Matrix Analysis (Lecture 3)

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Abstract

In the last two lectures, we analyze (left and right) eigenvalues and eigenvectors of a matrix, introduce a similarity transformation $A \to S^{-1}AS$ for a specified matrix A, and arise the diagonalizability of a matrix in M_n. From now on, we restrict our study to a special case of similarity called unitary similarity. This certain type of similarity requires the nonsingular S to embrace a simple property: $S^{-1} = S^*$. In this lecture, we are supposed to introduce basic properties of unitary matrices and some classical unitary matrices that are of greater use in the subsequent lectures. More importantly, the well-known *QR factorization*, which is of considerable theoretical and computational importance, will also be scrutinized.

1 Introduction (Page 83)

The chapter 2 of Horn's book begins with a general introduction of transformations involved unitary matrices or conjugate transposes of nonsingular matrices. As defined in Section 1.1 in Lecture 1 and Definition 1.1 in Lecture 2, a similarity transformation $A \to S^{-1}AS$ is conducted via a nonsingular matrix S. When the inverse of this matrix has a special form, that is, $S^{-1} = S^*$, the corresponding similarity transformation becomes $A \to S^*AS$, where S is a so-called unitary matrix. It turns out that similarity via a unitary matrix is not only conceptually simpler than general similarity (the conjugate transpose is much easier to compute than the inverse), but also exhibits superior

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stability properties in numerical computations. A fundamental property of unitary similarity is that every $A \in M_n$ is unitarily similar to an upper triangular matrix whose diagonal entries are the eigenvalues of A (Schur form or Schur triangularization; see Lecture 4).

The transformation $A \to S^*AS$, in which S is nonsingular but not necessarily unitary, is called **congruence*.

Remark. *congruence is not necessarily a similarity transformation. However, similarity by a unitary matrix is both a similarity and a *congruence.

For $A \in M_{n,m}$, the transformation $A \to UAV$, in which $U \in M_n$ and $V \in M_n$ are both unitary, is called *unitary equivalence*. The upper triangular form achievable under unitary similarity can be greatly refined under unitary equivalence and generalized to rectangular matrices: Every $A \in M_{m,n}$ is unitarily equivalent to a nonnegative diagonal matrix whose diagonal entries (the singular values of A) are of great significance.

2 Unitary matrices and the QR factorization (Page 83-91, Page 15-16, Page 19-20)

We have come across orthogonal vectors when examining left and right eigenvectors associated with different eigenvalues. Here we reiterate the definition of orthogonality.

Definition 2.1. *A list of vectors $x_1, ..., x_k \in \mathbf{C}^n$ is* orthogonal *if $x_i^* x_j = 0$ for all $i \neq j, i, j \in \{1, ..., k\}$. If, in addition, $x_i^* x_i = 1$ for all $i = 1, ..., k$ (that is, the vectors are* normalized*), then the list is* orthonormal.

Convention. It is often convenient to say that "$x_1, ..., x_k$ are orthogonal (respectively, orthonormal)" instead of the more formal statement "the list of vectors $v_1, ..., v_k$ is orthogonal (orthonormal, respectively)."

Example 2.2 (normalization)**.** If $y_1, ..., y_k \in \mathbf{C}^n$ are orthogonal and nonzero, the vectors $x_1, ..., x_k$ defined by $x_i = (y_i^* y_i)^{-\frac{1}{2}} y_i, i = 1, ..., k$ are orthonormal.

Definition 2.3. *Given any set $S \subset \mathbf{C}^n$, its* orthogonal complement *is the set $S^\perp = \{x \in \mathbf{C}^n : x^*y = 0$ for all $y \in S\}$ if S is nonempty; if S is empty, then $S^\perp = \mathbf{C}^n$.*

Remark. (a) In either case, $S^\perp = (\operatorname{span} S)^\perp$. Even if S is not a subspace, $S^\perp$ is always a subspace. We have $(S^\perp)^\perp = \operatorname{span} S$, and $(S^\perp)^\perp = S$ if S is a

subspace.
(b) It is always the case that $\dim S^{\perp} + \dim(S^{\perp})^{\perp} = n$. If S_1 and S_2 are subspaces, then $(S_1 + S_2)^{\perp} = S_1^{\perp} \cap S_2^{\perp}$.

An orthogonal list of vectors embraces many benign properties, which make them computationally simple.

Theorem 2.4. *Every orthogonal list of vectors in* $\mathbf{C}^n$ *is linearly independent.*

Proof. Suppose that $\{y_1, ..., y_k\}$ is an orthogonal set. Normalize them as Example 2.2 did and obtain an orthonormal list of vectors $\{x_1, ..., x_k\}$. Assume that $0 = \alpha_1 x_1 + \cdots + \alpha_k x_k$. Then $0 = (\alpha_1 x_1 + \cdots + \alpha_k x_k)^*(\alpha_1 x_1 + \cdots + \alpha_k x_k) = \sum_{i,j} \bar{\alpha}_i \alpha_j x_i^* x_j = \sum_{i=1}^{k} |\alpha_i|^2 x_i^* x_i = \sum_{i=1}^{k} |\alpha_i|^2$ because the vectors x_i are orthonormal. Thus, all $\alpha_i = 0$ and hence $\{x_1, ..., x_k\}$ is a linearly independent set, which in turn means that $\{y_1, ..., y_k\}$ is linearly independent. $\square$

Example 2.5. The fact that an orthogonal list of vectors $x_1, ..., x_k \in \mathbf{C}^n$ is linearly independent allows for two cases, either $k \leq n$ or at least $k - n$ of the vectors x_i are zero vectors. This is because there are at most n linearly independent vectors in $\mathbf{C}^n$, so the cardinality of a nonzero orthogonal set must satisfy $k \leq n$. If $k > n$, we can choose n vector from the list such that $\mathrm{span}\{x_1, ..., x_n\} = \mathbf{C}^n$, since $x_1, ..., x_k$ are linearly independent. Then $\{x_{n+1}, ..., x_k\} \subseteq (\mathrm{span}\{x_1, ..., x_n\})^{\perp} = (\mathbf{C}^n)^{\perp} = \{0\}$, yielding that $x_{n+1} = \cdots = x_n = 0$.

A linearly independent list need not be orthonormal, but one can apply the Gram-Schmidt orthonormalization procedure to it and obtain an orthonormal list with the same span.

Example 2.6 (Gram-Schmidt orthonormalization)**.** We first define the scalar $\langle x, y \rangle = y^* x$ as the *Euclidean inner product* (*standard inner product, usual inner product, scalar product, dot product*) of $x, y \in \mathbf{C}^n$. And the *Euclidean norm (usual norm, Euclidean length)* function on $\mathbf{C}^n$ is the real-valued function $||x||_2 = \langle x, x \rangle^{\frac{1}{2}} = (x^* x)^{\frac{1}{2}}$.

The *Gram-Schmidt process* starts with a list of vectors $v_1, ..., v_n$ and (if the given list is linearly independent) produces an orthonormal list of vectors $z_1, ..., z_n$ such that $\mathrm{span}\{z_1, ..., z_n\} = \mathrm{span}\{x_1, ..., x_n\}$ for each $k = 1, ..., n$. The vectors z_i may be calculated in turn as follows: Let $y_1 = x_1$ and normalize it: $z_1 = \frac{y_1}{||y_1||_2}$. Let $y_2 = x_2 - \langle x_2, z_1 \rangle z_1$ (y_2 is orthogonal to z_1) and normalize it: $z_2 = \frac{y_2}{||y_2||_2}$. Once $z_1, ..., z_{k-1}$ have been determined, the vector

$$y_k = x_k - \langle x_k, z_{k-1} \rangle z_{k-1} - \langle x_k, z_{k-2} \rangle z_{k-2} - \cdots - \langle x_k, z_1 \rangle z_1$$

is orthogonal to $z_1, ..., z_{k-1}$; normalize it: $z_k = \frac{y_k}{||y_k||_2}$. Continue until $k = n$. If we denote $Z = [z_1 \cdots z_n]$ and $X = [x_1 \cdots x_n]$, the Gram-Schmidt process gives a factorization $X = ZR$, where the square matrix $R = [r_{ij}]$ is nonsingular and upper triangular; that is, $r_{ij} = 0$ whenever $i > j$.

The Gram-Schmidt precess may be applied to any finite list of vectors, independent or not. If $x_1, ..., x_n$ are linearly independent, the Gram-Schmidt process produces a vector $y_k = 0$ for the least value of k for which x_k is a linear combination of $x_1, ..., x_{k-1}$.

Since any nonzero subspace of $\mathbf{R}^n$ or $\mathbf{C}^n$ always has a linearly independent list of vectors that spans the subspace, one can apply the Gram-Schmidt orthonormalization to obtain its orthonormal basis.

We are now prepared to make a formal definition for the main concept of this lecture, unitary matrices, and investigate their properties.

Definition 2.7. *A matrix $U \in M_n$ is unitary if $U^*U = I$. A matrix $U \in M_n(\mathbf{R})$ is real orthogonal if $U^TU = I$.*

Example 2.8. The matrices $U = \frac{1}{\sqrt{2}} \begin{bmatrix} I_n & iI_n \\ iI_n & I_n \end{bmatrix}$, $V = \frac{1}{\sqrt{2}} \begin{bmatrix} -iI_n & -iI_n \\ I_n & -I_n \end{bmatrix}$, and $Q = \frac{1}{\sqrt{2}} \begin{bmatrix} I_n & I_n \\ I_n & -I_n \end{bmatrix}$ are all unitary. In particular, Q is also real orthogonal.

We list some of the basic equivalent conditions for U to be unitary in the next theorem.

Theorem 2.9. *If $U \in M_n$, the following statements 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 are orthonormal.

(f) The rows of U are orthonormal.

(g) For all $x \in \mathbf{C}^n, ||x||_2 = ||Ux||_2$, that is, x and Ux have the same Euclidean norm.

Proof.

$$\begin{array}{ccccccccccc} (e) & \Leftrightarrow & (a) & \Leftrightarrow & (b) & \Leftrightarrow & (c) & \Leftrightarrow & (d) & \Leftrightarrow & (f) \\ & & \Updownarrow & & & & & & & & \\ & & (g) & & & & & & & & \end{array}$$

(a) implies (b) since U^{-1} (when it exists) is the unique matrix; the definition of unitary says that U is nonsingular and $U^{-1} = U^*$. Since $BA = I$ if and only if $AB = I$ (for $A, B \in M_n$), (b) implies (c). Since $(U^*)^* = U$, (c) implies that U^* is unitary; that is, (c) implies (d). The converse of each of these implications is similarly observed, so (a)-(d) are equivalent.

Partition $U = [u_1 \cdots u_n]$ according to its columns. Then $U^*U = I$ indicates that $u_i^* u_i = 1$ for all $i = 1, ..., n$ and $u_i^* u_j = 0$ for all $i \neq j$. Thus, $U^*U = I$ is another way of saying that the columns of U are orthonormal, and hence (a) is equivalent to (e). Likewise, (d) and (f) are equivalent.

If U is unitary and $y = Ux$, then $y^*y = x^*U^*Ux = x^*Ix = x^*x$, so (a) implies (g). To prove the converse, let $U^*U = A = [a_{ij}]$, let $z, w \in \mathbf{C}^n$ be given, and take $x = z + w$ in (g). Then $x^*x = z^*z + w^*w + 2\operatorname{Re} z^*w$ and $y^*y = x^*Ax = z^*Az + w^*Aw + 2\operatorname{Re} z^*Aw$; (g) ensures that $z^*z = z^*Az$ and $w^*w = w^*Aw$, and hence $\operatorname{Re} z^*w = \operatorname{Re} z^*Aw$ for any z and w.
Take $z = e_p$ and $w = ie_q$ and compute $\operatorname{Re} ie_p^T e_q = 0 = \operatorname{Re} ie_p^T Ae_q = \operatorname{Re} ia_{pq} = -\operatorname{Im} a_{pq}$, so every entry of A is real. Finally, take $z = e_p$ and $w = e_q$ and compute $e_p^T e_q = \operatorname{Re} e_p^T e_q = \operatorname{Re} e_p^T Ae_q = a_{pq}$, which tells us that $A = I$ and U is unitary. □

Remark. When proving (g) $\Rightarrow$ (a), we choose $x = w + z$ instead of just taking arbitrary x because if we take $x = e_1$, then $1 = x^*x = x^*Ax = a_{11}$ and only the diagonal entries of A can be determined by consecutively changing the value of x.

An important geometrical fact is that any two lists containing equal numbers of orthonormal vectors are related via a unitary transformation.

Theorem 2.10. *If $X = [x_1 \cdots x_n] \in M_{n,k}$ and $Y = [y_1 \cdots y_n] \in M_{n,k}$ have orthonormal columns, then there is a unitary $U \in M_n$ such that $Y = UX$. If X and Y are real, then U may be taken to be real.*

Proof. Extend each of the orthonormal lists $x_1, ..., x_k$ and $y_1, ..., y_k$ to orthonormal bases of $\mathbf{C}^n$ by furnishing each list with linearly independent vectors and applying Gram-Schmidt orthonormalization. That is, construct unitary matrices $V = [X\ X_2]$ and $W = [Y\ Y_2] \in M_n$. Then $U = WV^*$ is unitary and $[Y\ Y_2] = W = UV = [UX\ UX_2]$, so $Y = UX$. If X and Y are real, the matrices $[X\ X_2]$ and $[Y\ Y_2]$ may be chosen to be real orthogonal (their columns are orthonormal bases of $\mathbf{R}^n$). $\square$

If a unitary matrix is presented as a 2-by-2 block matrix, then the ranks of its off-diagonal blocks are equal; the ranks of its diagonal blocks are related by a simple formula. To prove this result, we rely on the *law of complementary nullities*.

Lemma 2.11. *Suppose that $A \in M_n$ is nonsingular, let α and β be nonempty subsets of $\{1, ..., n\}$, and write $|\alpha| = r$ and $|\beta| = s$ for the cardinalities of α and β. The* law of complementary nullities *is*

$$\text{nullity}(A[\alpha, \beta]) = \text{nullity}(A^{-1}[\beta^c, \alpha^c]) \tag{1}$$

which is equivalent to the rank identity

$$\text{rank}(A[\alpha, \beta]) = \text{rank}(A^{-1}[\beta^c, \alpha^c]) + r + s - n \tag{2}$$

Proof. Since we can permute rows and columns to place first the r rows indexed by α and the s columns indexed by β, it suffices to consider the presentations

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \text{ and } A^{-1} = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

where A_{11} and B_{11}^T are r-by-s and A_{22} and B_{22}^T are $(n-r)$-by-$(n-s)$.

The underlying principle here is very simple. Suppose that the nullity of A_{11} is k. If $k \geq 1$, let the columns of $X \in M_{s,k}$ is a basis for the null space of A_{11}. Since A is nonsingular,

$$A \begin{bmatrix} X \\ 0 \end{bmatrix} = \begin{bmatrix} A_{11}X \\ A_{21}X \end{bmatrix} = \begin{bmatrix} 0 \\ A_{21}X \end{bmatrix}$$

has full rank, so $A_{21}X$ has k independent columns. But

$$\begin{bmatrix} B_{12}(A_{21}X) \\ B_{22}(A_{21}X) \end{bmatrix} = A^{-1} \begin{bmatrix} 0 \\ A_{21}X \end{bmatrix} = A^{-1}A \begin{bmatrix} X \\ 0 \end{bmatrix} = \begin{bmatrix} X \\ 0 \end{bmatrix}$$

so $B_{22}(A_{21}X) = 0$ and hence nullity $B_{22} \geq k =$ nullity A_{11}, a statement that is trivially correct if $k = 0$. Symmetrically, a similar argument starting with B_{22} shows that nullity $A_{11} \geq$ nullity B_{22}.

By the *rank-nullity* theorem, we obtain that $s - \operatorname{rank} A_{11} = n - r - \operatorname{rank} B_{22}$. $\square$

Theorem 2.12. *Let a unitary $U \in M_n$ be partitioned as $U = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix}$, where $U_{11} \in M_k$. Then $\operatorname{rank} U_{12} = \operatorname{rank} U_{21}$ and $\operatorname{rank} U_{22} = \operatorname{rank} U_{11} + n - 2k$. In particular, $U_{12} = 0$ if and only if $U_{21} = 0$, in which case U_{11} and U_{22} are unitary.*

Proof. Applying the law of complementary nullities (1) and using the fact that $U^{-1} = \begin{bmatrix} U_{11}^* & U_{12}^* \\ U_{21}^* & U_{22}^* \end{bmatrix}$, we have that $\operatorname{nullity} U_{12} = \operatorname{nullity} U_{21}^*$, $\operatorname{nullity} U_{11} = \operatorname{nullity} U_{22}^*$. Since $U_{11} \in M_k, U_{12} \in M_{k,n-k}, U_{21} \in M_{n-k,k}, U_{22} \in M_{n-k,n-k}$ and conjugate transposition preserves the rank, we conclude that $\operatorname{rank} U_{12} = \operatorname{rank} U_{21}$ and $k - \operatorname{rank} U_{11} = n - k - \operatorname{rank} U_{22}$.

In the case when $U_{12} = U_{21} = 0$, $U^*U = I$ ensures that

$$\begin{bmatrix} U_{11}^* & 0 \\ 0 & U_{22}^* \end{bmatrix} \begin{bmatrix} U_{11} & 0 \\ 0 & U_{22} \end{bmatrix} = I,$$

yielding that $U_{11}^* U_{11} = U_{22}^* U_{22} = I$. □

Corollary 2.13. *A unitary matrix is upper triangular if and only if it is diagonal.*

Proof. ($\Leftarrow$) A diagonal matrix is obviously upper triangular.
($\Rightarrow$) Partition the upper triangular unitary matrix U into

$$U = \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}, \quad u_{11} \in M_1, U_{12} \in M_{1,n-1}, U_{22} \in M_{n-1}.$$

By Theorem 2.12, $U_{12} = 0$. Since U_{22} is still upper triangular, by repeating the same argument $n-1$ times, we prove that U is diagonal. □

Besides these properties, the set of unitary matrices forms a group under the standard matrix multiplication.

Theorem 2.14. *The set of unitary (respectively, real orthogonal) matrices in M_n forms a group. This group is generally referred to as the n-by-n unitary (respectively, real orthogonal) group, a subgroup of $GL(n, \mathbf{C})$.*

Proof. (Closure): If $U, V \in M_n$ are unitary, i.e., $U^*U = V^*V = I$, then $(UV)^*(UV) = V^*U^*UV = V^*IV = V^*V = I$, yielding that UV is also unitary.

(Associativity): The standard matrix multiplication are associative.
(Identity): Since the identity matrix I_n is unitary, it serves as the identity for this subgroup.
(Inverse): The inverse of a unitary matrix U is its conjugate transpose A^*, which is also unitary by (d) in Theorem 2.9.
The argument can be inherited to the case when matrices are real orthogonal without any effort. $\square$

The group of unitary matrices in M_n has another very important property. The defining identity $U^*U = I$ means that every column of U has Euclidean norm 1, and hence no entry of $U = [u_{ij}]$ can have absolute value greater than 1. If we think of the set of unitary matrices as a subset of $\mathbf{C}^{n^2}$, this says that it is a *bounded* subset. (In fact, it is bounded by n.) If $U_k = [u_{ij}^{(k)}]$ is an infinite sequence of unitary matrices, $k = 1, 2, ...,$ such that $\lim_{k\to\infty} u_{ij}^{(k)} = u_{ij}$ exists for all $i, j = 1, 2, ..., n$, then from the identity $U_k^* U_k = I$ for all $k = 1, 2, ...,$ we see that $\lim_{k\to\infty} U_k^* U_k = U^*U = I$, where $U = [u_{ij}]$ and the limit is taken componentwisely. Thus, the limit matrix U is also unitary. This says that the set of unitary matrices is a *closed* subset of $\mathbf{C}^{n^2}$.

Since a closed and bounded subset of a finite dimensional Euclidean space is a *compact* set, we conclude that the set (group) of unitary matrices in M_n is compact. For our purposes, the most important consequence of this observation is the following *selection principle* for unitary matrices.

Lemma 2.15. *Let $U_1, U_2, ... \in M_n$ be a given infinite sequence of unitary matrices. There exists an infinite subsequence $U_{k_1}, U_{k_2}, ..., 1 \leq k_1 < k_2 < \cdots,$ such that all of the entries of U_{k_i} converge (as sequences of complex numbers) to the entries of a unitary matrix as $i \to \infty$.*

Proof. All that is required here is the fact that from any infinite sequence in a compact set, one may always select a convergent subsequence. We have already observed that if a sequence of unitary matrices converges to some matrix, then the limit matrix must be unitary. $\square$

Remark. (a) The selection principle (2.15) applies as well to the real orthogonal group; that is, an infinite sequence of real orthogonal matrices has an infinite subsequences that converges to a real orthogonal matrix.
(b) The unitary limit guaranteed by the lemma need not be unique; it can depend on the subsequence chosen.

Example 2.16. Consider the sequence of unitary matrices $U_k = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}^k$, $k = 1, 2, \ldots$ Then $U_k = \begin{cases} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \text{if } k \text{ is odd,} \\ \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \text{if } k \text{ is even;} \end{cases}$ that is, there are two possible limits of subsequences.

A unitary matrix U has the property that U^{-1} *equals* U^*. One way to generalize the notion of a unitary matrix is to require that U^{-1} be *similar* to U^*. The set of such matrices is easily characterized as the range of the mapping $A \to A^{-1}A^*$ for all nonsingular $A \in M_n$.

Theorem 2.17. *Let $A \in M_n$ be nonsingular. Then A^{-1} is similar to A^* if and only if there is a nonsingular $B \in M_n$ such that $A = B^{-1}B^*$.*

Proof. ($\Leftarrow$) If $A = B^{-1}B^*$ for some nonsingular $B \in M_n$, then $A^{-1} = (B^*)^{-1}B$ and $B^*A^{-1}(B^*)^{-1} = B(B^*)^{-1} = (B^{-1}B^*)^* = A^*$, so A^{-1} is similar to A^* via the similarity matrix B^*.
($\Rightarrow$) If A^{-1} is similar to A^*, then there is a nonsingular $S \in M_n$ such that $SA^{-1}S^{-1} = A^*$ and hence $S = A^*SA$. Set $S_\theta = e^{i\theta}S$ for $\theta \in \mathbf{R}$ so that $S_\theta = A^*S_\theta A$ and $S_\theta^* = A^*S_\theta^*A$. Adding these two identities gives $H_\theta = A^*H_\theta A$, where $H_\theta = S_\theta + S_\theta^*$ is Hermitian.
If H_θ were singular, there would be a nonzero $x \in \mathbf{C}^n$ such that $0 = H_\theta x = S_\theta x + S_\theta^* x$, so $-x = S_\theta^{-1}S_\theta^*x = e^{-2i\theta}S^{-1}S^*x$ and $S^{-1}S^*x = -e^{2i\theta}x$. Choose a value of $\theta = \theta_0 \in [0, 2\pi)$ such that $-e^{2i\theta_0}$ is not an eigenvalue of $S^{-1}S^*$; the resulting Hermitian matrix $H = H_{\theta_0}$ is nonsingular and has the property that $H = A^*HA$.

Now choose any complex α such that $|\alpha| = 1$ and α is not an eigenvalue of A^*. Set $B = \beta(\alpha I - A^*)H$, where the complex parameter $\beta \neq 0$ is to be chosen, and observe that B is nonsingular. Since we want to have $A = B^{-1}B^*$, that is, $BA = B^*$, we compute $B^* = H(\bar{\beta}\bar{\alpha}I - \bar{\beta}A)$, and $BA = \beta(\alpha I - A^*)HA = \beta(\alpha HA - A^*HA) = \beta(\alpha HA - H) = H(\alpha\beta A - \beta I)$. We are done if we can select a nonzero β such that $\beta = -\bar{\beta}\bar{\alpha}$, but if $\alpha = e^{i\psi}$, then $\beta = e^{i(\pi-\psi)/2}$ will do. $\square$

Plane rotations and Householder matrices are special (and very simple) unitary matrices that play an important role in establishing some basic matrix factorizations. More importantly, Householder matrices are considered as the fundamental ingredient of *QR factorization*.

Example 2.18 (Plane rotations)**.** Let $1 \le i < j \le n$ and let

$$U(\theta; i, j) = \begin{bmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ & & & \cos\theta & & & & -\sin\theta & & & \\ & & & & 1 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 1 & & & & \\ & & & \sin\theta & & & & \cos\theta & & & \\ & & & & & & & & 1 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & 1 \end{bmatrix}$$

denote the result of replacing the (i, i) and (j, j) entries of n-by-n identity matrix by $\cos\theta$, replacing its (i, j) entry by $-\sin\theta$ and replacing its (j, i) entry by $\sin\theta$. The matrix $U(\theta; i, j)$ is called a *plane rotation* or *Givens rotation*. It is easy to verify that $U(\theta; i, j)$ is real orthogonal for any pair of indices i, j with $1 \le i < j \le n$ and any parameter $\theta \in [0, 2\pi)$, i.e., $U(\theta; i, j)^{-1} = U(\theta; i, j)^T = U(-\theta; i, j)$. Indeed, the matrix $U(\theta; i, j)$ carries out a rotation (through an angle θ) in the i, j coordinate plane of $\mathbf{R}^n$. Left multiplication by $U(\theta; i, j)$ affects only rows i and j of the matrix multiplied; right multiplication by $U(\theta; i, j)$ affects only columns i and j of the matrix multiplied.

Example 2.19 (Householder matrices)**.** Let $w \in \mathbf{C}^n$ be a nonzero vector. The *Householder matrix* $U_w \in M_n$ is defined by $U_w = I - 2(w^*w)^{-1}ww^*$. If w is a unit vector, then $U_w = I - 2ww^*$. A Householder matrix embrace the following important properties.
(a) A Householder matrix U_w is both unitary and Hermitian, so $U_w^{-1} = U_w$.

Proof. By definition, $U_w^* = I - 2(w^*w)^{-1}(ww^*)^* = I - 2(w^*w)^{-1}ww^* = U_w$,

$$\begin{aligned} U_w^* U_w = U_w^2 &= [I - 2(w^*w)^{-1}ww^*][I - 2(w^*w)^{-1}ww^*] \\ &= I - 4(w^*w)^{-1}(ww^*) + 4(w^*w)^{-2}[w(w^*w)w^*] \\ &= I - 4(w^*w)^{-1}(ww^*) + 4(w^*w)^{-1}(ww^*) \\ &= I, \end{aligned}$$

showing that $U_w^{-1} = U_w^* = U_w$. $\square$

Remark. In a similar fashion, we can show that the Householder matrix U_w is real orthogonal and symmetric when $w \in \mathbf{R}^n$ is a nonzero vector.

(b) A Householder matrix U_w acts as the identity on the subspace $w^\perp$ and that it acts as a reflection on the one-dimensional subspace spanned by w; that is, $U_w x = x$ if $x \perp w$ and $U_w w = -w$.

Proof. If $x \perp w$, namely, $w^*x = 0$, we have that $U_w x = [I - 2(w^*w)^{-1}ww^*]x = x - 2(w^*w)^{-1}w(w^*x) = x$. Additionally, $U_w w = [I - 2(w^*w)^{-1}ww^*]w = w - 2(w^*w)^{-1}w(w^*w) = -w$. $\square$

(c) The eigenvalues of a Householder matrix $U_w \in M_n$ are always $-1, \overbrace{1, ..., 1}^{n-1}$ and $\det U_w = -1$ for all n. Thus, for all n and every nonzero $w \in \mathbf{R}^n$, the Householder matrix $U_w \in M_n(\mathbf{R})$ is a real orthogonal matrix that is never a proper rotation matrix *(a real orthogonal matrix whose determinant is +1).*

Proof. Using Formula (19) in Lecture 1 or Example 1.26 in Lecture 2 and the fact that $\text{adj}(\alpha I) = \alpha^{n-1}I$, we compute

$$\begin{aligned} p_{U_w}(t) = \det(tI - U_w) &= \det[(t-1)I + 2(w^*w)^{-1}ww^*] \\ &= \det[(t-1)I] + 2(w^*w)^{-1}w^*\text{adj}[(t-1)I]w \\ &= (t-1)^n + 2(t-1)^{n-1}(w^*w)^{-1}w^*w \\ &= (t-1)^{n-1}(t+1), \end{aligned}$$

yielding that $U_w \in M_n$ has eigenvalues (-1) with multiplicity 1 and 1 with multiplicity $(n-1)$ and thus $\det(U_w) = \prod_{i=1}^{n} \lambda_i(U_w) = -1$, where $\lambda_i(U_w)$ is the i^{th} eigenvalue of U_w. $\square$

Definition 2.20. *A linear transformation $T : \mathbf{C}^n \to \mathbf{C}^m$ is called a Euclidean isometry if $||x||_2 = ||Tx||_2$ for all $x \in \mathbf{C}^n$.*

Theorem 2.9 (g) says that a square complex matrix $U \in M_n$ is a Euclidean isometry (via $U : x \to Ux$) if and only if it is unitary. However, the proof of Theorem 2.9 (g) did not explicitly give us a construction of the unitary matrix that takes any given vector in $\mathbf{C}^n$ into any other in $\mathbf{C}^n$ that has the same Euclidean norm. Fortunately, Householder matrices and unitary scalar matrices shed light on such an elegant construction.

Theorem 2.21. *Let $x, y \in \mathbf{C}^n$ be given and suppose that $||x||_2 = ||y||_2 > 0$. If $y = e^{i\theta}x$ for some real θ, let $U(y,x) = e^{i\theta}I_n$; otherwise, let $\phi \in [0, 2\pi)$ be such that $x^*y = e^{i\phi}|x^*y|$ (take $\phi = 0$ if $x^*y = 0$); let $w = e^{i\phi}x - y$; and let $U(y,x) = e^{i\phi}U_w$, where $U_w = I - 2(w^*w)^{-1}ww^*$ is a Householder matrix. Then $U(y,x)$ is unitary and essentially Hermitian, $U(y,x)x = y$, and $U(y,x)z \perp y$ whenever $z \perp x$. If x and y are real, then $U(y,x)$ is real orthogonal: $U(y,x) = I$ if $y = x$, and $U(y,x)$ is the real Householder matrix U_{x-y} otherwise.*

Proof. The assertions are readily verified if x and y are linearly dependent, that is, if $y = e^{i\theta}x$ for some real θ.
If x and y are linearly independent, the Cauchy-Schwarz inequality $|y^*x| \leq ||x||_2||y||_2$ and its equality condition guarantee that $x^*x \neq |x^*y|$. In order to verify that $U(y,x)x = y$, and $U(y,x)z \perp y$ whenever $z \perp x$, we first compute some small items involved in the whole calculating process:

$$\begin{aligned} w^*w &= (e^{i\phi}x - y)^*(e^{i\phi} - y) = x^*x - e^{-i\phi}x^*y - e^{i\phi}y^*x + y^*y \\ &= 2(x^*x - \mathrm{Re}(e^{-i\phi}x^*y)) = 2(x^*x - |x^*y|) \end{aligned}$$

and

$$w^*x = e^{-i\phi}x^*x - y^*x = e^{-i\phi}x^*x - e^{-i\phi}|y^*x| = e^{i\phi}(x^*x - |x^*y|)$$

and

$$y^*w = (e^{i\phi}y^*x - y^*y) = (|y^*x| - y^*y).$$

Therefore,

$$U(y,x)x = e^{i\phi}U_wx = e^{i\phi}(x - 2(w^*w)^{-1}ww^*x) = e^{i\phi}(x - (e^{i\phi}x - y)e^{-i\phi}) = y.$$

If $z \perp x$, then $w^*z = -y^*z$ and

$$\begin{aligned} y^*U(y,x)z &= e^{i\phi}\Big(y^*z - \frac{1}{x^*x - |x^*y|}(|y^*x| - y^*y)(-y^*z)\Big) \\ &= e^{i\phi}(y^*z + (-y^*z)) = 0. \end{aligned}$$

Since U_w is unitary and Hermitian, $U(y,x) = (e^{i\phi}I)U_w$ is unitary (as a product of two unitary matrices) and essentially Hermitian. $\square$

Remark. A matrix $A \in M_n$ is said to be *essentially Hermitian* if $e^{i\theta}A$ is Hermitian for some $\theta \in \mathbf{R}^n$.

Example 2.22. Let $y \in \mathbf{C}^n$ be a given unit vector and let e_1 be the first column of the n-by-n identity matrix. We construct $U(y, e_1)$ using the recipe in the preceding Theorem 2.21 and conclude that its first column should be y, since $y = U(y, e_1)e_1$. More generally, let $x \in \mathbf{C}^n$ be a given nonzero vector and therefore, the matrix $U(||x||_2 e_1, x)$ constructed in the preceding Theorem 2.21 is an essentially Hermitian unitary matrix that takes x into $||x||_2 e_1$.

We now apply the construction of the Euclidean isometry in Theorem 2.21 to deduce the well-known *QR factorization*.

Theorem 2.23. *(QR factorization) Let $A \in M_{n,m}$ be given.*

- *(a) If $n \geq m$, there is a $Q \in M_{n,m}$ with orthonormal columns and an upper triangular $R \in M_m$ with nonnegative main diagonal entries such that $A = QR$. In particular, if $m = n$, then the factor Q is unitary.*
- *(b) If* rank $A = m$, *then the factors Q and R in (a) are uniquely determined and the main diagonal entries of R are all positive.*
- *(c) There is a unitary $Q \in M_n$ and an upper triangular $R \in M_{n,m}$ with nonnegative diagonal entries such that $A = QR$.*
- *(d) If A is real, then the factors Q and R in (a),(b), and (d) may be taken to be real.*

Proof. (a) Let $a_1 \in \mathbf{C}^n$ be the first column of A, let $r_1 = ||a_1||_2$, and let U_1 be a unitary matrix such that $U_1 a_1 = r_1 e_1$. Theorem 2.21 gives an explicit construction for such a matrix, namely, $U(r_1 e_1, a_1)$. Partition

$$U_1 A = \begin{bmatrix} r_1 & \bigstar \\ 0 & A_2 \end{bmatrix}$$

where $A_2 \in M_{n-1,m-1}$. Let $a_2 \in \mathbf{C}^{n-1}$ be the first column of A_2 and let $r_2 = ||a_2||_2$. Use Theorem 2.21 again to construct a unitary $V_2 = U(r_2e_1, a_2) \in M_{n-1}$ such that $V_2a_2 = r_2e_1$ and let $U_2 = I_1 \oplus V_2$. Then

$$U_2U_1A = \begin{bmatrix} r_2 & & \bigstar \\ 0 & r_2 & \\ 0 & 0 & A_3 \end{bmatrix}$$

Repeat this construction m times to obtain

$$U_mU_{m-1}\cdots U_2U_1A = \begin{bmatrix} R \\ 0 \end{bmatrix}$$

where $R \in M_n$ is upper triangular. Its main diagonal entries are $r_1, ..., r_m$; they are all nonnegative. Let $U = U_mU_{m-1}\cdots U_2U_1$.
Partition $U^* = U_1^*U_2^*\cdots U_{m-1}^*U_m^* = [Q\ Q_2]$, where $Q \in M_{n,m}$ has orthonormal columns (it contains the first m columns of a unitary matrix). Then $A = QR$, as desired. In particular, if $m = n$, Q becomes a square matrix with orthonormal columns, which is thus unitary.
(b) If A has full column rank, then R is nonsingular, so its main diagonal entries are all positive. Suppose that rank $A = m$ and $A = QR = \tilde{Q}\tilde{R}$, where R and $\tilde{R}$ are upper triangular and have positive main diagonal entries, and Q and $\tilde{Q}$ have orthonormal columns. Then $A^*A = R^*(Q^*Q)R = R^*IR = R^*R$ and also $A^*A = \tilde{R}^*\tilde{R}$, so $R^*R = \tilde{R}^*\tilde{R}$ and $\tilde{R}^{-*}R^* = \tilde{R}R^{-1}$. This says that a lower triangular matrix equals an upper triangular matrix, so both must be diagonal: $\tilde{R}R^{-1} = D$ is diagonal, and it must have positive main diagonal entries because the main diagonal entries of both $\tilde{R}$ and R^{-1} are positive. But $\tilde{R} = DR$ implies that $D = \tilde{R}R^{-1} = \tilde{R}^{-*}R^* = (DR)^{-*}R^* = D^{-1}R^{-*}R^* = D^{-1}$, showing that $D^2 = I$ and hence $D = I$. We conclude that $\tilde{R} = R$ and hence $\tilde{Q} = Q$.
(c) If $n \geq m$, we may start with the factorization in (a), let $Q' = [Q\ Q_2] \in M_n$ be unitary, let $R' = \begin{bmatrix} R \\ 0 \end{bmatrix} \in M_{n,m}$, and observe that $A = QR = Q'R'$.
If $n < m$, we may undertake the construction in (a) (left multiplication by a sequence of scalar multiples of Householder transformations) and stops after n steps, when the factorization $U_n\cdots U_1A = [R\ \bigstar]$ is achieved and R is upper triangular. Entries in the $\bigstar$ block need not be zero.
(d) The assertion follows from the assurance in Theorem 2.21 that the unitary matrices U_i involved in the constructions in (a) and (c) may all be chosen to be real. □

Corollary 2.24. *(Cholesky factorization) Any $B \in M_n$ of the form $B = A^*A, A \in M_n$, may be written as $B = LL^*$, where $L \in M_n$ is lower triangular and has nonnegative diagonal entries.*

Proof. By Theorem 2.23, we factorize A into $A = QR$, where $Q \in M_n$ is unitary and $R \in M_n$ with nonnegative diagonal entries is upper triangular. Then $B = A^*A = (QR)^*QR = R^*Q^*QR = R^*IR = R^*R$. Choose $L = R^*$, which is lower triangular and has nonnegative diagonal entries. $\square$

Remark. (a) Theorem 2.23 (b) illuminates that if A is nonsingular, all the diagonal entries of L should be positive and L is unique.
(b) Every positive definite or semidefinite matrix may be factored in this way.

Some variants of the QR factorization of $A \in M_{n,m}$ can be useful in practice and we are supposed to discuss them in detail.

Corollary 2.25. *Let $A \in M_{n,m}$ be given. If $n \leq m$, then there is a $Q \in M_{n,m}$ with orthonormal rows and a lower triangular $L \in M_n$ with nonnegative main diagonal entries such that $A = LQ$.*

Proof. If $n \leq m$, then $A^* \in M_{m,n}$ and $A^* = \tilde{Q}R$ by Theorem 2.23, where $Q \in M_{m,n}$ has orthonormal columns and $R \in M_n$ is upper triangular. Then $A = R^*\tilde{Q}^*$ and the results follow by replacing R^* by L and $\tilde{Q}^*$ by Q. $\square$

Remark. If $Q' = \begin{bmatrix} Q \\ Q_2 \end{bmatrix}$ is unitary, we have the factorization of the form $A = [L\ 0]Q'$.

Corollary 2.26. *Let $A \in M_{n,m}$ be given.*

(a) There is a $Q \in M_{n,m}$ with orthonormal columns and a lower triangular $L \in M_m$ such that $A = QL$. If $\tilde{Q} = [Q\ Q_2]$ is unitary, we have a factorization of the form $A = \tilde{Q} \begin{bmatrix} L \\ 0 \end{bmatrix}$.

(b) If $n \leq m$, there is an upper triangular $R \in M_n$, $Q \in M_{n,m}$ with orthonormal rows, and a unitary $\tilde{Q} = \begin{bmatrix} Q \\ Q_2 \end{bmatrix} \in M_n$ such that $A = RQ = [R\ 0]\tilde{Q}$.

Proof. (a) Let K_p be the (real orthogonal and symmetric) p-by-p reversal matrix

$$\begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}$$

which has the pleasant property that $K_p^2 = I_p$. For square matrices $R \in M_p$, the matrix $L = K_p R K_p$ is lower triangular if R is upper triangular; the main diagonal entries of L are those of R, with the order reversed.

If $n \geq m$ and $AK_m = Q'R$ as in Theorem 2.23 (a), then $A = (Q'K_m)(K_m R K_m)$, which is a factorization of the form with $Q' \in M_{n,m}$ whose columns are orthonormal and an upper triangular $R \in M_n$. Thus, $Q = Q'K_m$ has the reversed order of columns of Q, which are still orthonormal, and $L = (K_m R K_m)$ is lower triangular.

If $n \leq m$ and we apply Theorem 2.23 (d) to AK_m, we obtain that $A = (QK_n)(K_n[R \bigstar]K_m)$, which is a factorization of the form

$$A = \tilde{Q}L,$$

where $\tilde{Q} \in M_n$ is unitary and $L \in M_{n,m}$ is lower triangular.
(b) If $n \leq m$ and we apply Theorem 2.23 (a) to A^*, we have that $A^*K_n = \tilde{Q}\tilde{R}$ and $A^* = (\tilde{Q}K_n)(K_n\tilde{R}K_n)$, i.e., $A = (K_n\tilde{R}K_n)^*(\tilde{Q}K_n)^*$. Thus, $R = (K_n\tilde{R}K_n)^*$ is upper triangular and $Q = (\tilde{Q}K_n)^*$ has orthonormal rows. $\square$

References

[1] Roger A. Horn, Charles R. Johnson (2012) *Matrix Analysis, Second Edition.* Cambridge University Press.