Chapter 4

Unitary Matrices

4.1 Basics

This chapter considers a very important class of matrices that are quite useful in proving a number of structure theorems about all matrices. Called *unitary* matrices, they comprise a class of matrices that have the remarkable properties that as transformations they preserve length, and preserve the angle between vectors. This is of course true for the identity transformation. Therefore it is helpful to regard unitary matrices as "generalized identities," though we will see that they form quite a large class. An important example of these matrices, the rotations, have already been considered. In this chapter, the underlying field is usually $\mathbb{C}$, the underlying vector space is $\mathbb{C}_n$, and almost without exception the underlying norm is $\|\cdot\|_2$. We begin by recalling a few important facts.

Recall that a set of vectors $x_1, \ldots, x_k \in \mathbb{C}_n$ is called **orthogonal** if $x_j^* x_m = \langle x_m, x_j \rangle = 0$ for $1 \leq j \neq m \leq k$. The set is **orthonormal** if

$$x_j^* x_m = \delta_{mj} = \begin{cases} 1 & j = m \\ 0 & j \neq m. \end{cases}$$

An orthogonal set of vectors can be made orthonormal by scaling:

$$x_j \longrightarrow \frac{1}{(x_j^* x_j)^{1/2}} x_j.$$

Theorem 4.1.1. *Every set of orthonormal vectors is linearly independent.*

Proof. The proof is routine, using a common technique. Suppose $S = \{x_j\}_{j=1}^k$ is orthonormal and linearly dependent. Then, without loss of generality (by relabeling if needed), we can assume

$$u_k = \sum_{j=1}^{k-1} c_j u_j.$$

Compute $u_k^* u_k$ as

$$\begin{aligned}1 = u_k^* u_k &= u_k^* \left(\sum_{j=1}^{k-1} c_j u_j \right) \\ &= \sum_{j=1}^{k-1} c_j u_k^* u_j = 0.\end{aligned}$$

This contradiction proves the result. □

Corollary 4.1.1. *If $S = \{u_1 \dots u_k\} \subset \mathbb{C}_n$ is orthonormal then $k \le n$.*

Corollary 4.1.2. *Every k-dimensional subspace of $\mathbb{C}_n$ has an orthonormal basis.*

Proof. Apply the Gram–Schmidt process to any basis to orthonormalize it. □

Definition 4.1.1. A matrix $U \in M_n$ is said to be **unitary** if $U^*U = I$. [If $U \in M_n(R)$ and $U^TU = I$, then U is called real **orthogonal**.]

Note: A linear transformation $T\colon\ \mathbb{C}_n \to \mathbb{C}_n$ is called an **isometry** if $\|Tx\| = \|x\|$ for all $x \in \mathbb{C}_n$.

Proposition 4.1.1. *Suppose that $U \in M_n$ is unitary. (i) Then the columns of U form an orthonormal basis of $\mathbb{C}_n$, or R_n , if U is real. (ii) The spectrum $\sigma(u) \subset \{z \mid |z| = 1\}$. (iii) $|\det U| = 1$.*

Proof. The proof of (i) is a consequence of the definition. To prove (ii), first denote the columns of U by u_i, $i = 1, \dots, n$. If λ is an eigenvalue of U with pertaining eigenvector x, then $\|Ux\| = \|\sum x_i u_i\| = (\sum |x_i|^2)^{1/2} = \|x\| = |\lambda|\|x\|$. Hence $|\lambda| = 1$. Finally, (iii) follows directly because $\det U = \prod \lambda_i$. Thus $|\det U| = \prod |\lambda_i| = 1$. □

This important result is just one of many equivalent results about unitary matrices. In the result below, a number of equivalences are established.

Theorem 4.1.2. *Let $U \in M_n$. The following are equivalent.*

(a) U is unitary.

(b) U is nonsingular and $U^* = U^{-1}$.

(c) $UU^* = I$.

(d) U^* is unitary.

(e) The columns of U form an orthonormal set.

(f) The rows of U form an orthonormal set.

(g) U is an isometry.

(h) U carries every set of orthonormal vectors to a set of orthonormal vectors.

Proof. (a) $\Rightarrow$ (b) follows from the definition of unitary **and** the fact that the inverse is unique.
(b) $\Rightarrow$ (c) follows from the fact that a left inverse is also a right inverse.
(a) $\Rightarrow$ (d) $UU^* = (U^*)^*U^* = I$.
(d) $\Rightarrow$ (e) (e) $\equiv$ (b) $\Rightarrow$ $u_j^* u_k \delta_{jk}$, where $u_1 \dots u_n$ are the columns of U. Similarly (b) $\Rightarrow$ (e).
(d) $\equiv$ (f) same reasoning.
(e) $\Rightarrow$ (g) We know the columns of U are orthonormal. Denoting the columns by $u_1 \dots u_n$, we have

$$Ux = \sum_1^n x_i u_i$$

where $x = (x_1, \dots, x_n)^T$. It is an easy matter to see that

$$\|Ux\|^2 = \sum_1^n |x_i|^2 = \|x\|^2.$$

(g) $\Rightarrow$ (e). Consider $x = e_j$. Then $Ux = u_j$. Hence $1 = \|e_j\| = \|Ue_j\| = \|u_j\|$. The columns of U have norm one. Now let $x = \alpha e_i + \beta e_j$ be chosen such that $\|x\| = \|\alpha e_i + \beta e_j\| = \sqrt{|\alpha|^2 + |\beta|^2} = 1$. Then

$$\begin{aligned} 1 &= \|Ux\|^2 \\ &= \|U(\alpha e_i + \beta e_j)\|^2 \\ &= \langle U(\alpha e_i + \beta e_j), U(\alpha e_i + \beta e_j)\rangle \\ &= |\alpha|^2 \langle Ue_i, Ue_i\rangle + |\beta|^2 \langle Ue_j, Ue_j\rangle + \alpha\bar{\beta}\langle Ue_i, Ue_j\rangle + \bar{\alpha}\beta\langle Ue_j, Ue_i\rangle \\ &= |\alpha|^2 \langle u_i, u_i\rangle + |\beta|^2 \langle u_j, u_j\rangle + \alpha\bar{\beta}\langle u_i, u_j\rangle + \bar{\alpha}\beta\langle u_j, u_i\rangle \\ &= |\alpha|^2 + |\beta|^2 + 2\Re\left(\alpha\bar{\beta}\langle u_i, u_j\rangle\right) \\ &= 1 + 2\Re\left(\alpha\bar{\beta}\langle u_i, u_j\rangle\right) \end{aligned}$$

Thus $\Re\left(\alpha\bar{\beta}\langle u_i, u_j\rangle\right) = 0$. Now suppose $\langle u_i, u_j\rangle = s + it$. Selecting $\alpha = \beta = \frac{1}{\sqrt{2}}$ we obtain that $\Re\langle u_i, u_j\rangle = 0$, and selecting $\alpha = i\beta = \frac{1}{\sqrt{2}}$ we obtain that $\Im\langle u_i, u_j\rangle = 0$. Thus $\langle u_i, u_j\rangle = 0$. Since the coordinates i and j are arbitrary, it follows that the columns of U are orthogonal.
(g) $\Rightarrow$ (h) Suppose $\{v_1, \dots, v_n\}$ is orthogonal. For any two of them $\|U(v_j + v_k)\|^2 = \|v_j + v_k\|^2$. Hence $\langle Uv_j, Uv_k\rangle = 0$.
(h)$\Rightarrow$ (e) The orthormal set of the standard unit vectors e_j, $j = 1, \dots, n$ is carried to the columns of U. That is $Ue_j = u_j$, the j^{th} column of U. Therefore the columns of U are orthonormal. □

Corollary 4.1.3. *If $U \in M_n(\mathbb{C})$ is unitary, then the transformation defined by U preserves angles.*

Proof. We have for any vectors x, $y \in \mathbb{C}_n$ that the angle θ is completely determined from the inner product via $\cos\theta = \frac{\langle x,y\rangle}{\|x\|\|y\|}$. Since U is unitary (and thus an isometry) it follows that

$$\langle Ux, Uy\rangle = \langle U^*Ux, y\rangle = \langle x, y\rangle$$

This proves the result. □

Example 4.1.1. Let $T(\theta) = \left[\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right]$ where θ is any real. Then $T(\theta)$ is *real* orthogonal.

Proposition 4.1.1. *If $U \in M_2(R)$ is real orthogonal, then U has the form $T(\theta)$ for some θ or the form*

$$U = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} T(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}$$

Finally, we can easily establish the diagonalizability of unitary matrices.

Theorem 4.1.3. *If $U \in M_n$ is unitary, then it is diagonalizable.*

Proof. To prove this we need to revisit the proof of Theorem 3.5.2. As before, select the first vector to be a normalized eigenvector u_1 pertaining to λ_1. Now choose the remaining vectors to be orthonormal to u_1. This makes the matrix P_1 with all these vectors as columns a unitary matrix. Therefore $B_1 = P^{-1}UP$ is also unitary. However it has the form

$$B_1 = \begin{bmatrix} \lambda & \alpha_1 & \dots & \alpha_{n-1} \\ 0 & & & \\ \vdots & & A_2 & \\ 0 & & & \end{bmatrix} \quad \text{where } \mathrm{A}_2 \text{ is } (\mathrm{n}-1) \times (\mathrm{n}-1)$$

Since it is unitary, it must have orthogonal columns by Theorem 4.1.2. It follows then that $\alpha_1 = \alpha_2 = \cdots = \alpha_n = 0$ and

$$B_1 = \begin{bmatrix} \lambda & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & A_2 & \\ 0 & & & \end{bmatrix}$$

At this point one may apply and inductive hypothesis to conclude that A_2 is similar to a diagonal matrix. Thus by the manner in which the full similarity was constructed, we see that A must also be similar to a diagonal matrix. □

Corollary 4.1.1. *Let $U \in M_n$ be unitary. Then*

(i) Then U has a set of n orthogonal eigenvectors.

(ii) Let $\{\lambda_1, \dots, \lambda_n\}$ and $\{v_1, \dots, v_n\}$ denote respectively the eigenvalues and their pertaining orthonormal eigenvectors of U. Then U has the representation as the sum of rank one matrices given by

$$U = \sum_{j=1}^{n} \lambda_j v_j v_j^T$$

This representation is often called the **spectral respresentation** *or spectral decomposition of U.*

4.1.1 Groups of matrices

Invertible and unitary matrices have a fundamental structure that makes possible a great many general statements about their nature and the way they act upon vectors other vectors matrices. A group is a set with a mathematical operation, product, that obeys some minimal set of properties so as to resemble the nonzero numbers under multiplication.

Definition 4.1.2. A **group** G is a set with a binary operation $G \times G \to G$ which assigns to every pair a, b of elements of G a unique element ab in G. The operation, called the **product**, satisfies four properties:

1. Closure. If $a,\, b \in G$, then $ab \in G$.

2. Associativity. If $a,\, b,\, c \in G$, then $a(bc) = (ab)c$.

3. Identity. There exists an element $e \in G$ such that $ae = ea = a$ for every $a \in G$. e is called the *identity* of G.

4. Inverse. For each $a \in G$, there exists an element $\hat{a} \in G$ such that $a\hat{a} = \hat{a}a = e$. $\hat{a}$ is called the inverse of a and is often denoted by a^{-1}.

A subset of G that is itself a group under the same product is called a **subgroup** of G.

It may be interesting to note that removal of any of the properties 2-4 leads to other categories of sets that have interest, and in fact applications, in their own right. Moreover, many groups have additional properties such as commutativity, i.e. $ab = ba$ for all $a,\, b \in G$. Below are a few examples of matrix groups. Note matrix addition is not involved in these definitions.

Example 4.1.2. As usual M_n is the vector space of $n \times n$ matrices. The product in these examples is the usual matrix product.

- The group $GL(n, F)$ is the group of invertible $n \times n$ matrices. This is the so-called **general linear** group. The subset of M_n of invertible lower (resp. upper) triangular matrices is a subgroup of $GL(n, F)$.

- The **unitary** group U_n of unitary matrices in $M_n(\mathbb{C})$.

- The **orthogonal** group O_n orthogonal matrices in $M_n(R)$. The subgroup of O_n denoted by SO_n consists of orthogonal matrices with determinant 1.

Because element inverses are required, it is obvious that the only subsets of invertible matrices in M_n will be groups. Clearly, $GL(n, F)$ is a group because the properties follow from those matrix of multiplication. We have already established that invertible lower triangular matrices have lower triangular inverses. Therefore, they form a subgroup of $GL(n, F)$. We consider the unitary and orthogonal groups below.

Proposition 4.1.2. *For any integer $n = 1, 2, \ldots$ the set of unitary matrices U_n (resp. real orthogonal) forms a group. Similarly O_n is a group, with subgroup SO_n.*

Proof. The result follows if we can show that unitary matrices are closed under multiplication. Let U and V be unitary. Then

$$\begin{aligned} (UV)^*(UV) &= V^*U^*UV \\ &= V^*V = I \end{aligned}$$

For orthogonal matrices the proof is essentially identical. That SO_n is a group follows from the determinant equality $\det(AB) = \det A \det B$. Therefore it is a subgroup of O_n. □

4.1.2 Permutation matrices

Another example of matrix groups comes from the idea of permutations of integers.

Definition 4.1.3. The matrix $P \in M_n(\mathbb{C})$ is called a **permutation** matrix if each row and each column has exactly one 1, the rest of the entries being zero.

Example 4.1.3. Let

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad Q = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

P and Q are permutation matrices.

Another way to view a permutation matrix is with the game of chess. On an $n \times n$ chess board place n rooks in positions where *none* of them attack one another. Viewing the board as an $n \times n$ matrix with ones where the rooks are and zeros elsewhere, this matrix will be a permutation matrix.

Of course there are $n!$ such placements, exactly the number of permutations of the integers $\{1, 2, \ldots, n\}$.

Permutation matrices are closely linked with permutations as discussed in Chapter 2.5. Let σ be a permutation of the integers $\{1, 2, \ldots, n\}$. Define the matrix A by

$$a_{ij} = \begin{cases} 1 & \text{if} \quad j = \sigma(i) \\ 0 & \text{if} \quad \text{otherwise} \end{cases}$$

Then A is a permutation matrix. We could also use the Dirac notation to express the same matrix, that is to say $a_{ij} = \delta_{i\sigma(j)}$. The product of permutation matrices is again a permutation matrix. This is apparent by straight multiplication. Let P and Q be two $n \times n$ permutation matrices with pertaining permutations σ_P and σ_Q of the integers $\{1, 2, \ldots, n\}$. Then the i^{th} row of P is $e_{\sigma_P(i)}$ and the i^{th} row of Q is $e_{\sigma_Q(i)}$. (Recall the e_i are the usual standard vectors.) Now the i^{th} row of the product PQ can be computed by

$$\sum_{j=1}^{n} p_{ij} e_{\sigma_Q(j)} = \sum_{j=1}^{n} \delta_{i\sigma(j)} e_{\sigma_Q(j)} = e_{\sigma_Q(\sigma_P(i))}$$

Thus the multiplication i^{th}row of PQ is a standard vector. Since the $\sigma_P(i)$ ranges over the integers $\{1, 2, \ldots, n\}$, it is true also that $\sigma_Q(\sigma_P(i))$ does likewise. Therefore the "product" $\sigma_Q(\sigma_P(i))$ is also a permutation. We conclude that the standard vectors constitute the rows of PQ. Thus permutation matrices are orthogonal under multiplication. Moreover the inverse of every permutation is permutation matrix, with the inverse describe through the inverse of the pertaining permutation of $\{1, 2, \ldots, n\}$. Therefore, we have the following result.

Proposition 4.1.3. *Permutation matrices are orthogonal. Permutation matrices form a subgroup of* O_n.

4.1.3 Unitary equivalence

Definition 4.1.4. A matrix $B \in M_n$ is said to be *unitarily equivalent* to A if there is a unitary matrix $U \in M_n$ such that

$$B = U^* A U.$$

(In the real case we say B is orthogonally equivalent to A.)

Theorem 4.1.4. *If B and A are unitarily equivalent. Then*

$$\sum_{i,j=1}^{n} |b_{ij}|^2 = \sum_{i,j=1}^{n} |a_{ij}|^2.$$

Proof. We have $\sum_{i,j=1}^{n} |a_{ij}|^2 = \text{tr } A^*A$, and

$$\begin{aligned}\Sigma|b_{ij}|^2 &= \text{tr } B^*B = \text{tr } (U^*AU)^*U^*AU = \text{tr } U^*A^*AU \\ &= \text{tr } A^*A,\end{aligned}$$

since the trace is invariant under similarity transformations. □

Alternatively, we have $BU^* = U^*A$. Since U (and U^*) are isometries we have each column of U^*A has the same norm as the norm of the same column of A. The same holds for the rows of BU^*, whence the result.

Example 4.1.4. $B = \begin{bmatrix} 3 & 1 \\ -2 & 0 \end{bmatrix}$ and $A = \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}$ are similar but not unitarily equivalent. A and B are similar because (1) they have the same spectrum, $\sigma(A) = \sigma(B) = \{1, 2\}$ and (2) they have two linearly independent eigenvectors. They are not unitarily equivalent because the conditions of the above theorem are not met.

Remark 4.1.1. Unitary equivalence is a finer classification than similarity. Indeed, consider the two sets $S(A) = \{B \mid B \text{ is similar to } A\}$ and $U(A) = \{B|B \text{ is unitarily equivalent to } A\}$, then

$$U(A) \subset S(A).$$

(Can you show that $U(A) \subsetneqq S(A)$ for some large class of $A \in M_n$?)

4.1.4 Householder transformations

An important class of unitary transformations are elementary reflections. These can be realized as transformations that reflect one vector to its negative and leave invariant the orthocomplement of vectors.

Definition 4.1.5. Simple Householder transformation.) Suppose $w \in \mathbb{C}^n$, $\|w\| = 1$. Define the **Householder** transformation H_w by

$$H_w = I - 2ww^*$$

Computing

$$\begin{aligned} H_w H_w^* &= (I - 2ww^*)(I - 2ww^*)^* \\ &= I - 2ww^* - 2ww^* + 4ww^*ww^* \\ &= I - 4ww^* + 4\langle w, w\rangle ww^* = I \end{aligned}$$

it follows that H_w is unitary.

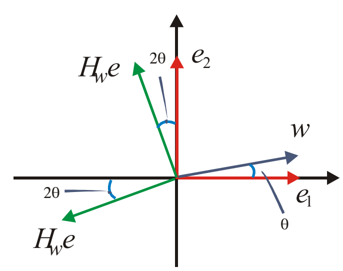
Example 4.1.5. Consider the vector $w = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}$ and the Householder transformation

$$\begin{aligned} H_w &= I - 2ww^T = \begin{bmatrix} 1 - 2\cos^2\theta & -2\cos\theta\sin\theta \\ -2\cos\theta\sin\theta & 1 - 2\sin^2\theta \end{bmatrix} \\ &= \begin{bmatrix} -\cos 2\theta & -\sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{bmatrix} \end{aligned}$$

The transformation properties for the standard vectors are

$$\begin{aligned} H_w\ e_1 &= \begin{bmatrix} -\cos 2\theta \\ -\sin 2\theta \end{bmatrix} \qquad \text{and} \\ H_w\ e_2 &= \begin{bmatrix} \cos 2\theta \\ -\sin 2\theta \end{bmatrix} \end{aligned}$$

This is shown below. It is evident that this unitary transformation is not a rotation. Though, it can be imagined as a "rotation with a one dimensional reflection."



Householder transformation H_w

Example 4.1.6. Let θ be real. For any $n \geq 2$ and $1 \leq i, j \leq n$ with $i \neq j$

define

$$
U_n(\theta,i,j)\quad
\begin{array}{c} \\ \\ \\ i \\ \\ \\ \\ j \\ \\ \\ \\ \end{array}
\begin{bmatrix}
1 & & 0 & \cdots & & & & \vdots & & & 0 \\
 & \ddots & & \vdots & & & & \vdots & & & \\
0 & & 1 & \vdots & & & & \vdots & & & \\
\cdots & \cdots & \cdots & \cos\theta & \cdots & \cdots & \cdots & -\sin\theta & \cdots & \cdots & \cdots \\
 & & & & 1 & & & & & & \\
 & & & \vdots & & \ddots & & \vdots & & & \\
 & & & & & & 1 & & & & \\
\cdots & \cdots & \cdots & \sin\theta & \cdots & \cdots & \cdots & \cos\theta & \cdots & \cdots & \cdots \\
 & & & \vdots & & & & \vdots & 1 & & \vdots \\
 & & & \vdots & & & & \vdots & 0 & \ddots & 0 \\
0 & & & \vdots & & & & \vdots & \vdots & & 1
\end{bmatrix}
$$

$$
\qquad\qquad\qquad\qquad\qquad i \qquad\qquad\qquad\qquad j
$$

Then $U_n(\theta; i, j)$ is a rotation and is unitary.

Proposition 4.1.4 (Limit theorems). *(i) Show that the unitary matrices are closed with respect to any norm. That is, if the sequence* $\{U_n\} \subset M_n(\mathbb{C})$ *are all unitary and the* $\lim_{n\to\infty} U_n = U$ *in the* $\|\cdot\|_2$ *norm, then* U *is also unitary.*

(ii) The unitary matrices are closed under pointwise convergence. That is, if the sequence $\{U\_n\} \subset M_n(\mathbb{C})$ *are all unitary and* $\lim_{n\to\infty} U_n = U$ *for each* (ij)*entry, then* U *is also unitary.*

Householder transformations can also be used to triangularize a matrix. The procedure successively removes the lower triangular portion of a matrix column by column in a way similar to Gaussian elimination. The elementary row operations are replaced by elementary reflectors. The result is a triangular matrix $T = H_{v_n} \cdots H_{v_2} H_{v_1} A$. Since these reflectors are unitary, the factorization yields an effective method for solving linear systems. The actual process is rather straightforward. Construct the vector v such that

$$
\left(I - 2vv^T\right) A = \left(I - 2vv^T\right) \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} \hat{a}_{11} & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ 0 & \hat{a}_{22} & \cdots & \hat{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \hat{a}_{n2} & \cdots & \hat{a}_{nn} \end{bmatrix}
$$

This is accomplished as follows. This means we wish to find a vector v such that

$$\left(I - 2vv^T\right)[a_{11}, a_{21}, \cdots, a_{n1}]^T = [\hat{a}_{11}, 0, \cdots, 0]^T$$

For notational convenience and to emphasize the construction is vector based, relabel the column vector $[a_{11}, a_{21}, \cdots, a_{n1}]^T$ as $[x_1, x_2, \ldots, x_n]^T$

$$v_j = \frac{x_j}{2\langle v, x\rangle}$$

for $j = 2, 3, \ldots, n$. Define

$$v_1 = \frac{x_1 + \alpha}{2\langle v, x\rangle}$$

Then

$$\begin{aligned}
\langle v, x\rangle &= \frac{\langle x, x\rangle}{2\langle v, x\rangle} + \frac{\alpha x_1}{2\langle v, x\rangle} = \frac{\|x\|^2}{2\langle v, x\rangle} + \frac{\alpha x_1}{2\langle v, x\rangle} \\
4\langle v, x\rangle^2 &= 2\|x\|^2 + 2\alpha x_1
\end{aligned}$$

where $\|\cdot\|$ denotes the Euclidean norm. Also, for H_v to be unitary we need

$$\begin{aligned}
1 &= \langle v, v\rangle = \frac{1}{4\langle v, x\rangle^2}\left(\|x\|^2 + 2\alpha x_1 + \alpha^2\right) \\
4\langle v, x\rangle^2 &= \|x\|^2 + 2\alpha x_1 + \alpha^2
\end{aligned}$$

Equating the two expressions for $4\langle v, x\rangle^2$ gives

$$\begin{aligned}
2\|x\|^2 + 2\alpha x_1 &= \|x\|^2 + 2\alpha x_1 + \alpha^2 \\
\alpha^2 &= \|x\|^2 \\
\alpha &= \pm\|x\|
\end{aligned}$$

We now have that

$$\begin{aligned}
4\langle v, x\rangle^2 &= 2\|x\|^2 \pm 2\|x\| x_1 \\
\langle v, x\rangle &= \left(\frac{1}{2}\left(\|x\|^2 \pm \|x\| x_1\right)\right)^{\frac{1}{2}}
\end{aligned}$$

This makes $v_1 = \frac{x_1 \pm \|x\|}{\left(\frac{1}{2}\left(\|x\|^2 \pm \|x\| x_1\right)\right)^{\frac{1}{2}}}$. With the construction of H_v to "eliminate" the first column of A, we relabel the vector v as v_1 (with the small

possibility of notational confusion) and move to describe H_{v_2} using a transformation of the same kind with a vector of the type $v = (0, x_2, x_3, \ldots, x_n)$. Such a selection will not affect the structure of the first column. Continue this until the matrix is triangularized. The upshot is that every matrix can be factored as $A = UT$, where U is unitary and T is upper triangular.
The main result for this section is the factorization theorem. As it turns out, every Unitary matrix can be written as a product of elementary reflectors. The proof requires a slightly more general notion of reflector.

Definition 4.1.6. The general form of the Householder matrix, also called an **elementary reflector**, has the form

$$H_v = I - \tau v v^*$$

where the vector $v \in C_n$.

In order for H_v to be unitary, it must be true that

$$\begin{aligned} H_v H_v^* &= (I - \tau v v^*)(I - \tau v v^*)^* \\ &= (I - \tau v v^*)(I - \bar{\tau} v v^*) \\ &= I - \tau v v^* - \bar{\tau} v v^* + |\tau|^2 (v^* v) v v^* \\ &= I - 2\mathrm{Re}(\tau) v v^* + |\tau|^2 |v|^2 v v^* \\ &= I \end{aligned}$$

Therefore, for $v \neq 0$ we must have

$$\begin{aligned} -2\mathrm{Re}(\tau) v v^* + |\tau|^2 |v|^2 v v^* &= \left(-2\mathrm{Re}(\tau) + |\tau|^2 |v|^2\right) v v^* \\ &= 0 \end{aligned}$$

or

$$-2\mathrm{Re}(\tau) + |\tau|^2 |v|^2 = 0$$

Now suppose that $Q \in M_n(R)$ is orthogonal and that the spectrum $\sigma(Q) \subset \{-1, 1\}$. Suppose Q has a complete set of normalized orthogonal eigenvectors[1], it can be expressed as $Q = \sum_{i=1}^{n} \lambda_i v_i v_i^T$ where the set $v_1, \ldots, v_n$ are the eigenvectors and $\lambda_i \subset \sigma(Q)$. Now assume the eigenvectors have been arranged so that this simplifies to

$$Q = -\sum_{i=1}^{k} v_i v_i^T + \sum_{i=k+1}^{n} v_i v_i^T$$

[1]This is in fact a theorem that will be established in Chapter 4.2. It follows as a consequence of Schur's theorem

Here we have just arrange the eigenvectors with eigenvalue -1 to come first. Define

$$H_j = I - 2v_j v_j^T \ , \qquad j = 1, \ldots, k$$

It follows that

$$Q = \prod_{j=1}^{k} H_j = \prod_{j=1}^{k} \left(I - 2v_j v_j^T\right)$$

for it is easy to check that

$$Uv_m = \prod_{j=1}^{k} H_j = \begin{cases} -v_m & \text{if} \quad m \leq k \\ v_m & \text{if} \quad m > k \end{cases}$$

Since we have agreement with Q on a basis, the equality follows. In words we may say that an orthogonal matrix U with spectrum $\sigma(Q) \subset \{-1, 1\}$ with can be written as a product of reflectors. With this simple case out of the way, we consider more general case we write $Q = \sum_{i=1}^{n} \lambda_i v_i v_i^T$. where the set $v_1, \ldots, v_n$ are the eigenvectors and $\lambda_i \subset \sigma(Q)$. We wish to represent Q similar to the above formula as a product of elementary reflectors.

$$Q = \prod_{j=1}^{k} H_j = \prod_{j=1}^{k} \left(I - \tau_j w_j w_j^*\right)$$

where $w_i = \alpha_i v_i$ for some scalars α_i. On the one hand it must be true that $-2\text{Re}(\tau_i) + |\tau_i|^2 |w_i|^2 = 0$ for each $i = 1, \ldots n$, and on the other hand it must follow that

$$\left(I - \tau_i w_i w_i^*\right) v_m = \begin{cases} \lambda_i v_i & \text{if} \quad m = i \\ v_m & \text{if} \quad m \neq i \end{cases}$$

The second of these relations is automatically satisfied by the orthogonality of the eigenvectors. The second relation can needs to be solved. This simplifies to $\left(I - \tau_i w_i w_i^*\right) v_i = \left(1 - \tau_i |\alpha_i|^2\right) v_i = \lambda_i v_i$. Therefore, it is necessary to solve the system

$$\begin{aligned} -2\text{Re}(\tau_i) + |\tau_i|^2 |v_i|^2 &= 0 \\ 1 - \tau_i |\alpha_i|^2 &= \lambda_i \end{aligned}$$

Having done so there results the factorization.

Theorem 4.1.5. *Let $Q \in M_n$ be real orthogonal or unitary. Then Q can be factored as the product of elementary reflectors $Q = \prod_{j=1}^{n} \left(I - \tau_j w_j w_j^*\right)$, where the w_j are the eigenvectors of Q.*

Note that the product written here is up to n whereas the earlier product was just up to k. The difference here is slight, for by taking the scalar (α) equal zero when necessary, it is possible to equate the second form to the first form when the spectrum is contained in the set $\{-1, 1\}$.

4.2 Schur's theorem

It has already been established in Theorem 3.5.2 that every matrix is similar to a triangular matrix. A far stronger result is possible. Called Schur's theorem, this result proves that the similarity is actually unitary similarity.

Theorem 4.2.1 (Schur's Theorem). *Every matrix $A \in M_n(\mathbb{C})$ is unitarily equivalent to a triangular matrix.*

Proof. We proceed by induction on the size of the matrix n. First suppose the A is 2×2. Then for a given eigenvalue λ and normalized eigenvector v form the matrix P with its first column v and second column any vector orthogonal to v with norm one. Then P is an unitary matrix and $P^*AP = \begin{bmatrix} \lambda & * \\ 0 & * \end{bmatrix}$. This is the desired triangular form. Now assume the Schur factorization is possible for matrices up to size $(n-1) \times (n-1)$. For the given $n \times n$ matrix A select any eigenvalue λ . With its pertaining normalized eigenvector v construct the matrix P with v in the first column and an orthonormal complementary basis in the remaining $n-1$ columns. Then

$$P^*AP = \begin{bmatrix} \lambda & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ 0 & \hat{a}_{22} & \cdots & \hat{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \hat{a}_{n2} & \cdots & \hat{a}_{nn} \end{bmatrix} = \begin{bmatrix} \lambda & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ 0 & & & \\ \vdots & & A_2 & \\ 0 & & & \end{bmatrix}$$

The eigenvalues of A_2 together with λ constitute the eigenvalues of A. By the inductive hypothesis there is an $(n-1) \times (n-1)$ unitary matrix $\hat{Q}$ such that $\hat{Q}^* A_2 \hat{Q} = T_2$, where T_2 is triangular. Now embed $\hat{Q}$ in an $n \times n$ matrix

Q as shown below

$$Q = \begin{bmatrix} \lambda & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \hat{Q} & \\ 0 & & & \end{bmatrix}$$

It follows that

$$Q^*P^*APQ = \begin{bmatrix} \lambda & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & T_2 & \\ 0 & & & \end{bmatrix} = T$$

is triangular, as indicated. Therefore the factorization is complete upon defining the similarity transformation $U = PQ$. Of course, the eigenvalues of A_2 together with λ constitute the eigenvalues of A, and therefore by similarity the diagonal of T contains only eigenvalues of A. □

The triangular matrix above is not unique as is easy to see by mixing or permuting the eigenvalues. An important consequence of Schur's theorem pertains to unitary matrices. Suppose that B is unitary and we apply the Schur factorization to write $B = U^*TU$. Then $T = UBU^*$. It follows that the upper triangular matrix is itself unitary, which is to say $T^*T = I$. It is a simple fact to prove this implies that T is in fact a diagonal matrix. Thus, the following result is proved.

Corollary 4.2.1. *Every unitary matrix is diagonalizable. Moreover, every unitary matrix has n orthogonal eigenvectors.*

Proposition 4.2.1. *If $B, A \in M_2$ are similar and $tr(B^*B) = tr(A^*A)$, then B and A are unitarily equivalent.*

This result higher dimensions.

Theorem 4.2.2. *Suppose that $A \in M_n(\mathbb{C})$ has distinct eigenvalues $\lambda_1 \dots \lambda_k$ with multiplicities $n_1, n_2, \dots, n_k$ respectively. Then A is similar to a matrix of the form*

$$\begin{bmatrix} T_1 & & & 0 \\ & T_2 & & \\ 0 & & \ddots & \\ & & & T_k \end{bmatrix}$$

where $T_i \in M_{n_i}$ is upper triangular with diagonal entries λ_i.

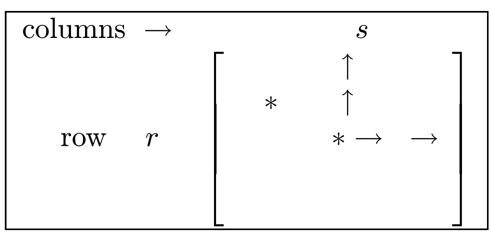
Proof. Let E_1 be eigenspace of λ_1. Assume $\dim E_1 = m_1$. Let $u_1 \dots u_{m_1}$ be an orthogonal basis of E_1, and suppose $v_1 \dots v_{n-m_1}$ is an orthonormal basis of $\mathbb{C}^n - E_1$. Then with $P = [u_1 \dots u_{m_1}, v_1 \dots v_{n-m_1}]$ we have $P^{-1}AP$ has the block structure

$$\left[\begin{array}{c|c} T_1 & 0 \\ \hline 0 & A_2 \end{array}\right].$$

Continue this way, as we have done before. However, if $\dim E_i < m_i$ we must proceed a different way. First apply Schur's Theorem to triangularize. Arrange the first m_1 eigenvalues to the first m_1 diagonal entries of T, the similar triangular matrix. Let $E_{r,s}$ be the matrix with a 1 in the r, s position and 0's elsewhere. We assume throughout that $r \neq s$. Then, it is easy to see that $I + \alpha E_{r,s}$ is invertible and that $(I + \alpha E_{rs})^{-1} = I - \alpha E_{rs}$. Now if we define

$$(I + \alpha E_{rs})^{-1}\, T\, (I + \alpha E_{rs})$$

we see that $t_{rs} \to t_{rs} + \alpha(t_{rr} - t_{ss})$. We know $t_{rr} - t_{ss} \neq 0$ if r and s pertain to values with different eigenvalues. Now this value is changed, but so also are the values above and to the right of t_{rs}. This is illustrated below.



To see how to use these similarity transformation to zero out the upper blocks, consider the special case with just two blocks

$$A = \left[\begin{array}{c|c} T_1 & T_{12} \\ \hline 0 & T_2 \end{array}\right]$$

We will give a procedure to use elementary matrices αE_{ij} to zero-out each of the entries in T_{12}. The matrix T_{12} has $m_1 \cdot m_2$ entries and we will need to use exactly that many of the matrices αE_{ij}. In the diagram below we illustrate the order of removal (zeroing-out) of upper entries

$$\left[\begin{array}{c|cccc}
 & m_1 & 2m_1 & \cdots & m_1 \cdot m_2 \\
 & \vdots & \vdots & & \vdots \\
T_1 & & & & \\
 & 2 & \vdots & & \\
 & 1 & m_1+1 & \cdots & \cdots \\
\hline
 & & & & \\
0 & T_2 & & & \\
 & & & &
\end{array}\right]$$

When performed in this way we develop $m_1{\cdot}m_2$ constants α_{ij}. We proceed in the upper right block (T_{12}) in the left-most column and bottom entry, that is position (m_1, m_1+1). For the (m_1, m_1+1) position we use the elementary matrix $\alpha E_{m_1,m_1+1}$ to zero out this position. This is possible because the diagonal entries of T_1 and T_2 are different. Now use the elementary matrix $\alpha E_{m_1-1,m_1+1}$ to zero-out the position (m_1-1, m_1+1). Proceed up this column to the first row each time using a new α. We are finished when all the entries in column m_1+1 from row m_1 to row 1 are zero. Now focus on the next column to the right, column m_1+2. Proceed in the same way from the (m_1, m_1+2) position to the $(1, m_1+1)$ position, using elementary matrices $\alpha E_{k,m_1+2}$ zeroing out the entries (k, m_1+2) positions, $k = m_1, \ldots, 1$. Ultimately, we can zero out every entry in the upper right block with this marching left-to-right, bottom-to-top procedure.

In the general scheme with $k \times k$ blocks, next use the matrices T_2 and T_3 to zero-out the block matrix T_{23}.(See below.)

$$T = \left[\begin{array}{ccc|ccc}
T_1 & 0 & T_{13} & \cdots & \cdots & \\
 & T_2 & T_{23} & & & \\
 & & T_3 & & & \\
\hline
 & & & \ddots & & \\
 & 0 & & & T_{k-1} & T_{k-1,k} \\
 & & & & & T_k
\end{array}\right]$$

After that it is possible using blocks T_1 and T_3 to zero-out the block T_{13}. This is the general scheme for the entire triangular structure, moving down the super-diagonal $(j.j+1)$ blocks and then up the (block) columns. In this way we can zero-out any value not in the square diagonal blocks pertaining to the eigenvalues $\lambda_1 \ldots \lambda_k$. $\square$

Remark 4.2.1. If $A \in M_n(R)$ and $\sigma(A) \subset R$, then all operations can be carried out with real numbers.

Lemma 4.2.1. *Let $\mathcal{J} \subset M_n$ be a commuting family. Then there is a vector $x \in \mathbb{C}^n$ for which x is an eigenvector for every $A \in \mathcal{J}$.*

Proof. Let $W \subset \mathbb{C}^n$ be a subspace of minimal dimension that is invariant under $\mathcal{J}$. Since $\mathbb{C}^n$ is invariant, we know W exists. Since $\mathbb{C}^n$ is invariant, we know W exists. Suppose there is an $A \in \mathcal{J}$ for which there is a vector in W which is not an eigenvector of A. Define $W_0 = \{y \in W \mid Ay = \lambda y \text{ for some } \lambda\}$. That is, W_0 is a set of eigenvectors of A. Since W is invariant under A, it follows that $W_0 \neq \phi$. Also, by assumption. $W_0 \subsetneqq W$. For any $x \in W_0$

$$ABx = (AB)x = B(Ax) = \lambda Bx$$

and so $Bx \in W_0$. It follows that W_0 is $\mathcal{J}$ invariant, and W_0 has lower positive dimension than W. □

As a consequence we have the following result.

Theorem 4.2.3. *Let $\mathcal{J}$ be a commuting family in M_n. If $A \in \mathcal{J}$ is diagonalizable, then $\mathcal{J}$ is simultaneously diagonalizable.*

Proof. Since A is diagonalizable there are n linearly independent eigenvectors of A and if S is in M_n and consists of those eigenvectors the matrix $S^{-1}AS$ is diagonal. Since eigenvectors of A are the same as eigenvectors of $B \in \mathcal{J}$, it follows that $S^{-1}BS$ is also diagonal. Thus $S^{-1}\mathcal{J}S = \mathcal{D} :=$ all diagonal matrices. □

Theorem 4.2.4. *Let $\mathcal{J} \subset M_n$ be a commuting family. There is a unitary matrix $U \in M_n$ such that U^*AU is upper triangular for each $A \in \mathcal{J}$.*

Proof. From the proof of Schur's Theorem we have that the eigenvectors chosen for U are the same for all $A \in \mathcal{J}$. This follows because after the first step we have reduced A and B to

$$\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix}$$

respectively. Commutativity is preserved under simultaneous similarity and therefore A_{22} and B_{22} commutes. Therefore at the second step the same eigenvector can be selected for *all* $B_{22} \subset \mathcal{J}_2$, a commuting family. □

Theorem 4.2.5. *If $A \in M_n(R)$, there is a real orthogonal matrix $Q \in M_n(R)$ such that*

$$(\star) \qquad Q^T A Q = \begin{bmatrix} A_1 & & & \\ & A_2 & \star & \\ 0 & & \ddots & \\ & & & A_k \end{bmatrix} \qquad 1 \le k \le n$$

where each A_i is a real 1×1 matrix or a real 2×2 matrix with a non real pair of complex conjugate eigenvalues.

Theorem 4.2.6. *Let $\mathcal{J} \subset M_n(R)$ be a commuting family. There is a real orthogonal matrix $Q \in M_n(R)$ for which $Q^T AQ$ has the form $(\star)$ for every $A \in \mathcal{J}$.*

Theorem 4.2.7. *Suppose $A, B \in M_n(\mathbb{C})$ have eigenvalues $\alpha_1, \dots, \alpha_n$ and $\beta_1, \dots, \beta_n$ respectively. If A and B commute then there is a permutation $i_1 \dots i_n$ of the integers $1, \dots, n$ for which the eigenvalues of $A+B$ are $\alpha_j + \beta_{i_j}$, $j = 1, \dots, n$. Thus $\sigma(A+B) \subset \sigma(A) + \sigma(B)$.*

Proof. Since $\mathcal{J} = \{A, B\}$ forms a commuting family we have that every eigenvector of A is an eigenvector of B, and conversely. Thus if $Ax = \alpha_j x$ we must have that $Bx = B_{i_j} x$. But how do we get the permutation? The answer is to simultaneously triangularize with $U \in M_n$. We have

$$U^* AU = T \quad \text{and} \quad U^* BU = R.$$

Since

$$U^*(A+B)U = T + R$$

we have that the eigenvalues pair up as described. □

Note: We don't necessarily need A and B to commute. We need only the hypothesis that A and B are simultaneously diagonalizable.

If A and B *do not* commute little can be said of $\sigma(A+B)$. In particular $\sigma(A+B) \subsetneqq \sigma(A) + \sigma(B)$. Indeed, by summing upper triangular and lower triangular matrices we can exhibit a range of possibilities. Let $A = \left[\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right]$, $B = \left[\begin{smallmatrix} 0 & 0 \\ 1 & 0 \end{smallmatrix}\right]$, $\sigma(A+B) = \{-1, 1\}$ but $\sigma(A) = \sigma(B) = \{0\}$.

Corollary 4.2.1. *Suppose $A, B \in M_n$ are commuting matrices with eigenvalues*
$\alpha_1, \dots, \alpha_n$ and $\beta_1, \dots, \beta_n$ respectively. If $\alpha_i \ne -\beta_j$ for all $1 \le i, j \le n$, then $A + B$ is nonsingular.

Note: Giving conditions for the nonsingularity of $A+B$ in terms of various conditions on A and B is a very different problem. It has many possible answers.

4.3 Exercises

1. Characterize all diagonal unitary matrices and all diagonal orthogonal matrices in M_n.

2. Let $T(\theta) = \left[\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right]$ where θ is any real. Then $T(\theta)$ is *real* orthogonal. Prove that if $U \in M_2(R)$ is real orthogonal, then U has the form $T(\theta)$ for some θ or
$$U = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} T(\theta),$$
and conversely.

3. Let us define the $n \times n$ matrix P to be a w-permutation matrix if for every vector $x \in R_n$, the vector Px has the same components as x in value and number, though possibly permuted. Show that w-permutation matrices are permutation matrices.

4. In R_2 identify all Householder transformations that are rotations.

5. Given any unit vector w in the plane formed by e_i and e_j. Express the Householder matrix for this vector.

6. Show that the set of unitary matrices on $\mathbb{C}_n$ forms a subgroup of the subset of $GL(n, \mathbb{C})$.

7. In R_2, prove that the product of two (Householder) reflections is a rotation. (Hint. If the reflection angles are θ_1 and θ_2, then the rotation angle is $2\,(\theta_1 - \theta_2)$.)

8. Prove that the unitary matrices are closed the norm. That is, if the sequence $\{U_n\} \subset M_n(\mathbb{C})$ are all unitary and $\lim_{n\to\infty} U_n = U$ in the $\|\cdot\|_2$ norm, then U is also unitary.

9. Let $A \in M_n$ be invertible. Define $G = A^k,\ (A^{-1})^k,\ k = 1, 2, \ldots.$ Show that G is a subgroup of M_n. Here the group multiplication is matrix multiplication.

10. Prove that the unitary matrices are closed under pointwise convergence. That is, if the sequence $\{U\_n\} \subset M_n(\mathbb{C})$ are all unitary and $\lim_{n\to\infty} U_n = U$ for each (ij)entry, then U is also unitary.

11. Suppose that $A \in M_n$ and that $AB = BA$ for all $B \in M_n$. Show that A is a multiple of the identity.

12. Prove that a unitary matrix U can be written as $V^{-1}W^{-1}VW$ for unitary V, W if and only if $\det U = 1$. (Bellman, 1970)

13. Prove that the only triangular unitary matrices are diagonal matrices.

14. We know that given any bounded sequence of numbers, there is a convergent subsequence. (Bolzano-Weierstrass Theorem). Show that the same is true for matrices for any given matrix norm. In particular, show that if U_n is any sequence of unitary matrices, then there is a convergent subsequence.

15. The *Hadamard Gate* (from quantum computing) is defined by the matrix $H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$. Show that this transformation is a Householder matrix. What are its eigenvalues and eigenvectors?

16. Show that the unitary matrices do not form a subspace $M_n(\mathbb{C})$.

17. Prove that if a matrix $A \in M_n(\mathbb{C})$ preserves the orthonormality of one orthonormal basis, then it must be unitary.

18. Call the matrix A a **checkerboard matrix** if either

    (I) $a_{ij} = 0$ if $i + j$ is even <u>or</u> (II) $a_{ij} = 0$ if $i + j$ is odd

    We call the matrices of type I **even checkerboard** and type II **odd checkerboard**. Define $CH\,(n)$ to be all $n \times n$ invertible checkerboard matrices. The questions below all pertain to square matrices.

    (a) Show that if n is odd there are no invertible even checkerboard matrices.

    (b) Prove that every unitary matrix U has determinant with modulus one. (That is, $|\det U| = 1$.)

    (c) Prove that n is odd the product of odd checkerboard matrices is odd.

(d) Prove that if n is even then the product of an even and an odd checkerboard matrix is odd, while the product of two even (or odd) checkerboard matrices is even.

(e) Prove that if n is even then the inverse of any checkerboard matrix is a checkerboard matrix of the same type. However, in light of (a), it is only true that if n is an invertible odd checkerboard matrix, its inverse is odd.

(f) Suppose that $n = 2m$. Characterize all the odd checkerboard invertible matrices.

(g) Prove that $CH\,(n)$ is a subgroup of $GL\,(n)$.

(h) Prove that the invertible odd checkerboard matrices of any size n forms a subgroup of $CH\,(n)$.

In connection with chess, checkerboard matrices give the type of chess board on which the maximum number of mutually non-attacking knights can be placed on the even ($i+j$ is even) or odd ($i+j$ is odd) positions.

19. Prove that every unitary matrix can be written as the product of a unitary diagonal matrix and another unitary matrix whose first column has nonnegative entries.