(U)$ is again imbedded in a convex polyhedron. It was shown [3] by one of the authors that the range of $\eta(U)$ for $U \in S_3$ is determined by the conditions

$$\sum_{i=1}^{3} \eta_i - 2\eta_l < 1 \quad (l=1,2,3), \quad (3a)$$

$$\sum_{i=1}^{3} \eta_i > 1. \quad (3b)$$

The condition (3a) is condition (b) of Theorem I for $n=3$, but we have now the extra condition (3b). The polyhedron defined by (3a) and (3b) is a regular tetrahedron (see Fig. 2 of Ref. [3]). The conditions (3a), (3b) imply that $\eta \in K_3$, so we need not impose condition (a) of Theorem I.

The result (3a), (3b) can be generalized to arbitrary $n \geq 3$. We introduce [1] the symbol $S^m$ for the set of all $m$-term sequences $\sigma$ of integers for which $1 \leq \sigma_1 < \cdots < \sigma_m \leq n$. Also $S^0$ is the empty set. The general result can now be stated as follows:

**Theorem II.** If $n \geq 3$ and $U \in S_n$, then $\eta(U)$ satisfies the conditions:

(i) $\eta(U) \in K_n$,

(ii) $\sum_{i=1}^{n} \eta_i - 2\eta_l \leq n - 2 \quad (l=1,\ldots,n)$,

(iii) $\sum_{i=1}^{n} \eta_i - 2 \sum_{i=1}^{n-3} \eta_{\sigma_i} \geq 4 - n, \quad \sigma \in S^n - 3$. 
Conditions (i), (ii) and (iii) define a convex polyhedron that contains the range of $\eta(U)$ for $U \in \mathbb{S}_n$. We have only proved [3] that $\eta(U)$ maps onto the polyhedron for $n = 3$, but we believe that this is the case also for $n > 3$.

In the case of $n = 4$, conditions (ii) and (iii) can be written in the more transparent form

$$0 \leq \sum_{i=1}^{4} \eta_i - 2\eta_i \leq 2, \quad (l = 1, \ldots, 4).$$

The conditions (ii) and (iii) define $n$ and $(\begin{smallmatrix} n \\ 3 \end{smallmatrix})$ hyperplanes in $E_n$ respectively. Let $H_1$ and $H_2$ be any two of these hyperplanes. The set $H_1 \cap H_2 \cap K_n$ turns out to be either the empty set or a line segment on the boundary of $K_n$, i.e., $H_1 \cap H_2 \cap K_n$ contains no interior points of $K_n$. The conditions (ii) and (iii) do not imply (i) except for $n = 3$.

Condition (iii) shows that $\eta(U) \neq 0$ for all $U$ in $\mathbb{S}_3$. However, this only holds for $n = 3$. For any $n > 2$ and $n \neq 3$ there exists a $U_0 \in \mathbb{S}_n$ such that $\eta(U_0) = 0$. Thus for even $n$ we can take $U_0$ to be the $n/2$-term direct sum $\rho \oplus \rho \oplus \cdots \oplus \rho$, where $\rho$ is the matrix

$$\rho = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{4}$$

For $n = 5$ a possible $U_0$ is the matrix

$$\frac{1}{2} \begin{bmatrix} 0 & 1 & Z & Z^{-1} & 1 \\ 1 & 0 & Z^{-1} & Z & 1 \\ Z & Z^{-1} & 0 & 1 & 1 \\ Z^{-1} & Z & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}, \tag{5}$$

with

$$Z = \frac{1}{2} (1 + \sqrt{3} i),$$

and for odd $n$ greater than 5 we can take $U_0$ to be the direct sum of (5) and a $U_0$ in $\mathbb{S}_{n-5}$. As a consequence of this there is no non-trivial lower bound on $\sum_{i=1}^{n} \eta_i$ for $n \neq 3$.

Before going to the proof of Theorem II we shall briefly mention a physical application of the theorem. The $S$-matrix describing a system of two-body reactions $A_i + B_i \rightarrow A_j + B_j$ $(i, j = 1, \ldots, n)$ for fixed energy and angular momentum is a unitary symmetric matrix. The norm squared of the
matrix elements gives the transition rates of the reactions. Therefore bounds of the type (ii) and (iii) of Theorem II can give useful [3] restrictions on the transition rates.

PROOF OF THEOREM II

The basic idea in our proof of Theorem II is taken from Horn's proof of Theorem I.

Conditions (i) and (ii) of Theorem II follow from conditions (a) and (b) of Theorem I, so we only have to prove condition (iii). For \( n > 4 \) it is clearly sufficient to prove (iii) for \( \sigma = (4, 5, \ldots, n) \). All the other inequalities follow by rearrangement of the basis vectors.

Let \( n > 3 \) be given and let \( r \) be the number defined by

\[
U \in S_n \left\{ \sum_{i=1}^{n} \varepsilon_i |U_n| \right\},
\]

where \( \varepsilon_i = 1 \) for \( i < 3 \), and \( \varepsilon_i = -1 \) for \( i > 3 \). The condition (iii) is equivalent to \( r > 4 - n \). We shall show that in fact \( r = 4 - n \). Clearly

\[
r > 3 - n.
\]

We can easily find a \( U \in S_n \) for which the parenthesis on the right of (6) is \( 4 - n \). Take for example the direct sum \( \rho \oplus I_1 \) for \( n = 3 \) and \( \rho \oplus \rho \oplus I_{n-4} \) for \( n > 3 \), where \( I_k \) is the \( k \)-dimensional unit matrix and \( \rho \) is given by (4). Hence

\[
r \leq 4 - n.
\]

We shall show that there exists a real matrix \( R \) in \( S_n \) for which

\[
r = \text{tr} R.
\]

A real matrix in \( S_n \) has eigenvalues \( \pm 1 \), and therefore \( \text{tr} R \) can only take on the values \( -n, 2-n, 4-n, \ldots, n-2, n \). By (7), (8), and (9) it then follows that \( r = 4 - n \), which is what we want to prove.

To obtain \( R \) we use a matrix \( S \) in \( S_n \) for which

\[
r = \sum_{i=1}^{n} \varepsilon_i |S_i|.
\]
The existence of such a matrix $S$ follows from the fact that $S_n$ is compact and $\eta(U)$ is continuous in the standard topology for the group $\mathbb{U}_n$. Let $S_{kk} = \eta_k \exp(2i\delta_k)$ be the diagonal elements of $S$. We form a new matrix $\hat{S}$ by multiplying the $k$th row and column of $S$ by $\exp(-i\delta_k)$ for $k \leq 3$ and by $i\exp(-i\delta_k)$ for $k > 3$. The matrix $\hat{S}$ has then the diagonal elements $\hat{S}_{kk} = \eta_k$, so $r = \text{tr} \hat{S}$. Also $\hat{S} \in S_n$.

If for $n > 3$ we have $\eta_i = 0$ for some $i > 3$, then $r > 4 - n$, which implies condition (iii). We can therefore assume that $\eta_i \neq 0$ for $n > 3$ and $i > 3$.

Let $V^{pq}$ ($p \leq n, q \leq n, p \neq q$) be the matrix in $S_n$ given by

\[
(V^{pq})_{ij} = \delta_{ij} \quad \text{for} \quad i \neq p, q \text{ or } j \neq p, q.
\]

\[
(V^{pq})_{pp} = \cos \theta e^{2i\alpha}, \quad (V^{pq})_{qq} = \cos \theta,
\]

\[
(V^{pq})_{pq} = (V^{pq})_{qp} = i \sin \theta e^{i\alpha}.
\]

The matrix $W^{pq} = V^{pq} \hat{S} V^{pq}$ belongs to $S_n$, and $(W^{pq})_{ii} = \varepsilon_i \eta_i$ for $i \neq p, q$. From the definition (6) of $r$ and by the use of (10) it follows that

\[
\varepsilon_p |(W^{pq})_{pp}| + \varepsilon_q |(W^{pq})_{qq}| \gtrless \varepsilon_p \eta_p + \varepsilon_q \eta_q.
\]

This inequality holds for arbitrary $\alpha$ and $\theta$. For $\alpha = 0$ and to first order in $\theta$ it gives

\[
\varepsilon_p |\varepsilon_p \eta_p + 2i\theta \hat{S}_{pq}| + \varepsilon_q |\varepsilon_q \eta_q + 2i\theta \hat{S}_{pq}| \gtrless \varepsilon_p \eta_p + \varepsilon_q \eta_q,
\]

which for $\eta_p \neq 0$ and $\eta_q \neq 0$ reduces to

\[
\theta \text{Im} \hat{S}_{pq} \leq 0.
\]

Since the sign of $\theta$ is arbitrary, (12) implies that $\text{Im} \hat{S}_{pq} = 0$. Therefore, if $\eta_i \neq 0$ for all $i$, we have that $\hat{S}$ is real and we can use $R = \hat{S}$.

Consider now the case where $\eta_p = 0$ ($p \leq 3$) but $\eta_q \neq 0$. Then

\[
|\langle W^{pq} \rangle_{pp}| = |\varepsilon_q \hat{S}_{pq} i e^{i\alpha} \sin 2\theta - \eta_p \sin^2 \theta|,
\]

\[
|\langle W^{pq} \rangle_{qq}| = |\varepsilon_q \hat{S}_{pq} i e^{i\alpha} \sin 2\theta + \eta_q \cos^2 \theta|.
\]
We choose $\alpha$ such that $\varepsilon_Y \hat{S}_{pq} e^{i\alpha}$ is real and positive, and we choose $\theta$ ($0 < \theta < \pi / 2$) such that

$$2|\hat{S}_{pq}| \cot \theta < \eta_q \quad \text{if} \quad q < 3,$$

(13a)

and

$$2|\hat{S}_{pq}| \cot \theta > \eta_q \quad \text{if} \quad q > 3.$$  

(13b)

We can only impose condition (13b) if $\hat{S}_{pq} \neq 0$. If the conditions (13a) or (13b) are fulfilled, we have $(W^{pq})_{pp} \neq 0$ and $(W^{pq})_{qq} \neq 0$, and Eq. (10) is satisfied with $S$ replaced by $W^{pq}$. This means that if $\eta_q \neq 0$ for some $q$ ($q < 3$), we can by successive transformations construct a new matrix $\hat{W}$ with non-zero diagonal elements and such that $r = \text{tr} \hat{W}$. The problem is then reduced to the case considered above.

For $n = 3$ it is a simple exercise to see that not all $\eta_i$ can be zero. (It is only at this point that the restriction to $S_n$ is essential.) For $n > 3$ we may have $\eta_i = 0$ for $i = 1, 2, 3$. If also $\hat{S}_{ij} = 0$ for all $i < 3$ and $q > 3$, this implies that the principal submatrix $(\hat{S}_{ij})$ with $i, j = 1, 2, 3$ is a matrix in $S_3$ with all diagonal elements zero. Since no such matrix exists, we have $\hat{S}_{ij} \neq 0$ for some $i < 3$ and $q > 3$. We can then impose the condition (13b) and construct the corresponding matrix $W^{pq}$ with $(W^{pq})_{ij} \neq 0$. Thereby the problem is reduced to our previous case. This concludes the proof of the theorem.

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REFERENCES


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