Basic Properties of Matrices

In this chapter, we build on the notions introduced on page 5, and discuss a wide range of basic topics related to matrices with real elements. Some of the properties carry over to matrices with complex elements, but the reader should not assume this. Occasionally, for emphasis, we will refer to “real” matrices, but unless it is stated otherwise, we are assuming the matrices are real.

The topics and the properties of matrices that we choose to discuss are motivated by applications in the data sciences. In Chapter 8, we will consider in more detail some special types of matrices that arise in regression analysis and multivariate data analysis, and then in Chapter 9 we will discuss some specific applications in statistics.

3.1 Basic Definitions and Notation

It is often useful to treat the rows or columns of a matrix as vectors. Terms such as linear independence that we have defined for vectors also apply to rows and/or columns of a matrix. The vector space generated by the columns of the $n \times m$ matrix $A$ is of order $n$ and of dimension $m$ or less, and is called the column space of $A$, the range of $A$, or the manifold of $A$. This vector space is denoted by

$$\mathcal{V}(A)$$

or

$$\text{span}(A).$$

(The argument of $\mathcal{V}(\cdot)$ or $\text{span}(\cdot)$ can be either a matrix or a set of vectors. Recall from Section 2.1.3 that if $G$ is a set of vectors, the symbol $\text{span}(G)$ denotes the vector space generated by the vectors in $G$.) We also define the row space of $A$ to be the vector space of order $m$ (and of dimension $n$ or less) generated by the rows of $A$; notice, however, the preference given to the column space.
Many of the properties of matrices that we discuss hold for matrices with an infinite number of elements, but throughout this book we will assume that the matrices have a finite number of elements, and hence the vector spaces are of finite order and have a finite number of dimensions.

Similar to our definition of multiplication of a vector by a scalar, we define the multiplication of a matrix $A$ by a scalar $c$ as

$$cA = (ca_{ij}).$$

The $a_{ii}$ elements of a matrix are called **diagonal elements**; an element $a_{ij}$ with $i < j$ is said to be “above the diagonal”, and one with $i > j$ is said to be “below the diagonal”. The vector consisting of all of the $a_{ii}$’s is called the **principal diagonal** or just the diagonal. The elements $a_{i,i+c}$ are called “codiagonals” or “minor diagonals”. If the matrix has $m$ columns, the $a_{i,m+1-i}$ elements of the matrix are called **skew diagonal elements**. We use terms similar to those for diagonal elements for elements above and below the skew diagonal elements. These phrases are used with both square and nonsquare matrices. The diagonal begins in the first row and first column (that is, $a_{11}$), and ends at $a_{kk}$, where $k$ is the minimum of the number of rows and the number of columns.

If, in the matrix $A$ with elements $a_{ij}$ for all $i$ and $j$, $a_{ij} = a_{ji}$, $A$ is said to be **symmetric**. A symmetric matrix is necessarily square. A matrix $A$ such that $a_{ij} = -a_{ji}$ is said to be **skew symmetric**. The diagonal entries of a skew symmetric matrix must be 0. If $a_{ij} = \bar{a}_{ji}$ (where $\bar{a}$ represents the conjugate of the complex number $a$), $A$ is said to be **Hermitian**. A Hermitian matrix is also necessarily square, and, of course, a real symmetric matrix is Hermitian. A Hermitian matrix is also called a **self-adjoint** matrix.

### Diagonal, Hollow, and Diagonally Dominant Matrices

If all except the principal diagonal elements of a matrix are 0, the matrix is called a **diagonal matrix**. A diagonal matrix is the most common and most important type of sparse matrix. If all of the principal diagonal elements of a matrix are 0, the matrix is called a **hollow matrix**. A skew symmetric matrix is hollow, for example. If all except the principal skew diagonal elements of a matrix are 0, the matrix is called a **skew diagonal matrix**.

An $n \times m$ matrix $A$ for which

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| \quad \text{for each } i = 1, \ldots, n$$

(3.1)
is said to be **row diagonally dominant**; one for which $|a_{jj}| > \sum_{i \neq j} |a_{ij}|$ for each $j = 1, \ldots, m$ is said to be **column diagonally dominant**. (Some authors refer to this as **strict** diagonal dominance and use “diagonal dominance” without qualification to allow the possibility that the inequalities in the definitions
are not strict.) Most interesting properties of such matrices hold whether the dominance is by row or by column. If \( A \) is symmetric, row and column diagonal dominances are equivalent, so we refer to row or column diagonally dominant symmetric matrices without the qualification; that is, as just diagonally dominant.

**Matrices with Special Patterns of Zeroes**

If all elements below the diagonal are 0, the matrix is called an *upper triangular matrix*; and a *lower triangular matrix* is defined similarly. If all elements of a column or row of a triangular matrix are zero, we still refer to the matrix as triangular, although sometimes we speak of its form as *trapezoidal*. Another form called trapezoidal is one in which there are more columns than rows, and the additional columns are possibly nonzero. The four general forms of triangular or trapezoidal matrices are shown below, using an intuitive notation with \( X \) and 0 to indicate the pattern.

\[
\begin{bmatrix}
X & X & X \\
0 & X & X \\
0 & 0 & X
\end{bmatrix}
\quad \begin{bmatrix}
X & X & X \\
0 & X & X \\
0 & 0 & 0
\end{bmatrix}
\quad \begin{bmatrix}
X & X & X \\
0 & X & X \\
0 & 0 & 0
\end{bmatrix}
\quad \begin{bmatrix}
X & X & X \\
0 & 0 & X \\
0 & 0 & 0
\end{bmatrix}
\]

In this notation, \( X \) indicates that the element is possibly not zero. It does not mean each element is the same. In some cases, \( X \) and 0 may indicate “submatrices”, which we discuss in the section on partitioned matrices.

If all elements are 0 except \( a_{i,i+c_k} \) for some small number of integers \( c_k \), the matrix is called a *band matrix* (or *banded matrix*). In many applications, \( c_k \in \{-w_l, -w_l + 1, \ldots, -1, 0, 1, \ldots, w_u - 1, w_u\} \). In such a case, \( w_l \) is called the *lower band width* and \( w_u \) is called the *upper band width*. These patterned matrices arise in time series and other stochastic process models as well as in solutions of differential equations, and so they are very important in certain applications. Although it is often the case that interesting band matrices are symmetric, or at least have the same number of codiagonals that are nonzero, neither of these conditions always occurs in applications of band matrices. If all elements below the principal skew diagonal elements of a matrix are 0, the matrix is called a *skew upper triangular matrix*. A common form of Hankel matrix, for example, is the skew upper triangular matrix (see page 334). Notice that the various terms defined here, such as triangular and band, also apply to nonsquare matrices.

Band matrices occur often in numerical solutions of partial differential equations. A band matrix with lower and upper band widths of 1 is a *tridiagonal matrix*. If all diagonal elements and all elements \( a_{i,i\pm 1} \) are nonzero, a tridiagonal matrix is called a “matrix of type 2”. The inverse of a covariance matrix that occurs in common stationary time series models is a matrix of type 2 (see page 334).
Using the intuitive notation of $X$ and $0$ as above, a band matrix may be written as

$$
\begin{bmatrix}
X & X & 0 & \cdots & 0 & 0 \\
X & X & X & \cdots & 0 & 0 \\
0 & X & X & \cdots & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \cdots & X & X \\
\end{bmatrix}
$$

Computational methods for matrices may be more efficient if the patterns are taken into account.

A matrix is in upper *Hessenberg form*, and is called a *Hessenberg matrix*, if it is upper triangular except for the first subdiagonal, which may be nonzero. That is, $a_{ij} = 0$ for $i > j + 1$:

$$
\begin{bmatrix}
X & X & X & \cdots & X \\
X & X & X & \cdots & X \\
0 & X & X & \cdots & X \\
0 & 0 & X & \cdots & X \\
\vdots & \vdots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \cdots & X \\
\end{bmatrix}
$$

A symmetric matrix that is in Hessenberg form is necessarily *tridiagonal*.

Hessenberg matrices arise in some methods for computing eigenvalues (see Chapter 7).

Many matrices of interest are *sparse*: that is, they have a large proportion of elements that are 0. The matrices discussed above are generally not considered sparse. (“A large proportion” is subjective, but generally means more than 75%, and in many interesting cases is well over 95%.) Efficient and accurate computations often require that the sparsity of a matrix be accommodated explicitly.

### 3.1.1 Matrix Shaping Operators

In order to perform certain operations on matrices and vectors, it is often useful first to reshape a matrix. The most common reshaping operation is the transpose, which we define in this section. Sometimes we may need to rearrange the elements of a matrix or form a vector into a special matrix. In this section, we define three operators for doing this.

**Transpose**

The *transpose* of a matrix is the matrix whose $i^{th}$ row is the $i^{th}$ column of the original matrix and whose $j^{th}$ column is the $j^{th}$ row of the original matrix. We use a superscript “$T$” to denote the transpose of a matrix; thus, if $A = (a_{ij})$, then
\[ A^T = (a_{ji}). \] (3.2)

(In other literature, the transpose is often denoted by a prime, as in \( A' = (a_{ji}) = A^T \).)

If the elements of the matrix are from the field of complex numbers, the conjugate transpose, also called the adjoint, is more useful than the transpose. (“Adjoint” is also used to denote another type of matrix, so we will generally avoid using that term. This meaning of the word is the origin of the other term for a Hermitian matrix, a “self-adjoint matrix”.) We use a superscript “H” to denote the conjugate transpose of a matrix; thus, if \( A = (a_{ij}) \), then \( A^H = (\bar{a}_{ji}) \). We also use a similar notation for vectors. If the elements of \( A \) are all real, then \( A^H = A^T \). (The conjugate transpose is often denoted by an asterisk, as in \( A^* = (\bar{a}_{ji}) = A^H \). This notation is more common if a prime is used to denote the transpose. We sometimes use the notation \( A^+ \) to denote a \( g_2 \) inverse of the matrix \( A \); see page 117.)

If (and only if) \( A \) is symmetric, \( A = A^T \); if (and only if) \( A \) is skew symmetric, \( A^T = -A \); and if (and only if) \( A \) is Hermitian, \( A = A^H \).

### Diagonal Matrices and Diagonal Vectors: diag(·) and vecdiag(·)

A square diagonal matrix can be specified by the \( \text{diag}(·) \) constructor function that operates on a vector and forms a diagonal matrix with the elements of the vector along the diagonal:

\[
\text{diag}((d_1, d_2, \ldots, d_n)) = \begin{bmatrix}
d_1 & 0 & \cdots & 0 \\
0 & d_2 & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & 0 & \cdots & d_n
\end{bmatrix}.
\] (3.3)

(Notice that the argument of \( \text{diag} \) is a vector; that is why there are two sets of parentheses in the expression above, although sometimes we omit one set without loss of clarity.) The \( \text{diag} \) function defined here is a mapping \( \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n} \). Later we will extend this definition slightly.

A very important diagonal matrix has all 1s along the diagonal. If it has \( n \) diagonal elements, it is denoted by \( I_n \); so \( I_n = \text{diag}(1_n) \). This is called the identity matrix of order \( n \). The size is often omitted, and we call it the identity matrix, and denote it by \( I \).

The \( \text{vecdiag}(·) \) function forms a vector from the principal diagonal elements of a matrix. If \( A \) is an \( n \times m \) matrix, and \( k = \min(n, m) \),

\[
\text{vecdiag}(A) = (a_{11}, \ldots, a_{kk}).
\] (3.4)

The \( \text{vecdiag} \) function defined here is a mapping \( \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^{\min(n,m)} \).

Sometimes we overload \( \text{diag}(·) \) to allow its argument to be a matrix, and in that case, it is the same as \( \text{vecdiag}(·) \). Both the R and Matlab computing systems, for example, use this overloading; that is, they each provide a single function (called \text{diag} in each case).
Forming a Vector from the Elements of a Matrix: vec(\cdot) and vech(\cdot)

It is sometimes useful to consider the elements of a matrix to be elements of a single vector. The most common way this is done is to string the columns of the matrix end-to-end into a vector. The vec(\cdot) function does this:

\[
\text{vec}(A) = (a_1^T, a_2^T, \ldots, a_m^T),
\]

(3.5)

where \(a_1, a_2, \ldots, a_m\) are the column vectors of the matrix \(A\). The vec function is also sometimes called the “pack” function. (A note on the notation: the right side of equation (3.5) is the notation for a column vector with elements \(a_i^T\); see Chapter 1.) The vec function is a mapping \(\mathbb{R}^{n \times m} \mapsto \mathbb{R}^{nm}\).

For a symmetric matrix \(A\) with elements \(a_{ij}\), the “vech” function stacks the unique elements into a vector:

\[
\text{vech}(A) = (a_{11}, a_{21}, \ldots, a_{m1}, a_{22}, \ldots, a_{m2}, \ldots, a_{mm}).
\]

(3.6)

There are other ways that the unique elements could be stacked that would be simpler and perhaps more useful (see the discussion of symmetric storage mode on page 474), but equation (3.6) is the standard definition of vech(\cdot). The vech function is a mapping \(\mathbb{R}^{n \times n} \mapsto \mathbb{R}^{n(n+1)/2}\).

3.1.2 Partitioned Matrices

We often find it useful to partition a matrix into submatrices; for example, in many applications in data analysis, it is often convenient to work with submatrices of various types representing different subsets of the data.

We usually denote the submatrices with capital letters with subscripts indicating the relative positions of the submatrices. Hence, we may write

\[
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix},
\]

(3.7)

where the matrices \(A_{11}\) and \(A_{12}\) have the same number of rows, \(A_{21}\) and \(A_{22}\) have the same number of rows, \(A_{11}\) and \(A_{21}\) have the same number of columns, and \(A_{12}\) and \(A_{22}\) have the same number of columns. Of course, the submatrices in a partitioned matrix may be denoted by different letters. Also, for clarity, sometimes we use a vertical bar to indicate a partition:

\[
A = [B | C].
\]

The vertical bar is used just for clarity and has no special meaning in this representation.

The term “submatrix” is also used to refer to a matrix formed from a given matrix by deleting various rows and columns of the given matrix. In this terminology, \(B\) is a submatrix of \(A\) if for each element \(b_{ij}\) there is an \(a_{kl}\)
with \( k \geq i \) and \( l \geq j \) such that \( b_{ij} = a_{kl} \); that is, the rows and/or columns of the submatrix are not necessarily contiguous in the original matrix. This kind of subsetting is often done in data analysis, for example, in variable selection in linear regression analysis.

A square submatrix whose principal diagonal elements are elements of the principal diagonal of the given matrix is called a principal submatrix. If \( A_{11} \) in the example above is square, it is a principal submatrix, and if \( A_{22} \) is square, it is also a principal submatrix. Sometimes the term “principal submatrix” is restricted to square submatrices. If a matrix is diagonally dominant, then it is clear that any principal submatrix of it is also diagonally dominant.

A principal submatrix that contains the \((1,1)\) element and whose rows and columns are contiguous in the original matrix is called a leading principal submatrix. If \( A_{11} \) is square, it is a leading principal submatrix in the example above.

Partitioned matrices may have useful patterns. A “block diagonal” matrix is one of the form

\[
\begin{bmatrix}
X & 0 & \cdots & 0 \\
0 & X & \cdots & 0 \\
\vdots & & \ddots & \vdots \\
0 & 0 & \cdots & X 
\end{bmatrix},
\]

where 0 represents a submatrix with all zeros and \( X \) represents a general submatrix with at least some nonzeros.

The \( \text{diag}(\cdot) \) function previously introduced for a vector is also defined for a list of matrices:

\[
\text{diag}(A_1, A_2, \ldots, A_k)
\]

denotes the block diagonal matrix with submatrices \( A_1, A_2, \ldots, A_k \) along the diagonal and zeros elsewhere. A matrix formed in this way is sometimes called a direct sum of \( A_1, A_2, \ldots, A_k \), and the operation is denoted by \( \oplus \):

\[
A_1 \oplus \cdots \oplus A_k = \text{diag}(A_1, \ldots, A_k). \tag{3.8}
\]

Although the direct sum is a binary operation, we are justified in defining it for a list of matrices because the operation is clearly associative.

The \( A_i \) may be of different sizes and they may not be square, although in most applications the matrices are square (and some authors define the direct sum only for square matrices).

We will define vector spaces of matrices below and then recall the definition of a direct sum of vector spaces (page 18), which is different from the direct sum defined above in terms of \( \text{diag}(\cdot) \).

**Transposes of Partitioned Matrices**

The transpose of a partitioned matrix is formed in the obvious way; for example,
\[
\begin{bmatrix}
A_{11} & A_{12} & A_{13} \\
A_{21} & A_{22} & A_{23}
\end{bmatrix}^T =
\begin{bmatrix}
A_{11}^T & A_{21}^T \\
A_{12}^T & A_{22}^T \\
A_{13}^T & A_{23}^T
\end{bmatrix}.
\] (3.9)

### 3.1.3 Matrix Addition

The sum of two matrices of the same shape is the matrix whose elements are the sums of the corresponding elements of the addends. As in the case of vector addition, we overload the usual symbols for the operations on the reals to signify the corresponding operations on matrices when the operations are defined; hence, addition of matrices is also indicated by “+”, as with scalar addition and vector addition. We assume throughout that writing a sum of matrices \(A + B\) implies that they are of the same shape; that is, that they are conformable for addition.

The “+” operator can also mean addition of a scalar to a matrix, as in \(A + a\), where \(A\) is a matrix and \(a\) is a scalar. Although this meaning of “+” is generally not used in mathematical treatments of matrices, in this book we use it to mean the addition of the scalar to each element of the matrix, resulting in a matrix of the same shape. This meaning is consistent with the semantics of modern computer languages such as Fortran 90/95 and R.

The addition of two \(n \times m\) matrices or the addition of a scalar to an \(n \times m\) matrix requires \(nm\) scalar additions.

The matrix additive identity is a matrix with all elements zero. We sometimes denote such a matrix with \(n\) rows and \(m\) columns as \(0_{n \times m}\), or just as 0. We may denote a square additive identity as \(0_n\).

### The Transpose of the Sum of Matrices

The transpose of the sum of two matrices is the sum of the transposes:

\[
(A + B)^T = A^T + B^T.
\] (3.10)

The sum of two symmetric matrices is therefore symmetric.

### Rank Ordering Matrices

There are several possible ways to form a rank ordering of matrices of the same shape, but no complete ordering is entirely satisfactory. If all of the elements of the matrix \(A\) are positive, we write

\[
A > 0;
\] (3.11)

if all of the elements are nonnegative, we write

\[
A \geq 0.
\] (3.12)
The terms “positive” and “nonnegative” and these symbols are not to be confused with the terms “positive definite” and “nonnegative definite” and similar symbols for important classes of matrices having different properties (which we will introduce in equation (3.66) and discuss further in Section 8.3.)

**Vector Spaces of Matrices**

Having defined scalar multiplication and matrix addition (for conformable matrices), we can define a vector space of $n \times m$ matrices as any set that is closed with respect to those operations. The individual operations of scalar multiplication and matrix addition allow us to define an axpy operation on the matrices, as in equation (2.1) on page 12. Closure of this space implies that it must contain the additive identity, just as we saw on page 13. The matrix additive identity is the 0 matrix.

As with any vector space, we have the concepts of linear independence, generating set or spanning set, basis set, essentially disjoint spaces, and direct sums of matrix vector spaces (as in equation (2.10), which is different from the direct sum of matrices defined in terms of diag(·) as in equation (3.8)).

An important vector space of matrices is $\mathbb{R}^{n \times m}$. For matrices $X, Y \in \mathbb{R}^{n \times m}$ and $a \in \mathbb{R}$, the axpy operation is $aX + Y$.

If $n \geq m$, a set of $nm \ n \times m$ matrices whose columns consist of all combinations of a set of $n \ n$-vectors that span $\mathbb{R}^n$ is a basis set for $\mathbb{R}^{n \times m}$. If $n < m$, we can likewise form a basis set for $\mathbb{R}^{n \times m}$ or for subspaces of $\mathbb{R}^{n \times m}$ in a similar way. If \{${B_1, \ldots, B_k}$\} is a basis set for $\mathbb{R}^{n \times m}$, then any $n \times m$ matrix can be represented as $\sum_{i=1}^{k} c_i B_i$. Subsets of a basis set generate subspaces of $\mathbb{R}^{n \times m}$.

Because the sum of two symmetric matrices is symmetric, and a scalar multiple of a symmetric matrix is likewise symmetric, we have a vector space of the $n \times n$ symmetric matrices. This is clearly a subspace of the vector space $\mathbb{R}^{n \times n}$. All vectors in any basis for this vector space must be symmetric. Using a process similar to our development of a basis for a general vector space of matrices, we see that there are $n(n + 1)/2$ matrices in the basis (see Exercise 3.1).

### 3.1.4 Scalar-Valued Operators on Square Matrices: The Trace

There are several useful mappings from matrices to real numbers; that is, from $\mathbb{R}^{n \times m}$ to $\mathbb{R}$. Some important ones are norms, which are similar to vector norms and which we will consider later. In this section and the next, we define two scalar-valued operators, the trace and the determinant, that apply to square matrices.
3. Basic Properties of Matrices

The Trace: \( \text{tr}(\cdot) \)

The sum of the diagonal elements of a square matrix is called the trace of the matrix. We use the notation “\( \text{tr}(A) \)” to denote the trace of the matrix \( A \):

\[
\text{tr}(A) = \sum_i a_{ii}. \tag{3.13}
\]

The Trace of the Transpose of Square Matrices

From the definition, we see

\[
\text{tr}(A) = \text{tr}(A^T). \tag{3.14}
\]

The Trace of Scalar Products of Square Matrices

For a scalar \( c \) and an \( n \times n \) matrix \( A \),

\[
\text{tr}(cA) = c \text{tr}(A). \tag{3.15}
\]

This follows immediately from the definition because for \( \text{tr}(cA) \) each diagonal element is multiplied by \( c \).

The Trace of Partitioned Square Matrices

If the square matrix \( A \) is partitioned such that the diagonal blocks are square submatrices, that is,

\[
A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{3.16}
\]

where \( A_{11} \) and \( A_{22} \) are square, then from the definition, we see that

\[
\text{tr}(A) = \text{tr}(A_{11}) + \text{tr}(A_{22}). \tag{3.17}
\]

The Trace of the Sum of Square Matrices

If \( A \) and \( B \) are square matrices of the same order, a useful (and obvious) property of the trace is

\[
\text{tr}(A + B) = \text{tr}(A) + \text{tr}(B). \tag{3.18}
\]

3.1.5 Scalar-Valued Operators on Square Matrices: The Determinant

The determinant, like the trace, is a mapping from \( \mathbb{R}^{n \times n} \) to \( \mathbb{R} \). Although it may not be obvious from the definition below, the determinant has far-reaching applications in matrix theory.
The Determinant: \( \det(\cdot) \)

For an \( n \times n \) (square) matrix \( A \), consider the product \( a_{1j_1} \cdots a_{nj_n} \), where \( \pi_j = (j_1, \ldots, j_n) \) is one of the \( n! \) permutations of the integers from 1 to \( n \). Define a permutation to be even or odd according to the number of times that a smaller element follows a larger one in the permutation. (For example, \((1, 3, 2)\) is an odd permutation, and \((3, 1, 2)\) and \((1, 2, 3)\) are even permutations.) Let \( \sigma(\pi_j) = 1 \) if \( \pi_j = (j_1, \ldots, j_n) \) is an even permutation, and let \( \sigma(\pi_j) = -1 \) otherwise. Then the determinant of \( A \), denoted by \( \det(A) \), is defined by

\[
\det(A) = \sum_{\text{all permutations}} \sigma(\pi_j)a_{1j_1} \cdots a_{nj_n}.
\]  

(3.18)

Notation and Simple Properties of the Determinant

The determinant is also sometimes written as \( |A| \).

I prefer the notation \( \det(A) \), because of the possible confusion between \( |A| \) and the absolute value of some quantity. The latter notation, however, is recommended by its compactness, and I do use it in expressions such as the PDF of the multivariate normal distribution (see equation (9.1)) that involve nonnegative definite matrices (see page 82 for the definition). The determinant of a matrix may be negative, and sometimes, as in measuring volumes (see page 68 for simple areas and page 181 for special volumes called Jacobians), we need to specify the absolute value of the determinant, so we need something of the form \( |\det(A)| \).

The definition of the determinant is not as daunting as it may appear at first glance. Many properties become obvious when we realize that \( \sigma(\cdot) \) is always \( \pm 1 \), and it can be built up by elementary exchanges of adjacent elements. For example, consider \( \sigma(3, 2, 1) \). There are three elementary exchanges beginning with the natural ordering:

\[
(1, 2, 3) \rightarrow (2, 1, 3) \rightarrow (2, 3, 1) \rightarrow (3, 2, 1);
\]

hence, \( \sigma(3, 2, 1) = (-1)^3 = -1 \).

If \( \pi_j \) consists of the interchange of exactly two elements in \((1, \ldots, n)\), say elements \( p \) and \( q \) with \( p < q \), then there are \( q - p \) elements before \( p \) that are larger than \( p \), and there are \( q - p - 1 \) elements between \( q \) and \( p \) in the permutation each with exactly one larger element preceding it. The total number is \( 2q - 2p + 1 \), which is an odd number. Therefore, if \( \pi_j \) consists of the interchange of exactly two elements, then \( \sigma(\pi_j) = -1 \).

If the integers \( 1, \ldots, m \) occur sequentially in a given permutation and are followed by \( m + 1, \ldots, n \) which also occur sequentially in the permutation, they can be considered separately:

\[
\sigma(j_1, \ldots, j_n) = \sigma(j_1, \ldots, j_m)\sigma(j_{m+1}, \ldots, j_n).
\]  

(3.19)
Furthermore, we see that the product $a_{1j} \cdots a_{nj}$ has exactly one factor from each unique row-column pair. These observations facilitate the derivation of various properties of the determinant (although the details are sometimes quite tedious).

We see immediately from the definition that the determinant of an upper or lower triangular matrix (or a diagonal matrix) is merely the product of the diagonal elements (because in each term of equation (3.18) there is a 0, except in the term in which the subscripts on each factor are the same).

**Minors, Cofactors, and Adjugate Matrices**

Consider the $2 \times 2$ matrix

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}. $$

From the definition of the determinant, we see that

$$\det(A) = a_{11}a_{22} - a_{12}a_{21}. \quad (3.20)$$

Now let $A$ be a $3 \times 3$ matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}. $$

In the definition of the determinant, consider all of the terms in which the elements of the first row of $A$ appear. With some manipulation of those terms, we can express the determinant in terms of determinants of submatrices as

$$\det(A) = a_{11}(-1)^{1+1}\det\left( \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} \right) + a_{12}(-1)^{1+2}\det\left( \begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{bmatrix} \right) + a_{13}(-1)^{1+3}\det\left( \begin{bmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \right). \quad (3.21)$$

Notice that this is the same form as in equation (3.20):

$$\det(A) = a_{11}(1)\det(a_{22}) + a_{12}(-1)\det(a_{21}).$$

The manipulation in equation (3.21) of the terms in the determinant could be carried out with other rows of $A$.

The determinants of the $2 \times 2$ submatrices in equation (3.21) are called **minors or complementary minors** of the associated element. The definition
can be extended to \((n-1) \times (n-1)\) submatrices of an \(n \times n\) matrix, for \(n \geq 2\). We denote the minor associated with the \(a_{ij}\) element as

\[
\det \left( A_{-(i)(j)} \right),
\]  

(3.22)

in which \(A_{-(i)(j)}\) denotes the submatrix that is formed from \(A\) by removing the \(i^{th}\) row and the \(j^{th}\) column. The sign associated with the minor corresponding to \(a_{ij}\) is \((-1)^{i+j}\). The minor together with its appropriate sign is called the cofactor of the associated element; that is, the cofactor of \(a_{ij}\) is \((-1)^{i+j} \det \left( A_{-(i)(j)} \right)\). We denote the cofactor of \(a_{ij}\) as \(a_{(ij)}\):

\[
a_{(ij)} = (-1)^{i+j} \det \left( A_{-(i)(j)} \right).
\]  

(3.23)

Notice that both minors and cofactors are scalars.

The manipulations leading to equation (3.21), though somewhat tedious, can be carried out for a square matrix of any size larger than \(1 \times 1\), and minors and cofactors are defined as above. An expression such as in equation (3.21) is called an expansion in minors or an expansion in cofactors.

The extension of the expansion (3.21) to an expression involving a sum of signed products of complementary minors arising from \((n-1) \times (n-1)\) submatrices of an \(n \times n\) matrix \(A\) is

\[
\det(A) = \sum_{j=1}^{n} a_{ij}(-1)^{i+j} \det \left( A_{-(i)(j)} \right)
\]  

or

\[
\det(A) = \sum_{j=1}^{n} a_{ij}a_{(ij)},
\]  

(3.24)

(3.25)

These expressions are called Laplace expansions. Each determinant \(\det \left( A_{-(i)(j)} \right)\) can likewise be expressed recursively in a similar expansion.

Expressions (3.24) and (3.25) are special cases of a more general Laplace expansion based on an extension of the concept of a complementary minor of an element to that of a complementary minor of a minor. The derivation of the general Laplace expansion is straightforward but rather tedious (see Harville, 1997, for example, for the details).

Laplace expansions could be used to compute the determinant, but the main value of these expansions is in proving properties of determinants. For example, from the special Laplace expansion (3.24) or (3.25), we can quickly see that the determinant of a matrix with two rows that are the same is zero. We see this by recursively expanding all of the minors until we have only \(2 \times 2\) matrices consisting of a duplicated row. The determinant of such a matrix is 0, so the expansion is 0.
The expansion in equation (3.24) has an interesting property: if instead of the elements $a_{ij}$ from the $i^{th}$ row we use elements from a different row, say the $k^{th}$ row, the sum is zero. That is, for $k \neq i$,

$$
\sum_{j=1}^{n} a_{kj}(-1)^{i+j}\det(A_{-(i)(j)}) = \sum_{j=1}^{n} a_{kj}a_{(ij)} = 0.
$$

(3.26)

This is true because such an expansion is exactly the same as an expansion for the determinant of a matrix whose $k^{th}$ row has been replaced by its $i^{th}$ row; that is, a matrix with two identical rows. The determinant of such a matrix is 0, as we saw above.

A certain matrix formed from the cofactors has some interesting properties. We define the matrix here but defer further discussion. The adjugate of the $n \times n$ matrix $A$ is defined as

$$
\text{adj}(A) = (a_{(ji)}),
$$

(3.27)

which is an $n \times n$ matrix of the cofactors of the elements of the transposed matrix. (The adjugate is also called the adjoint or sometimes “classical adjoint”, but as we noted above, the term adjoint may also mean the conjugate transpose. To distinguish it from the conjugate transpose, the adjugate is also sometimes called the “classical adjoint”. We will generally avoid using the term “adjoint”.) Note the reversal of the subscripts; that is,

$$
\text{adj}(A) = (a_{(ij)})^T.
$$

The adjugate has an interesting property involving matrix multiplication (which we will define below in Section 3.2) and the identity matrix:

$$
A \text{adj}(A) = \text{adj}(A)A = \det(A)I.
$$

(3.28)

To see this, consider the $(i, j)^{th}$ element of $A \text{adj}(A)$. By the definition of the multiplication of $A$ and $\text{adj}(A)$, that element is $\sum_k a_{ik}(\text{adj}(A))_{kj}$. Now, noting the reversal of the subscripts in $\text{adj}(A)$ in equation (3.27), and using equations (3.24) and (3.26), we have

$$
\sum_k a_{ik}(\text{adj}(A))_{kj} = \begin{cases} 
\det(A) & \text{if } i = j \\
0 & \text{if } i \neq j;
\end{cases}
$$

that is, $A \text{adj}(A) = \det(A)I$.

The adjugate has a number of other useful properties, some of which we will encounter later, as in equation (3.137).

The Determinant of the Transpose of Square Matrices

One important property we see immediately from a manipulation of the definition of the determinant is

$$
\det(A) = \det(A^T).
$$

(3.29)
The Determinant of Scalar Products of Square Matrices

For a scalar $c$ and an $n \times n$ matrix $A$,

$$\det(cA) = c^n \det(A).$$

(3.30)

This follows immediately from the definition because, for $\det(cA)$, each factor in each term of equation (3.18) is multiplied by $c$.

The Determinant of an Upper (or Lower) Triangular Matrix

If $A$ is an $n \times n$ upper (or lower) triangular matrix, then

$$\det(A) = \prod_{i=1}^{n} a_{ii}.$$  

(3.31)

This follows immediately from the definition. It can be generalized, as in the next section.

The Determinant of Certain Partitioned Square Matrices

Determinants of square partitioned matrices that are block diagonal or upper or lower block triangular depend only on the diagonal partitions:

$$\det(A) = \det \left( \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \right) = \det \left( \begin{bmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{bmatrix} \right) = \det \left( \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \right) = \det(A_{11})\det(A_{22}).$$

(3.32)

We can see this by considering the individual terms in the determinant, equation (3.18). Suppose the full matrix is $n \times n$, and $A_{11}$ is $m \times m$. Then $A_{22}$ is $(n - m) \times (n - m)$, $A_{21}$ is $(n - m) \times m$, and $A_{12}$ is $m \times (n - m)$. In equation (3.18), any addend for which $(j_1, \ldots, j_m)$ is not a permutation of the integers $1, \ldots, m$ contains a factor $a_{ij}$ that is in a 0 diagonal block, and hence the addend is 0. The determinant consists only of those addends for which $(j_1, \ldots, j_m)$ is a permutation of the integers $1, \ldots, m$, and hence $(j_{m+1}, \ldots, j_n)$ is a permutation of the integers $m+1, \ldots, n$,

$$\det(A) = \sum \sum \sigma(j_1, \ldots, j_m, j_{m+1}, \ldots, j_n)a_{1j_1} \cdots a_{mj_m}a_{m+1,j_{m+1}} \cdots a_{nj_n},$$

where the first sum is taken over all permutations that keep the first $m$ integers together while maintaining a fixed ordering for the integers $m+1$ through $n$, and the second sum is taken over all permutations of the integers from $m+1$ through $n$ while maintaining a fixed ordering of the integers from 1 to $m$. Now, using equation (3.19), we therefore have for $A$ of this special form.
Basic Properties of Matrices

\[
\det(A) = \sum \sum \sigma(j_1, \ldots, j_m, j_{m+1}, \ldots, j_n) a_{1j_1} \cdots a_{mj_m} a_{m+1,j_{m+1}} \cdots a_{nj_n}
\]

\[
= \sum \sigma(j_1, \ldots, j_m) a_{1j_1} \cdots a_{mj_m} \sum \sigma(j_{m+1}, \ldots, j_n) a_{m+1,j_{m+1}} \cdots a_{nj_n}
\]

\[
= \det(A_{11}) \det(A_{22}),
\]

which is equation (3.32). We use this result to give an expression for the determinant of more general partitioned matrices in Section 3.4.2.

Another useful partitioned matrix of the form of equation (3.15) has \( A_{11} = 0 \) and \( A_{21} = -I \):

\[
A = \begin{bmatrix}
0 & A_{12} \\
-I & A_{22}
\end{bmatrix}.
\]

In this case, using equation (3.24), we get

\[
det(A) = (((-1)^n+1)(-1))^n \det(A_{12})
\]

\[
= (-1)^{n(n+3)} \det(A_{12})
\]

\[
= \det(A_{12}). \quad (3.33)
\]

We will consider determinants of a more general partitioning in Section 3.4.2, beginning on page 110.

The Determinant of the Sum of Square Matrices

Occasionally it is of interest to consider the determinant of the sum of square matrices. We note in general that

\[
det(A + B) \neq det(A) + det(B),
\]

which we can see easily by an example. (Consider matrices in \( \mathbb{R}^{2 \times 2} \), for example, and let \( A = I \) and \( B = \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix} \).)

In some cases, however, simplified expressions for the determinant of a sum can be developed. We consider one in the next section.

A Diagonal Expansion of the Determinant

A particular sum of matrices whose determinant is of interest is one in which a diagonal matrix \( D \) is added to a square matrix \( A \), that is, \( \det(A + D) \). (Such a determinant arises in eigenanalysis, for example, as we see in Section 3.8.2.)

For evaluating the determinant \( \det(A + D) \), we can develop another expansion of the determinant by restricting our choice of minors to determinants of matrices formed by deleting the same rows and columns and then continuing to delete rows and columns recursively from the resulting matrices. The expansion is a polynomial in the elements of \( D \); and for our purposes later, that is the most useful form.
Before considering the details, let us develop some additional notation. The matrix formed by deleting the same row and column of $A$ is denoted $A_{-i}(i)$ as above (following equation (3.22)). In the current context, however, it is more convenient to adopt the notation $A_{(i_1,...,i_k)}$ to represent the matrix formed from rows $i_1,...,i_k$ and columns $i_1,...,i_k$ from a given matrix $A$. That is, the notation $A_{(i_1,...,i_k)}$ indicates the rows and columns kept rather than those deleted; and furthermore, in this notation, the indexes of the rows and columns are the same. We denote the determinant of this $k \times k$ matrix in the obvious way, $\det(A_{(i_1,...,i_k)})$. Because the principal diagonal elements of this matrix are principal diagonal elements of $A$, we call $\det(A_{(i_1,...,i_k)})$ a principal minor of $A$.

Now consider $\det(A + D)$ for the $2 \times 2$ case:

$$\det \left( \begin{bmatrix} a_{11} + d_1 & a_{12} \\ a_{21} & a_{22} + d_2 \end{bmatrix} \right).$$

Expanding this, we have

$$\det(A + D) = (a_{11} + d_1)(a_{22} + d_2) - a_{12}a_{21}$$

$$= \det \left( \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \right) + d_1d_2 + a_{22}d_1 + a_{11}d_2$$

$$= \det(A_{(1,2)}) + d_1d_2 + a_{22}d_1 + a_{11}d_2.$$ Of course, $\det(A_{(1,2)}) = \det(A)$, but we are writing it this way to develop the pattern. Now, for the $3 \times 3$ case, we have

$$\det(A + D) = \det(A_{(1,2,3)})$$

$$+ \det(A_{(2,3)})d_1 + \det(A_{(1,3)})d_2 + \det(A_{(1,2)})d_3$$

$$+ a_{33}d_1d_2 + a_{22}d_1d_3 + a_{11}d_2d_3$$

$$+ d_1d_2d_3.$$

(3.34)

In the applications of interest, the elements of the diagonal matrix $D$ may be a single variable: $d$, say. In this case, the expression simplifies to

$$\det(A + D) = \det(A_{(1,2,3)}) + \sum_{i \neq j} \det(A_{(i,j)})d + \sum_i a_{ii}d^2 + d^3.$$ (3.35)

Carefully continuing in this way for an $n \times n$ matrix, either as in equation (3.34) for $n$ variables or as in equation (3.35) for a single variable, we can make use of a Laplace expansion to evaluate the determinant.

Consider the expansion in a single variable because that will prove most useful. The pattern persists; the constant term is $|A|$, the coefficient of the first-degree term is the sum of the $(n - 1)$-order principal minors, and, at the other end, the coefficient of the $(n - 1)^{th}$-degree term is the sum of the
first-order principal minors (that is, just the diagonal elements), and finally the coefficient of the \( n \)-th-degree term is 1.

This kind of representation is called a diagonal expansion of the determinant because the coefficients are principal minors. It has occasional use for matrices with large patterns of zeros, but its main application is in analysis of eigenvalues, which we consider in Section 3.8.2.

**Computing the Determinant**

For an arbitrary matrix, the determinant is rather difficult to compute. The method for computing a determinant is not the one that would arise directly from the definition or even from a Laplace expansion. The more efficient methods involve first factoring the matrix, as we discuss in later sections.

The determinant is not very often directly useful, but although it may not be obvious from its definition, the determinant, along with minors, cofactors, and adjoint matrices, is very useful in discovering and proving properties of matrices. The determinant is used extensively in eigenanalysis (see Section 3.8).

**A Geometrical Perspective of the Determinant**

In Section 2.2, we discussed a useful geometric interpretation of vectors in a linear space with a Cartesian coordinate system. The elements of a vector correspond to measurements along the respective axes of the coordinate system. When working with several vectors, or with a matrix in which the columns (or rows) are associated with vectors, we may designate a vector \( x_i \) as \( x_i = (x_{i1}, \ldots, x_{id}) \). A set of \( d \) linearly independent \( d \)-vectors define a parallelotope in \( d \) dimensions. For example, in a two-dimensional space, the linearly independent 2-vectors \( x_1 \) and \( x_2 \) define a parallelogram, as shown in Figure 3.1. The area of this parallelogram is the base times the height, \( bh \), where, in this case, \( b \) is the length of the vector \( x_1 \), and \( h \) is the length of \( x_2 \) times the sine of the angle \( \theta \). Thus, making use of equation (2.45) on page 36 for the cosine of the angle, we have

\[
\text{area} = bh \\
= \|x_1\|\|x_2\| \sin(\theta) \\
= \|x_1\|\|x_2\| \sqrt{1 - \left( \frac{(x_1, x_2)}{\|x_1\|\|x_2\|} \right)^2} \\
= \sqrt{\|x_1\|^2\|x_2\|^2 - (x_1, x_2)^2} \\
= \sqrt{(x_{11}^2 + x_{12}^2)(x_{21}^2 + x_{22}^2) - (x_{11}x_{21} - x_{12}x_{22})^2} \\
= |x_{11}x_{22} - x_{12}x_{21}| \\
= |\det(X)|, \quad (3.36)
\]
Figure 3.1. Volume (Area) of Region Determined by $x_1$ and $x_2$

where $x_1 = (x_{11}, x_{12})$, $x_2 = (x_{21}, x_{22})$, and

$$X = \begin{bmatrix} x_1 & x_2 \end{bmatrix} = \begin{bmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \end{bmatrix}.$$

Although we will not go through the details here, this equivalence of a volume of a parallelepiped that has a vertex at the origin and the absolute value of the determinant of a square matrix whose columns correspond to the vectors that form the sides of the parallelepiped extends to higher dimensions.

In making a change of variables in integrals, as in equation (4.37) on page 181, we use the absolute value of the determinant of the Jacobian as a volume element. Another instance of the interpretation of the determinant as a volume is in the generalized variance, discussed on page 318.

3.2 Multiplication of Matrices and Multiplication of Vectors and Matrices

The elements of a vector or matrix are elements of a field, and most matrix and vector operations are defined in terms of the two operations of the field. Of course, in this book, the field of most interest is the field of real numbers.

3.2.1 Matrix Multiplication (Cayley)

There are various kinds of multiplication of matrices that may be useful. The most common kind of multiplication is Cayley multiplication. If the number of columns of the matrix $A$, with elements $a_{ij}$, and the number of rows of the
matrix $B$, with elements $b_{ij}$, are equal, then the (Cayley) product of $A$ and $B$ is defined as the matrix $C$ with elements

$$c_{ij} = \sum_k a_{ik} b_{kj}. \quad (3.37)$$

This is the most common type of matrix product, and we refer to it by the unqualified phrase “matrix multiplication”.

Cayley matrix multiplication is indicated by juxtaposition, with no intervening symbol for the operation: $C = AB$.

If the matrix $A$ is $n \times m$ and the matrix $B$ is $m \times p$, the product $C = AB$ is $n \times p$:

$$C = \begin{bmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nm} \end{bmatrix} \begin{bmatrix} b_{11} & \cdots & b_{1p} \\ \vdots & \ddots & \vdots \\ b_{m1} & \cdots & b_{mp} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + \cdots + a_{1m}b_{m1} \\ \vdots \\ a_{n1}b_{11} + \cdots + a_{nm}b_{m1} \end{bmatrix}.$$

Cayley matrix multiplication is a mapping,

$$\mathbb{R}^{n \times m} \times \mathbb{R}^{m \times p} \mapsto \mathbb{R}^{n \times p}.$$

The multiplication of an $n \times m$ matrix and an $m \times p$ matrix requires $nmp$ scalar multiplications and $np(m - 1)$ scalar additions. Here, as always in numerical analysis, we must remember that the definition of an operation, such as matrix multiplication, does not necessarily define a good algorithm for evaluating the operation.

It is obvious that while the product $AB$ may be well-defined, the product $BA$ is defined only if $n = p$; that is, if the matrices $AB$ and $BA$ are square. We assume throughout that writing a product of matrices $AB$ implies that the number of columns of the first matrix is the same as the number of rows of the second; that is, they are conformable for multiplication in the order given.

It is easy to see from the definition of matrix multiplication (3.37) that in general, even for square matrices, $AB \neq BA$. It is also obvious that if $AB$ exists, then $B^T A^T$ exists and, in fact,

$$B^T A^T = (AB)^T. \quad (3.38)$$

The product of symmetric matrices is not, in general, symmetric. If (but not only if) $A$ and $B$ are symmetric, then $AB = (BA)^T$.

Because matrix multiplication is not commutative, we often use the terms “premultiply” and “postmultiply” and the corresponding nominal forms of these terms. Thus, in the product $AB$, we may say $B$ is premultiplied by $A$, or, equivalently, $A$ is postmultiplied by $B$.

Although matrix multiplication is not commutative, it is associative; that is, if the matrices are conformable,

$$A(BC) = (AB)C. \quad (3.39)$$
It is also \emph{distributive} over addition; that is,
\[ A(B + C) = AB + AC \quad (3.40) \]
and
\[ (B + C)A = BA + CA. \quad (3.41) \]
These properties are obvious from the definition of matrix multiplication.
(Note that left-sided distribution is not the same as right-sided distribution because the multiplication is not commutative.)

An \( n \times n \) matrix consisting of 1s along the diagonal and 0s everywhere else is a \emph{multiplicative identity} for the set of \( n \times n \) matrices and Cayley multiplication. Such a matrix is called the \emph{identity matrix of order} \( n \), and is denoted by \( I_n \), or just by \( I \). The columns of the identity matrix are unit vectors.

The identity matrix is a multiplicative identity for any matrix so long as the matrices are conformable for the multiplication. If \( A \) is \( n \times m \), then
\[ I_n A = AI_m = A. \]

\section*{Powers of Square Matrices}

For a square matrix \( A \), its product with itself is defined, and so we will use the notation \( A^2 \) to mean the Cayley product \( AA \), with similar meanings for \( A^k \) for a positive integer \( k \). As with the analogous scalar case, \( A^k \) for a negative integer may or may not exist, and when it exists, it has a meaning for Cayley multiplication similar to the meaning in ordinary scalar multiplication. We will consider these issues later (in Section 3.3.3).

For an \( n \times n \) matrix \( A \), if \( A^k \) exists for negative integral values of \( k \), we define \( A^0 \) by
\[ A^0 = I_n. \quad (3.42) \]

For a diagonal matrix \( D = \text{diag} ((d_1, \ldots, d_n)) \), we have
\[ D^k = \text{diag} ((d_1^k, \ldots, d_n^k)). \quad (3.43) \]

\section*{Matrix Polynomials}

Polynomials in square matrices are similar to the more familiar polynomials in scalars. We may consider
\[ p(A) = b_0 I + b_1 A + \cdots b_k A^k. \]

The value of this polynomial is a matrix.

The theory of polynomials in general holds, and in particular, we have the useful factorizations of monomials: for any positive integer \( k \),
\[ I - A^k = (I - A)(I + A + \cdots A^{k-1}), \quad (3.44) \]
and for an odd positive integer \( k \),
\[ I + A^k = (I + A)(I - A + \cdots A^{k-1}). \quad (3.45) \]
3.2.2 Multiplication of Matrices with Special Patterns

Various properties of matrices may or may not be preserved under matrix multiplication. We have seen already that the product of symmetric matrices is not in general symmetric.

Many of the various patterns of zeroes in matrices discussed on page 53 are preserved under matrix multiplication. Assume \( A \) and \( B \) are square matrices of the same number of rows.

- If \( A \) and \( B \) are diagonal, \( AB \) is diagonal;
- if \( A \) and \( B \) are upper triangular, \( AB \) is upper triangular;
- if \( A \) and \( B \) are lower triangular, \( AB \) is lower triangular;
- if \( A \) is upper triangular and \( B \) is lower triangular, in general, none of \( AB, BA, A^T A, B^T B, A A^T \), and \( BB^T \) is triangular.

Each of these statements can be easily proven using the definition of multiplication in equation (3.37).

The products of banded matrices are generally banded with a wider bandwidth. If the bandwidth is too great, obviously the matrix can no longer be called banded.

Multiplication of Partitioned Matrices

Multiplication and other operations with partitioned matrices are carried out with their submatrices in the obvious way. Thus, assuming the submatrices are conformable for multiplication,

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix}
\begin{bmatrix}
B_{11} & B_{12} \\
B_{21} & B_{22}
\end{bmatrix}
= 
\begin{bmatrix}
A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\
A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22}
\end{bmatrix}.
\]

It is clear that the product of conformable block diagonal matrices is block diagonal.

Sometimes a matrix may be partitioned such that one partition is just a single column or row, that is, a vector or the transpose of a vector. In that case, we may use a notation such as

\[
\begin{bmatrix} X \\ y \end{bmatrix}
\]

or

\[
\begin{bmatrix} X | y \end{bmatrix},
\]

where \( X \) is a matrix and \( y \) is a vector. We develop the notation in the obvious fashion; for example,

\[
\begin{bmatrix} X \\ y \end{bmatrix}^T \begin{bmatrix} X & y \end{bmatrix} = 
\begin{bmatrix}
X^T X & X^T y \\
y^T X & y^T y
\end{bmatrix}.
\]

(3.46)
3.2 Multiplication of Matrices

3.2.3 Elementary Operations on Matrices

Many common computations involving matrices can be performed as a sequence of three simple types of operations on either the rows or the columns of the matrix:

- the interchange of two rows (columns),
- a scalar multiplication of a given row (column), and
- the replacement of a given row (column) by the sum of that row (columns) and a scalar multiple of another row (column); that is, an axpy operation.

Such an operation on the rows of a matrix can be performed by premultiplication by a matrix in a standard form, and an operation on the columns of a matrix can be performed by postmultiplication by a matrix in a standard form. To repeat:

- premultiplication: operation on rows;
- postmultiplication: operation on columns.

The matrix used to perform the operation is called an elementary transformation matrix or elementary operator matrix. Such a matrix is the identity matrix transformed by the corresponding operation performed on its unit rows, $e_T^p$, or columns, $e_p$.

In actual computations, we do not form the elementary transformation matrices explicitly, but their formulation allows us to discuss the operations in a systematic way and better understand the properties of the operations. Products of any of these elementary operator matrices can be used to effect more complicated transformations.

Operations on the rows are more common, and that is what we will discuss here, although operations on columns are completely analogous. These transformations of rows are called elementary row operations.

Interchange of Rows or Columns; Permutation Matrices

By first interchanging the rows or columns of a matrix, it may be possible to partition the matrix in such a way that the partitions have interesting or desirable properties. Also, in the course of performing computations on a matrix, it is often desirable to interchange the rows or columns of the matrix. (This is an instance of “pivoting”, which will be discussed later, especially in Chapter 6.) In matrix computations, we almost never actually move data from one row or column to another; rather, the interchanges are effected by changing the indexes to the data.

Interchanging two rows of a matrix can be accomplished by premultiplying the matrix by a matrix that is the identity with those same two rows interchanged; for example,
The first matrix in the expression above is called an *elementary permutation matrix*. It is the identity matrix with its second and third rows (or columns) interchanged. An elementary permutation matrix, which is the identity with the \(p\)th and \(q\)th rows interchanged, is denoted by \(E_{pq}\). That is, \(E_{pq}\) is the identity, except the \(p\)th row is \(e_q^T\) and the \(q\)th row is \(e_p^T\). Note that \(E_{pq} = E_{qp}\).

Thus, for example, if the given matrix is \(4 \times m\), to interchange the second and third rows, we use

\[
E_{23} = E_{32} = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}.
\]

It is easy to see from the definition that an elementary permutation matrix is symmetric. Note that the notation \(E_{pq}\) does not indicate the order of the elementary permutation matrix; that must be specified in the context.

Premultiplying a matrix \(A\) by a (conformable) \(E_{pq}\) results in an interchange of the \(p\)th and \(q\)th rows of \(A\) as we see above. Any permutation of rows of \(A\) can be accomplished by successive premultiplications by elementary permutation matrices. Note that the order of multiplication matters. Although a given permutation can be accomplished by different elementary permutations, the number of elementary permutations that effect a given permutation is always either even or odd; that is, if an odd number of elementary permutations results in a given permutation, any other sequence of elementary permutations to yield the given permutation is also odd in number. Any given permutation can be effected by successive interchanges of adjacent rows.

Postmultiplying a matrix \(A\) by a (conformable) \(E_{pq}\) results in an interchange of the \(p\)th and \(q\)th columns of \(A\):

\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33} \\
a_{41} & a_{42} & a_{43}
\end{bmatrix}
\begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
= \begin{bmatrix}
a_{11} & a_{13} & a_{12} \\
a_{21} & a_{23} & a_{22} \\
a_{31} & a_{33} & a_{32} \\
a_{41} & a_{43} & a_{42}
\end{bmatrix}.
\]

Note that

\[
A = E_{pq}E_{pq}A = AE_{pq}E_{pq};
\]

that is, as an operator, an elementary permutation matrix is its own inverse operator: \(E_{pq}E_{pq} = I\).

Because all of the elements of a permutation matrix are 0 or 1, the trace of an \(n \times n\) elementary permutation matrix is \(n - 2\).

The product of elementary permutation matrices is also a *permutation matrix* in the sense that it permutes several rows or columns. For example,
premultiplying $A$ by the matrix $Q = E_{pq}E_{qr}$ will yield a matrix whose $p$th row is the $r$th row of the original $A$, whose $q$th row is the $p$th row of $A$, and whose $r$th row is the $q$th row of $A$. We often use the notation $E_\pi$ to denote a more general permutation matrix. This expression will usually be used generically, but sometimes we will specify the permutation, $\pi$.

A general permutation matrix (that is, a product of elementary permutation matrices) is not necessarily symmetric, but its transpose is also a permutation matrix. It is not necessarily its own inverse, but its permutations can be reversed by a permutation matrix formed by products of elementary permutation matrices in the opposite order; that is,

$$E_\pi^T E_\pi = I.$$  

As a prelude to other matrix operations, we often permute both rows and columns, so we often have a representation such as

$$B = E_{\pi_1} AE_{\pi_2},$$

(3.48)

where $E_{\pi_1}$ is a permutation matrix to permute the rows and $E_{\pi_2}$ is a permutation matrix to permute the columns. We use these kinds of operations to arrive at the important equation (3.105) on page 93, and combine these operations with others to yield equation (3.119) on page 99. These equations are used to determine the number of linearly independent rows and columns and to represent the matrix in a form with a maximal set of linearly independent rows and columns clearly identified.

**The Vec-Permutation Matrix**

A special permutation matrix is the matrix that transforms the vector $\text{vec}(A)$ into $\text{vec}(A^T)$. If $A$ is $n \times m$, the matrix $K_{nm}$ that does this is $nm \times nm$. We have

$$\text{vec}(A^T) = K_{nm}\text{vec}(A).$$

(3.49)

The matrix $K_{nm}$ is called the $nm$ vec-permutation matrix.

**Scalar Row or Column Multiplication**

Often, numerical computations with matrices are more accurate if the rows have roughly equal norms. For this and other reasons, we often transform a matrix by multiplying one of its rows by a scalar. This transformation can also be performed by premultiplication by an elementary transformation matrix. For multiplication of the $p$th row by the scalar, the elementary transformation matrix, which is denoted by $E_p(a)$, is the identity matrix in which the $p$th diagonal element has been replaced by $a$. Thus, for example, if the given matrix is $4 \times m$, to multiply the second row by $a$, we use
Basic Properties of Matrices

Postmultiplication of a given matrix by the multiplier matrix \( E_p(a) \) results in the multiplication of the \( p \)\(^{th} \) column by the scalar. For this, \( E_p(a) \) is a square matrix of order equal to the number of columns of the given matrix.

Note that the notation \( E_p(a) \) does not indicate the number of rows and columns. This must be specified in the context.

Note that, if \( a \neq 0 \),

\[
A = E_p(1/a)E_p(a)A,
\]

that is, as an operator, the inverse operator is a row multiplication matrix on the same row and with the reciprocal as the multiplier.

Axpy Row or Column Transformations

The other elementary operation is an axpy on two rows and a replacement of one of those rows with the result

\[
a_p \leftarrow aa_q + a_p.
\]

This operation also can be effected by premultiplication by a matrix formed from the identity matrix by inserting the scalar in the \((p, q)\) position. Such a matrix is denoted by \( E_{pq}(a) \). Thus, for example, if the given matrix is \( 4 \times m \), to add \( a \) times the third row to the second row, we use

\[
E_{23}(a) = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & a & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}.
\]

Premultiplication of a matrix \( A \) by such a matrix,

\[
E_{pq}(a)A,
\]

yields a matrix whose \( p \)\(^{th} \) row is \( a \) times the \( q \)\(^{th} \) row plus the original row.

Given the \( 4 \times 3 \) matrix \( A = (a_{ij}) \), we have

\[
E_{23}(a)A = \begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} + aa_{31} & a_{22} + aa_{32} & a_{23} + aa_{33} \\
a_{31} & a_{32} & a_{33} \\
a_{41} & a_{42} & a_{43}
\end{bmatrix}.
\]

Postmultiplication of a matrix \( A \) by an axpy operator matrix,

\[
AE_{pq}(a),
\]
yields a matrix whose $q^{th}$ column is $a$ times the $p^{th}$ column plus the original column. For this, $E_{pq}(a)$ is a square matrix of order equal to the number of columns of the given matrix. Note that the column that is changed corresponds to the second subscript in $E_{pq}(a)$.

Note that

$$A = E_{pq}(-a)E_{pq}(a);$$

(3.52)

that is, as an operator, the inverse operator is the same axpy elementary operator matrix with the negative of the multiplier.

A common use of axpy operator matrices is to form a matrix with zeros in all positions of a given column below a given position in the column. These operations usually follow an operation by a scalar row multiplier matrix that puts a 1 in the position of interest. For example, given an $n \times m$ matrix $A$ with $a_{ij} \neq 0$, to put a 1 in the $(i,j)$ position and 0s in all positions of the $j^{th}$ column below the $i^{th}$ row, we form the product

$$E_{mi}(-a_{mj}) \cdots E_{i+1,i}(-a_{i+1,j})E_i(1/a_{ij})A.$$

(3.53)

This process is called Gaussian elimination.

Gaussian elimination is often performed sequentially down the diagonal elements of a matrix. If at some point $a_{ii} = 0$, the operations of equation (3.53) cannot be performed. In that case, we may first interchange the $i^{th}$ row with the $k^{th}$ row, where $k > i$ and $a_{ki} \neq 0$. Such an interchange is called pivoting. We will discuss pivoting in more detail on page 229 in Chapter 6.

To form a matrix with zeros in all positions of a given column except one, we use additional matrices for the rows above the given element:

$$E_{mi}(-a_{mj}) \cdots E_{i+1,i}(-a_{i+1,j}) \cdots E_{i-1,i}(-a_{i-1,j}) \cdots E_1(-a_{1j})E_i(1/a_{ij})A.$$

We can likewise zero out all elements in the $i^{th}$ row except the one in the $(ij)^{th}$ position by similar postmultiplications.

These elementary transformations are the basic operations in Gaussian elimination, which is discussed in Sections 5.6 and 6.2.1.

Elementary Operator Matrices: Summary of Notation

Because we have introduced various notation for elementary operator matrices, it may be worthwhile to review the notation. The notation is useful and I will use it from time to time, but unfortunately, there is no general form for the notation. I will generally use an “$E$” as the root symbol for the matrix, but the specific type is indicated by various other symbols.

Referring back to the listing of the types of operations on page 73, we have the various elementary operator matrices:

- $E_{pq}$: the interchange of rows $p$ and $q$ ($E_{pq}$ is the same as $E_{qp}$)
- $E_\pi$: a general permutation of rows, where $\pi$ denotes a permutation
- $E_p(a)$: multiplication of row $p$ by $a$. 
• \( E_{pq}(a) \): the replacement of row \( p \) by the sum of row \( p \) and \( a \) times row \( q \).

Recall that these operations are effected by premultiplication. The same kinds of operations on the columns are effected by postmultiplication.

**Determinants of Elementary Operator Matrices**

The determinant of an elementary permutation matrix \( E_{pq} \) has only one term in the sum that defines the determinant (equation (3.18), page 61), and that term is 1 times \( \sigma \) evaluated at the permutation that exchanges \( p \) and \( q \). As we have seen (page 61), this is an odd permutation; hence, for an elementary permutation matrix \( E_{pq} \),

\[
\det(E_{pq}) = -1.
\]  

(3.54)

Because all terms in \( \det(E_{pq}A) \) are exactly the same terms as in \( \det(A) \) but with one different permutation in each term, we have

\[
\det(E_{pq}A) = -\det(A).
\]

More generally, if \( A \) and \( E_\pi \) are \( n \times n \) matrices, and \( E_\pi \) is any permutation matrix (that is, any product of \( E_{pq} \) matrices), then \( \det(E_\pi A) \) is either \( \det(A) \) or \( -\det(A) \) because all terms in \( \det(E_\pi A) \) are exactly the same as the terms in \( \det(A) \) but possibly with different signs because the permutations are different. In fact, the differences in the permutations are exactly the same as the permutation of 1, \ldots, \( n \) in \( E_\pi \); hence,

\[
\det(E_\pi A) = \det(E_\pi) \det(A).
\]

(In equation (3.60) below, we will see that this equation holds more generally.)

The determinant of an elementary row multiplication matrix \( E_p(a) \) is

\[
\det(E_p(a)) = a.
\]  

(3.55)

If \( A \) and \( E_p(a) \) are \( n \times n \) matrices, then

\[
\det(E_p(a)A) = a\det(A),
\]

as we see from the definition of the determinant, equation (3.18).

The determinant of an elementary axpy matrix \( E_{pq}(a) \) is 1,

\[
\det(E_{pq}(a)) = 1,
\]  

(3.56)

because the term consisting of the product of the diagonals is the only term in the determinant.

Now consider \( \det(E_{pq}(a)A) \) for an \( n \times n \) matrix \( A \). Expansion in the minors (equation (3.24)) along the \( p^{th} \) row yields
\[
\det(E_{pq}(a)A) = \sum_{j=1}^{n} (a_{pj} + aa_{qj})(-1)^{p+j} \det(A_{ij}) \\
= \sum_{j=1}^{n} a_{pj}(-1)^{p+j} \det(A_{ij}) + a \sum_{j=1}^{n} a_{qj}(-1)^{p+j} \det(A_{ij}).
\]

From equation (3.26) on page 64, we see that the second term is 0, and since the first term is just the determinant of \(A\), we have
\[
\det(E_{pq}(a)A) = \det(A). \tag{3.57}
\]

### 3.2.4 The Trace of a Cayley Product that Is Square

A useful property of the trace for the matrices \(A\) and \(B\) that are conformable for the multiplications \(AB\) and \(BA\) is
\[
\text{tr}(AB) = \text{tr}(BA). \tag{3.58}
\]

This is obvious from the definitions of matrix multiplication and the trace. Note that \(A\) and \(B\) may not be square (so the trace is not defined for them), but if they are conformable for the multiplications, then both \(AB\) and \(BA\) are square.

Because of the associativity of matrix multiplication, this relation can be extended as
\[
\text{tr}(ABC) = \text{tr}(BCA) = \text{tr}(CAB) \tag{3.59}
\]
for matrices \(A\), \(B\), and \(C\) that are conformable for the multiplications indicated. Notice that the individual matrices need not be square. This fact is very useful in working with quadratic forms, as in equation (3.68).

### 3.2.5 The Determinant of a Cayley Product of Square Matrices

An important property of the determinant is
\[
\det(AB) = \det(A) \det(B) \tag{3.60}
\]
if \(A\) and \(B\) are square matrices conformable for multiplication. We see this by first forming
\[
\det \left( \begin{bmatrix} I & A \\ 0 & I \end{bmatrix} \begin{bmatrix} A & 0 \\ -I & B \end{bmatrix} \right) = \det \left( \begin{bmatrix} 0 & AB \\ -I & B \end{bmatrix} \right) \tag{3.61}
\]
and then observing from equation (3.33) that the right-hand side is \(\det(AB)\). Now consider the left-hand side. The matrix that is the first factor on the left-hand side is a product of elementary axpy transformation matrices; that is, it is a matrix that when postmultiplied by another matrix merely adds multiples of rows in the lower part of the matrix to rows in the upper part of
the matrix. If $A$ and $B$ are $n \times n$ (and so the identities are likewise $n \times n$),
the full matrix is the product:

$$\begin{bmatrix}
I & A \\
0 & I
\end{bmatrix} = E_{1,n+1}(a_{11}) \cdots E_{1,2n}(a_{1n}) E_{2,n+1}(a_{21}) \cdots E_{2,2n}(a_{2n}) \cdots E_{n,2n}(a_{nn}).$$

Hence, applying equation (3.57) recursively, we have

$$\det \left( \begin{bmatrix} I & A \\ 0 & I \end{bmatrix} \begin{bmatrix} A & 0 \\ -I & B \end{bmatrix} \right) = \det \begin{bmatrix} A & 0 \\ -I & B \end{bmatrix},$$

and from equation (3.32) we have

$$\det \begin{bmatrix} A & 0 \\ -I & B \end{bmatrix} = \det(A)\det(B),$$

and so finally we have equation (3.60).

From equation (3.60), we see that if $A$ and $B$ are square matrices con-
formable for multiplication, then

$$\det(AB) = \det(BA). \quad (3.62)$$

(Recall, in general, even in the case of square matrices, $AB \neq BA$.) This
equation is to be contrasted with equation (3.58), $\text{tr}(AB) = \text{tr}(BA)$, which
does not even require that the matrices be square. A simple counterexample
for nonsquare matrices is $\det(xx^T) \neq \det(x^Tx)$, where $x$ is a vector with
at least two elements. (Here, think of the vector as an $n \times 1$ matrix. This
counterexample can be seen in various ways. One way is to use a fact that we
will encounter on page 105, and observe that $\det(xx^T) = 0$ for any $x$ with at
least two elements.)

### 3.2.6 Multiplication of Matrices and Vectors

It is often convenient to think of a vector as a matrix with only one ele-
ment in one of its dimensions. This provides for an immediate extension of
the definitions of transpose and matrix multiplication to include vectors as
either or both factors. In this scheme, we follow the convention that a vector
corresponds to a column; that is, if $x$ is a vector and $A$ is a matrix, $Ax$
or $x^TA$ may be well-defined, but neither $xA$ nor $Ax^T$ would represent anything,
except in the case when all dimensions are 1. (In some computer systems for
matrix algebra, these conventions are not enforced; see, for example the R
code in Figure 12.4 on page 491.) The alternative notation $x^Ty$ we introduced
earlier for the dot product or inner product, $\langle x, y \rangle$, of the vectors $x$ and $y$
is consistent with this paradigm.

Vectors and matrices are fundamentally different kinds of mathematical
objects. In general, it is not relevant to say that a vector is a “column” or
a “row”; it is merely a one-dimensional (or rank 1) object. We will continue to write vectors as \( x = (x_1, \ldots, x_n) \), but this does not imply that the vector is a “row vector”. Matrices with just one row or one column are different objects from vectors. We represent a matrix with one row in a form such as \( Y = [y_{11} \ldots y_{1n}] \), and we represent a matrix with one column in a form such as

\[
Y = \begin{bmatrix}
y_{11} \\
\vdots \\
y_{m1}
\end{bmatrix}
\]

(Compare the notation in equations (1.1) and (1.2) on page 4.)

The Matrix/Vector Product as a Linear Combination

If we represent the vectors formed by the columns of an \( n \times m \) matrix \( A \) as \( a_1, \ldots, a_m \), the matrix/vector product \( Ax \) is a linear combination of these columns of \( A \):

\[
Ax = \sum_{i=1}^{m} x_i a_i. \tag{3.63}
\]

(Here, each \( x_i \) is a scalar, and each \( a_i \) is a vector.)

Given the equation \( Ax = b \), we have \( b \in \text{span}(A) \); that is, the \( n \)-vector \( b \) is in the \( k \)-dimensional column space of \( A \), where \( k \leq m \).

3.2.7 Outer Products

The outer product of the vectors \( x \) and \( y \) is the matrix

\[
xy^T. \tag{3.64}
\]

Note that the definition of the outer product does not require the vectors to be of equal length. Note also that while the inner product is commutative, the outer product is not commutative (although it does have the property \( xy^T = (yx^T)^T \)).

A very common outer product is of a vector with itself:

\[
xx^T.
\]

The outer product of a vector with itself is obviously a symmetric matrix.

We should again note some subtleties of differences in the types of objects that result from operations. If \( A \) and \( B \) are matrices conformable for the operation, the product \( A^T B \) is a matrix even if both \( A \) and \( B \) are \( n \times 1 \) and so the result is \( 1 \times 1 \). For the vectors \( x \) and \( y \) and matrix \( C \), however, \( x^Ty \) and \( x^TCy \) are scalars; hence, the dot product and a quadratic form are not the same as the result of a matrix multiplication. The dot product is a scalar, and the result of a matrix multiplication is a matrix. The outer product of vectors is a matrix, even if both vectors have only one element. Nevertheless, as we have mentioned before, we will treat a one by one matrix or a vector with only one element as a scalar whenever it is convenient to do so.
3.2.8 Bilinear and Quadratic Forms; Definiteness

A variation of the vector dot product, \( x^T Ay \), is called a bilinear form, and the special bilinear form \( x^T Ax \) is called a quadratic form. Although in the definition of quadratic form we do not require \( A \) to be symmetric—because for a given value of \( x \) and a given value of the quadratic form \( x^T Ax \) there is a unique symmetric matrix \( A_s \) such that \( x^T A_s x = x^T Ax \)—we generally work only with symmetric matrices in dealing with quadratic forms. (The matrix \( A_s \) is \( \frac{1}{2}(A + A^T) \); see Exercise 3.3.) Quadratic forms correspond to sums of squares and hence play an important role in statistical applications.

Nonnegative and Positive Definite Matrices

A symmetric matrix \( A \) such that for any (conformable and real) vector \( x \) the quadratic form \( x^T Ax \) is nonnegative, that is,

\[
x^T Ax \geq 0,
\]

is called a nonnegative definite matrix. We denote the fact that \( A \) is nonnegative definite by

\[
A \succeq 0.
\]

(Note that we consider \( 0_{n \times n} \) to be nonnegative definite.)

A symmetric matrix \( A \) such that for any (conformable) vector \( x \neq 0 \) the quadratic form

\[
x^T Ax > 0
\]

is called a positive definite matrix. We denote the fact that \( A \) is positive definite by

\[
A \succ 0.
\]

(Recall that \( A \geq 0 \) and \( A > 0 \) mean, respectively, that all elements of \( A \) are nonnegative and positive.) When \( A \) and \( B \) are symmetric matrices of the same order, we write \( A \succeq B \) to mean \( A - B \succeq 0 \) and \( A \succ B \) to mean \( A - B \succ 0 \). Nonnegative and positive definite matrices are very important in applications. We will encounter them from time to time in this chapter, and then we will discuss more of their properties in Section 8.3.

In this book we use the terms “nonnegative definite” and “positive definite” only for symmetric matrices. In other literature, these terms may be used more generally; that is, for any (square) matrix that satisfies (3.65) or (3.66).

The Trace of Inner and Outer Products

The invariance of the trace to permutations of the factors in a product (equation (3.58)) is particularly useful in working with bilinear and quadratic forms. Let \( A \) be an \( n \times m \) matrix, \( x \) be an \( n \)-vector, and \( y \) be an \( m \)-vector. Because
the bilinear form is a scalar (or a $1 \times 1$ matrix), and because of the invariance, we have the very useful fact

$$x^T Ay = \text{tr}(x^T Ay) = \text{tr}(Ayx^T).$$

(3.67)

A common instance is when $A$ is square and $x = y$. We have for the quadratic form the equality

$$x^T Ax = \text{tr}(Ax^T).$$

(3.68)

In equation (3.68), if $A$ is the identity $I$, we have that the inner product of a vector with itself is the trace of the outer product of the vector with itself, that is,

$$x^T x = \text{tr}(xx^T).$$

(3.69)

Also, by letting $A$ be the identity in equation (3.68), we have an alternative way of showing that for a given vector $x$ and any scalar $a$, the norm $\|x - a\|$ is minimized when $a = \bar{x}$:

$$(x - a)^T (x - a) = \text{tr}(xx^T) + n(a - \bar{x})^2.$$  

(3.70)

(Here, “$\bar{x}$” denotes the mean of the elements in $x$. Compare this with equation (2.61) on page 44.)

3.2.9 Anisometric Spaces

In Section 2.1, we considered various properties of vectors that depend on the inner product, such as orthogonality of two vectors, norms of a vector, angles between two vectors, and distances between two vectors. All of these properties and measures are invariant to the orientation of the vectors; the space is isometric with respect to a Cartesian coordinate system. Noting that the inner product is the bilinear form $x^T I y$, we have a heuristic generalization to an anisometric space. Suppose, for example, that the scales of the coordinates differ; say, a given distance along one axis in the natural units of the axis is equivalent (in some sense depending on the application) to twice that distance along another axis, again measured in the natural units of the axis. The properties derived from the inner product, such as a norm and a metric, may correspond to the application better if we use a bilinear form in which the matrix reflects the different effective distances along the coordinate axes. A diagonal matrix whose entries have relative values corresponding to the inverses of the relative scales of the axes may be more useful. Instead of $x^T y$, we may use $x^T Dy$, where $D$ is this diagonal matrix.

Rather than differences in scales being just in the directions of the coordinate axes, more generally we may think of anisometries being measured by general (but perhaps symmetric) matrices. (The covariance and correlation matrices defined on page 316 come to mind. Any such matrix to be used in this
context should be positive definite because we will generalize the dot product, which is necessarily nonnegative, in terms of a quadratic form.) A bilinear form \( x^T Ay \) may correspond more closely to the properties of the application than the standard inner product.

We define orthogonality of two vectors \( x \) and \( y \) with respect to \( A \) by

\[
x^T Ay = 0.
\]

(3.71)

In this case, we say \( x \) and \( y \) are \( A \)-conjugate.

The \( L_2 \) norm of a vector is the square root of the quadratic form of the vector with respect to the identity matrix. A generalization of the \( L_2 \) vector norm, called an elliptic norm or a conjugate norm, is defined for the vector \( x \) as the square root of the quadratic form \( x^T Ax \) for any symmetric positive definite matrix \( A \). It is sometimes denoted by \( \|x\|_A \):

\[
\|x\|_A = \sqrt{x^T Ax}.
\]

(3.72)

It is easy to see that

\[
\|x\|_A
\]

satisfies the definition of a norm given on page 24. If \( A \) is a diagonal matrix with elements \( w_i \geq 0 \), the elliptic norm is the weighted \( L_2 \) norm of equation (2.31).

The elliptic norm yields an elliptic metric in the usual way of defining a metric in terms of a norm. The distance between the vectors \( x \) and \( y \) with respect to \( A \) is \( \sqrt{(x - y)^T A (x - y)} \). It is easy to see that this satisfies the definition of a metric given on page 30.

A metric that is widely useful in statistical applications is the Mahalanobis distance, which uses a covariance matrix as the scale for a given space. (The sample covariance matrix is defined in equation (8.70) on page 316.) If \( S \) is the covariance matrix, the Mahalanobis distance, with respect to that matrix, between the vectors \( x \) and \( y \) is

\[
\sqrt{(x - y)^T S^{-1} (x - y)}.
\]

(3.73)

3.2.10 Other Kinds of Matrix Multiplication

The most common kind of product of two matrices is the Cayley product, and when we speak of matrix multiplication without qualification, we mean the Cayley product. Three other types of matrix multiplication that are useful are Hadamard multiplication, Kronecker multiplication, and inner product multiplication.

The Hadamard Product

Hadamard multiplication is defined for matrices of the same shape as the multiplication of each element of one matrix by the corresponding element of the
other matrix. Hadamard multiplication immediately inherits the commutativity, associativity, and distribution over addition of the ordinary multiplication of the underlying field of scalars. Hadamard multiplication is also called array multiplication and element-wise multiplication. Hadamard matrix multiplication is a mapping

\[ \mathbb{R}^{n \times m} \times \mathbb{R}^{n \times m} \mapsto \mathbb{R}^{n \times m}. \]

The identity for Hadamard multiplication is the matrix of appropriate shape whose elements are all 1s.

### The Kronecker Product

Kronecker multiplication, denoted by \( \otimes \), is defined for any two matrices \( A_{n \times m} \) and \( B_{p \times q} \) as

\[
A \otimes B = \begin{bmatrix}
    a_{11}B & \ldots & a_{1m}B \\
    \vdots & \ddots & \vdots \\
    a_{n1}B & \ldots & a_{nm}B
\end{bmatrix}.
\]

The Kronecker product of \( A \) and \( B \) is \( np \times mq \); that is, Kronecker matrix multiplication is a mapping

\[ \mathbb{R}^{n \times m} \times \mathbb{R}^{p \times q} \mapsto \mathbb{R}^{np \times mq}. \]

The Kronecker product is also called the “right direct product” or just direct product. (A left direct product is a Kronecker product with the factors reversed. In some of the earlier literature, “Kronecker product” was used to mean a left direct product.) Note the similarity of the Kronecker product of matrices with the direct product of sets, defined on page 5, in the sense that the result is formed from ordered pairs of elements from the two operands.

Kronecker multiplication is not commutative, but it is associative and it is distributive over addition, as we will see below. (Again, this parallels the direct product of sets.)

The identity for Kronecker multiplication is the \( 1 \times 1 \) matrix with the element 1; that is, it is the same as the scalar 1.

We can understand the properties of the Kronecker product by expressing the \((i, j)\) element of \( A \otimes B \) in terms of the elements of \( A \) and \( B \),

\[
(A \otimes B)_{i,j} = A_{[i/p]+1, \ [j/q]+1} B_{i-p[i/p], \ j-q[i/q]}, \tag{3.74}
\]

where \([\cdot]\) is the greatest integer function.

Some additional properties of Kronecker products that are immediate results of the definition are, assuming the matrices are conformable for the indicated operations,
(aA) ⊗ (bB) = ab(A ⊗ B)
= (abA) ⊗ B
= A ⊗ (abB), for scalars \(a, b\), \(3.75\)

\((A + B) ⊗ (C) = A ⊗ C + B ⊗ C, \(3.76\)\)

\((A ⊗ B) ⊗ C = A ⊗ (B ⊗ C), \(3.77\)\)

\((A ⊗ B)^T = A^T ⊗ B^T, \(3.78\)\)

\((A ⊗ B)(C ⊗ D) = AC ⊗ BD. \(3.79\)\)

These properties are all easy to see by using equation \((3.74)\) to express the \((i, j)\) element of the matrix on either side of the equation, taking into account the size of the matrices involved. For example, in the first equation, if \(A\) is \(n \times m\) and \(B\) is \(p \times q\), the \((i, j)\) element on the left-hand side is

\[aA_{\lfloor i/p\rfloor + 1, \lfloor j/q\rfloor + 1}bB_{i-p\lfloor i/p\rfloor, j-q\lfloor i/q\rfloor}\]

and that on the right-hand side is

\[abA_{\lfloor i/p\rfloor + 1, \lfloor j/q\rfloor + 1}bB_{i-p\lfloor i/p\rfloor, j-q\lfloor i/q\rfloor}\]

They are all this easy! Hence, they are Exercise 3.6.

The determinant of the Kronecker product of two square matrices \(A_{n \times n}\) and \(B_{m \times m}\) has a simple relationship to the determinants of the individual matrices:

\[\det(A ⊗ B) = \det(A)^m \det(B)^n. \quad (3.80)\]

The proof of this, like many facts about determinants, is straightforward but involves tedious manipulation of cofactors. The manipulations in this case can be facilitated by using the vec-permutation matrix. See Harville (1997) for a detailed formal proof.

Another property of the Kronecker product of square matrices is

\[\text{tr}(A ⊗ B) = \text{tr}(A)\text{tr}(B). \quad (3.81)\]

This is true because the trace of the product is merely the sum of all possible products of the diagonal elements of the individual matrices.

The Kronecker product and the vec function often find uses in the same application. For example, an \(n \times m\) normal random matrix \(X\) with parameters \(M, \Sigma, \Psi\) can be expressed in terms of an ordinary \(np\)-variate normal random variable \(Y = \text{vec}(X)\) with parameters vec\((M)\) and \(\Sigma ⊗ \Psi\). (We discuss matrix random variables briefly on page 185. For a fuller discussion, the reader is referred to a text on matrix random variables such as Carmeli, 1983.)
A relationship between the vec function and Kronecker multiplication is
\[ \text{vec}(ABC) = (C^T \otimes A)\text{vec}(B) \]  
(3.82)
for matrices \( A, B, \) and \( C \) that are conformable for the multiplication indicated.

**The Inner Product of Matrices**

A product of two matrices of the same shape is defined as the sum of the dot products of the vectors formed from the columns of one matrix with vectors formed from the corresponding columns of the other matrix; that is, if \( a_1, \ldots, a_m \) are the columns of \( A \) and \( b_1, \ldots, b_m \) are the columns of \( B \), then the inner product of \( A \) and \( B \), denoted \( \langle A, B \rangle \), is
\[ \langle A, B \rangle = \sum_{j=1}^{m} a_j^T b_j. \]  
(3.83)

Similarly as for vectors (page 23), the inner product is sometimes called a “dot product”, and the notation \( A \cdot B \) is sometimes used to denote the matrix inner product. (I generally try to avoid use of the term dot product for matrices because the term may be used differently by different people. In Matlab, for example, “dot product”, implemented in the \texttt{dot} function, can refer either to \( 1 \times m \) matrix consisting of the individual terms in the sum in equation (3.83), or to the \( n \times 1 \) matrix consisting of the dot products of the vectors formed from the rows of \( A \) and \( B \). In the NumPy linear algebra package, the \texttt{dot} function implements Cayley multiplication! This is probably because someone working with Python realized the obvious fact that the defining equation of Cayley multiplication, equation (3.37) on page 70, is actually the dot product of the vector formed from the elements in the \( i \)th row in the first matrix and the vector formed from the elements in the \( j \)th column in the first matrix.)

For conformable matrices \( A, B, \) and \( C \), we can easily confirm that this product satisfies the general properties of an inner product listed on page 23:

- If \( A \neq 0 \), \( \langle A, A \rangle > 0 \), and \( \langle 0, A \rangle = \langle A, 0 \rangle = \langle 0, 0 \rangle = 0. \)
- \( \langle A, B \rangle = \langle B, A \rangle. \)
- \( \langle sA, B \rangle = s \langle A, B \rangle, \) for a scalar \( s. \)
- \( \langle (A + B), C \rangle = \langle A, C \rangle + \langle B, C \rangle. \)

As in the case of the inner product of vectors, the inner product of matrices defined as in equation (3.83) over the complex field is not an inner product because the first property listed above does not hold. As in the case of vectors, a generalized definition of an inner product using complex conjugates is an inner product.

As with any inner product (restricted to objects in the field of the reals), its value is a real number. Thus the matrix inner product is a mapping
\[ \mathbb{R}^{n \times m} \times \mathbb{R}^{n \times m} \mapsto \mathbb{R}. \]
We see from the definition above that the inner product of matrices satisfies
\[ \langle A, B \rangle = \text{tr}(A^T B), \]  
(3.84)
which could alternatively be taken as the definition.

Rewriting the definition of \( \langle A, B \rangle \) as \( \sum_{j=1}^{m} \sum_{i=1}^{n} a_{ij} b_{ij} \), we see that
\[ \langle A, B \rangle = \langle A^T, B^T \rangle. \]
(3.85)

Like any inner product, inner products of matrices obey the Cauchy-Schwarz inequality (see inequality (2.21), page 24),
\[ \langle A, B \rangle \leq \langle A, A \rangle^{\frac{1}{2}} \langle B, B \rangle^{\frac{1}{2}}, \]
(3.86)
with equality holding only if \( A = 0 \) or \( B = sA \) for some scalar \( s \).

In Section 2.1.8, we defined orthogonality and orthonormality of two or more vectors in terms of inner products. We can likewise define an orthogonal binary relationship between two matrices in terms of inner products of matrices. We say the matrices \( A \) and \( B \) of the same shape are orthogonal to each other if
\[ \langle A, B \rangle = 0. \]
(3.87)

We also use the term “orthonormal” to refer to matrices that are orthogonal to each other and for which each has an inner product with itself of 1. In Section 3.7, we will define orthogonality as a unary property of matrices. The term “orthogonal”, when applied to matrices, generally refers to that property rather than the binary property we have defined here.

On page 59 we identified a vector space of matrices and defined a basis for the space \( \mathbb{R}^{n \times m} \). If \( \{U_1, \ldots, U_k\} \) is a basis set for \( \mathcal{M} \subset \mathbb{R}^{n \times m} \), with the property that \( \langle U_i, U_j \rangle = 0 \) for \( i \neq j \) and \( \langle U_i, U_i \rangle = 1 \), and \( A \) is an \( n \times m \) matrix, with the Fourier expansion
\[ A = \sum_{i=1}^{k} c_i U_i, \]
(3.88)
we have, analogous to equation (2.50) on page 39,
\[ c_i = \langle A, U_i \rangle. \]
(3.89)
The \( c_i \) have the same properties (such as the Parseval identity, equation (2.51), for example) as the Fourier coefficients in any orthonormal expansion. Best approximations within \( \mathcal{M} \) can also be expressed as truncations of the sum in equation (3.88) as in equation (2.54). The objective of course is to reduce the truncation error. (The norms in Parseval’s identity and in measuring the goodness of an approximation are matrix norms in this case. We discuss matrix norms in Section 3.9 beginning on page 145.)
3.3 Matrix Rank and the Inverse of a Matrix

The linear dependence or independence of the vectors forming the rows or columns of a matrix is an important characteristic of the matrix.

The maximum number of linearly independent vectors (those forming either the rows or the columns) is called the **rank** of the matrix. We use the notation

$$\text{rank}(A)$$

to denote the rank of the matrix \(A\). (We have used the term “rank” before to denote dimensionality of an array. “Rank” as we have just defined it applies only to a matrix or to a set of vectors, and this is by far the more common meaning of the word. The meaning is clear from the context, however.)

Because multiplication by a nonzero scalar does not change the linear independence of vectors, for the scalar \(a\) with \(a \neq 0\), we have

$$\text{rank}(aA) = \text{rank}(A). \quad (3.90)$$

From results developed in Section 2.1, we see that for the \(n \times m\) matrix \(A\),

$$\text{rank}(A) \leq \min(n, m). \quad (3.91)$$

### Row Rank and Column Rank

We have defined matrix rank in terms of numbers of linearly independent rows or columns. This is because the number of linearly independent rows is the same as the number of linearly independent columns. Although we may use the terms “row rank” or “column rank”, the single word “rank” is sufficient because they are the same. To see this, assume we have an \(n \times m\) matrix \(A\) and that there are exactly \(p\) linearly independent rows and exactly \(q\) linearly independent columns. We can permute the rows and columns of the matrix so that the first \(p\) rows are linearly independent rows and the first \(q\) columns are linearly independent and the remaining rows or columns are linearly dependent on the first ones. (Recall that applying the same permutation to all of the elements of each vector in a set of vectors does not change the linear dependencies over the set.) After these permutations, we have a matrix \(B\) with submatrices \(W, X, Y,\) and \(Z\),

$$B = \begin{bmatrix} W_{p \times q} & X_{p \times m-q} \\ Y_{n-p \times q} & Z_{n-p \times m-q} \end{bmatrix}, \quad (3.92)$$

where the rows of \(R = [W|X]\) correspond to \(p\) linearly independent \(m\)-vectors and the columns of \(C = \begin{bmatrix} W \\ Y \end{bmatrix}\) correspond to \(q\) linearly independent \(n\)-vectors. Without loss of generality, we can assume \(p \leq q\). Now, if \(p < q\), it must be the case that the columns of \(W\) are linearly dependent because there are \(q\) of
them, but they have only \( p \) elements. Therefore, there is some \( q \)-vector \( a \) such that \( Wa = 0 \). Now, since the rows of \( R \) are the full set of linearly independent rows, any row in \( [Y \mid Z] \) can be expressed as a linear combination of the rows of \( R \), and any row in \( Y \) can be expressed as a linear combination of the rows of \( W \). This means, for some \( n - p \times p \) matrix \( T \), that \( Y = TW \). In this case, however, \( Ca = 0 \). But this contradicts the assumption that the columns of \( C \) are linearly independent; therefore it cannot be the case that \( p < q \). We conclude therefore that \( p = q \); that is, that the maximum number of linearly independent rows is the same as the maximum number of linearly independent columns.

Because the row rank, the column rank, and the rank of \( A \) are all the same, we have

\[
\text{rank}(A) = \dim(V(A)),
\]

(3.93)

\[
\text{rank}(A^T) = \text{rank}(A),
\]

(3.94)

\[
\dim(V(A^T)) = \dim(V(A)).
\]

(3.95)

(Note, of course, that in general \( V(A^T) \neq V(A) \); the orders of the vector spaces are possibly different.)

**Full Rank Matrices**

If the rank of a matrix is the same as its smaller dimension, we say the matrix is of **full rank**. In the case of a nonsquare matrix, we may say the matrix is of full row rank or full column rank just to emphasize which is the smaller number.

If a matrix is not of full rank, we say it is **rank deficient** and define the **rank deficiency** as the difference between its smaller dimension and its rank.

A full rank matrix that is square is called **nonsingular**, and one that is not nonsingular is called **singular**.

A square matrix that is either row or column diagonally dominant is nonsingular. The proof of this is Exercise 3.8. (It’s easy!)

A positive definite matrix is nonsingular. The proof of this is Exercise 3.9.

Later in this section, we will identify additional properties of square full rank matrices. (For example, they have inverses and their determinants are nonzero.)

**Rank of Elementary Operator Matrices and Matrix Products Involving Them**

Because within any set of rows of an elementary operator matrix (see Section 3.2.3), for some given column, only one of those rows contains a nonzero
element, the elementary operator matrices are all obviously of full rank (with
the proviso that \( a \neq 0 \) in \( E_p(a) \)).

Furthermore, the rank of the product of any given matrix with an ele-
mentary operator matrix is the same as the rank of the given matrix. To see this,
consider each type of elementary operator matrix in turn. For a given matrix
\( A \), the set of rows of \( E_{pq}A \) is the same as the set of rows of \( A \); hence, the rank
of \( E_{pq}A \) is the same as the rank of \( A \). Likewise, the set of columns of \( AE_{pq} \)
is the same as the set of columns of \( A \); hence, again, the rank of \( AE_{pq} \) is the
same as the rank of \( A \).

The set of rows of \( E_p(a)A \) for \( a \neq 0 \) is the same as the set of rows of \( A \),
except for one, which is a nonzero scalar multiple of the corresponding row
of \( A \); therefore, the rank of \( E_p(a)A \) is the same as the rank of \( A \). Likewise,
the set of columns of \( AE_p(a) \) is the same as the set of columns of \( A \), except
for one, which is a nonzero scalar multiple of the corresponding row of \( A \); there-
fore, again, the rank of \( AE_p(a) \) is the same as the rank of \( A \).

Finally, the set of rows of \( E_{pq}(a)A \) for \( a \neq 0 \) is the same as the set of rows of \( A \),
except for one, which is a nonzero scalar multiple of some row of \( A 
\)
added to the corresponding row of \( A \); therefore, the rank of \( E_{pq}(a)A \) is the
same as the rank of \( A \). Likewise, we conclude that the rank of \( AE_{pq}(a) \) is the
same as the rank of \( A \).

We therefore have that if \( P \) and \( Q \) are the products of elementary operator
matrices,

\[
\operatorname{rank}(P \!AQ) = \operatorname{rank}(A).
\]  

(3.96)

On page 101, we will extend this result to products by any full rank matrices.

3.3.1 The Rank of Partitioned Matrices, Products of
Matrices, and Sums of Matrices

The partitioning in equation (3.92) leads us to consider partitioned matrices
in more detail.

Rank of Partitioned Matrices and Submatrices

Let the matrix \( A \) be partitioned as

\[
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix},
\]

where any pair of submatrices in a column or row may be null (that is, where
for example, it may be the case that \( A = [A_{11}|A_{12}] \)). Then the number of
linearly independent rows of \( A \) must be at least as great as the number of
linearly independent rows of \([A_{11}|A_{12}] \) and the number of linearly independent
rows of \([A_{21}|A_{22}] \). By the properties of subvectors in Section 2.1.1, the number
of linearly independent rows of \([A_{11}|A_{12}] \) must be at least as great as the
number of linearly independent rows of \( A_{11} \) or \( A_{21} \). We could go through a
similar argument relating to the number of linearly independent columns and arrive at the inequality
\[ \text{rank}(A_{ij}) \leq \text{rank}(A). \]  
(3.97)

Furthermore, we see that
\[ \text{rank}(A) \leq \text{rank}([A_{11}|A_{12}]) + \text{rank}([A_{21}|A_{22}]) \]  
(3.98)
because rank(A) is the number of linearly independent columns of A, which is less than or equal to the number of linearly independent rows of [A_{11}|A_{12}] plus the number of linearly independent rows of [A_{12}|A_{22}]. Likewise, we have
\[ \text{rank}(A) \leq \text{rank}\left(\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}\right) + \text{rank}\left(\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}\right). \]  
(3.99)

In a similar manner, by merely counting the number of independent rows, we see that, if
\[ V([A_{11}|A_{12}]^T) \perp V([A_{21}|A_{22}]^T), \]
then
\[ \text{rank}(A) = \text{rank}([A_{11}|A_{12}]) + \text{rank}([A_{21}|A_{22}]); \]  
(3.100)
and, if
\[ V\left(\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}\right) \perp V\left(\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}\right), \]
then
\[ \text{rank}(A) = \text{rank}\left(\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}\right) + \text{rank}\left(\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}\right). \]  
(3.101)

**An Upper Bound on the Rank of Products of Matrices**

The rank of the product of two matrices is less than or equal to the lesser of the ranks of the two:
\[ \text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B)). \]  
(3.102)

We can show this by separately considering two cases for the \( n \times k \) matrix A and the \( k \times m \) matrix B. In one case, we assume \( k \) is at least as large as \( n \) and \( n \leq m \), and in the other case we assume \( k < n \leq m \). In both cases, we represent the rows of \( AB \) as \( k \) linear combinations of the rows of \( B \).

From equation (3.102), we see that the rank of an outer product matrix (that is, a matrix formed as the outer product of two vectors) is 1.

Equation (3.102) provides a useful upper bound on \( \text{rank}(AB) \). In Section 3.3.8, we will develop a lower bound on \( \text{rank}(AB) \).
3.3 Matrix Rank and the Inverse of a Matrix

An Upper and a Lower Bound on the Rank of Sums of Matrices

The rank of the sum of two matrices is less than or equal to the sum of their ranks; that is,

\[ \text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B). \]  
(3.103)

We can see this by observing that

\[ A + B = [A | B] \begin{bmatrix} I \\ I \end{bmatrix}, \]

and so \( \text{rank}(A + B) \leq \text{rank}([A | B]) \) by equation (3.102), which in turn is \( \leq \text{rank}(A) + \text{rank}(B) \) by equation (3.98).

Using inequality (3.103) and the fact that \( \text{rank}(-B) = \text{rank}(B) \), we write \( \text{rank}(A - B) \leq \text{rank}(A) + \text{rank}(B) \), and so, replacing \( A \) in (3.103) by \( A + B \), we have \( \text{rank}(A) \leq \text{rank}(A + B) + \text{rank}(B) \), or \( \text{rank}(A + B) \geq \text{rank}(A) + \text{rank}(B) \). By a similar procedure, we get \( \text{rank}(A - B) \) \( \geq \) \( \text{rank}(B) - \text{rank}(A) \), or

\[ \text{rank}(A + B) \geq |\text{rank}(A) - \text{rank}(B)|. \]  
(3.104)

3.3.2 Full Rank Partitioning

As we saw above, the matrix \( W \) in the partitioned \( B \) in equation (3.92) is square; in fact, it is \( r \times r \), where \( r \) is the rank of \( B \):

\[ B = \begin{bmatrix} W_{r \times r} & X_{r \times m-r} \\ Y_{n-r \times r} & Z_{n-r \times m-r} \end{bmatrix}. \]  
(3.105)

This is called a full rank partitioning of \( B \).

The matrix \( B \) in equation (3.105) has a very special property: the full set of linearly independent rows are the first \( r \) rows, and the full set of linearly independent columns are the first \( r \) columns.

Any rank \( r \) matrix can be put in the form of equation (3.105) by using permutation matrices as in equation (3.48), assuming that \( r \geq 1 \). That is, if \( A \) is a nonzero matrix, there is a matrix of the form of \( B \) above that has the same rank. For some permutation matrices \( E_{\pi_1} \) and \( E_{\pi_2} \),

\[ B = E_{\pi_1} A E_{\pi_2}. \]  
(3.106)

The inverses of these permutations coupled with the full rank partitioning of \( B \) form a full rank partitioning of the original matrix \( A \).

For a square matrix of rank \( r \), this kind of partitioning implies that there is a full rank \( r \times r \) principal submatrix, and the principal submatrix formed by including any of the remaining diagonal elements is singular. The principal minor formed from the full rank principal submatrix is nonzero, but if the order of the matrix is greater than \( r \), a principal minor formed from a submatrix larger than \( r \times r \) is zero.
3 Basic Properties of Matrices

The partitioning in equation (3.105) is of general interest, and we will use this type of partitioning often. We express an equivalent partitioning of a transformed matrix in equation (3.119) below.

The same methods as above can be used to form a full rank square submatrix of any order less than or equal to the rank. That is, if the $n \times m$ matrix $A$ is of rank $r$ and $q \leq r$, we can form

$$E_{πr}AE_{πc} = \begin{bmatrix} S_{q \times q} & T_{q \times m-q} \\ U_{n-q \times r} & V_{n-q \times m-q} \end{bmatrix},$$

(3.107)

where $S$ is of rank $q$.

It is obvious that the rank of a matrix can never exceed its smaller dimension (see the discussion of linear independence on page 12). Whether or not a matrix has more rows than columns, the rank of the matrix is the same as the dimension of the column space of the matrix. (As we have just seen, the dimension of the column space is necessarily the same as the dimension of the row space, but the order of the column space is different from the order of the row space unless the matrix is square.)

3.3.3 Full Rank Matrices and Matrix Inverses

We have already seen that full rank matrices have some important properties. In this section, we consider full rank matrices and matrices that are their Cayley multiplicative inverses.

**Solutions of Linear Equations**

Important applications of vectors and matrices involve systems of linear equations:

$$a_{11}x_1 + \cdots + a_{1m}x_m \equiv b_1$$
$$\vdots$$
$$a_{n1}x_1 + \cdots + a_{nm}x_m \equiv b_n$$

(3.108)

or

$$Ax \equiv b.$$  

(3.109)

In this system, $A$ is called the coefficient matrix. An $x$ that satisfies this system of equations is called a *solution* to the system. For given $A$ and $b$, a solution may or may not exist. From equation (3.63), a solution exists if and only if the $n$-vector $b$ is in the $k$-dimensional column space of $A$, where $k \leq m$. A system for which a solution exists is said to be *consistent*; otherwise, it is *inconsistent*.

We note that if $Ax = b$, for any conformable $y$,

$$y^T Ax = 0 \iff y^T b = 0.$$  

(3.110)
Consistent Systems

A linear system \( A_{n \times m} x = b \) is consistent if and only if

\[
\text{rank}([A \mid b]) = \text{rank}(A).
\] (3.111)

We can see this by recognizing that the space spanned by the columns of \( A \) is the same as that spanned by the columns of \( A \) and the vector \( b \); therefore \( b \) must be a linear combination of the columns of \( A \). Furthermore, the linear combination is the solution to the system \( Ax = b \). (Note, of course, that it is not necessary that it be a unique linear combination.)

Equation (3.111) is equivalent to the condition

\[
[A \mid b]y = 0 \iff Ay = 0.
\] (3.112)

A special case that yields equation (3.111) for any \( b \) is

\[
\text{rank}(A_{n \times m}) = n,
\] (3.113)

and so if \( A \) is of full row rank, the system is consistent regardless of the value of \( b \). In this case, of course, the number of rows of \( A \) must be no greater than the number of columns (by inequality (3.91)). A square system in which \( A \) is nonsingular is clearly consistent.

A generalization of the linear system \( Ax = b \) is \( AX = B \), where \( B \) is an \( n \times k \) matrix. This is the same as \( k \) systems \( Ax_1 = b_1, \ldots, Ax_k = b_k \), where the \( x_i \) and the \( b_i \) are the columns of the respective matrices. Consistency of \( AX = B \), as above, is the condition for a solution in \( X \) to exist. (This condition is also called “compatibility” of the system; that is, the linear system \( AX = B \) is said to be compatible if it is consistent.)

It is clear that the system \( AX = B \) is consistent if each of the \( Ax_i = b_i \) systems is consistent. Furthermore, if the system is consistent, then every linear relationship among the rows of \( A \) exists among the rows of \( B \); that is, for any \( c \) such that \( c^T A = 0 \), then \( c^T B = 0 \). To see this, let \( c \) be such that \( c^T A = 0 \). We then have \( c^T AX = c^T B = 0 \), and so the same linear relationship that exists among the rows of \( A \) exists among the rows of \( B \).

We discuss methods for solving linear systems in Section 3.5 and in Chapter 6. In the next section, we consider a special case of \( n \times n \) (square) \( A \) when equation (3.113) is satisfied (that is, when \( A \) is nonsingular).

Matrix Inverses

Let \( A \) be an \( n \times n \) nonsingular matrix, and consider the linear systems

\[
Ax_i = e_i,
\]

where \( e_i \) is the \( i \)th unit vector. For each \( e_i \), this is a consistent system by equation (3.111).
We can represent all \( n \times n \) such systems as

\[
A \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} = \begin{bmatrix} e_1 & \cdots & e_n \end{bmatrix}
\]

or

\[AX = I_n,\]

and this full system must have a solution; that is, there must be an \( X \) such that \( AX = I_n \). Because \( AX = I \), we call \( X \) a “right inverse” of \( A \). The matrix \( X \) must be \( n \times n \) and nonsingular (because \( I \) is); hence, it also has a right inverse, say \( Y \), and \( XY = I \). From \( AX = I \), we have \( AXY = Y \), so \( A = Y \), and so finally \( XA = I \); that is, the right inverse of \( A \) is also the “left inverse”. We will therefore just call it the inverse of \( A \) and denote it as \( A^{-1} \). This is the Cayley multiplicative inverse. Hence, for an \( n \times n \) nonsingular matrix \( A \), we have a matrix \( A^{-1} \) such that

\[A^{-1}A = AA^{-1} = I_n. \tag{3.114}\]

The inverse of the nonsingular square matrix \( A \) is unique. (This follows from the argument above about a “right inverse” and a “left inverse”.)

We have already encountered the idea of a matrix inverse in our discussions of elementary transformation matrices. The matrix that performs the inverse of the elementary operation is the inverse matrix.

From the definitions of the inverse and the transpose, we see that

\[(A^{-1})^T = (A^T)^{-1}, \tag{3.115}\]

and because in applications we often encounter the inverse of a transpose of a matrix, we adopt the notation

\[A^{-T}\]

to denote the inverse of the transpose.

In the linear system (3.109), if \( n = m \) and \( A \) is nonsingular, the solution is

\[x = A^{-1}b. \tag{3.116}\]

For scalars, the combined operations of inversion and multiplication are equivalent to the single operation of division. From the analogy with scalar operations, we sometimes denote \( AB^{-1} \) by \( A/B \). Because matrix multiplication is not commutative, we often use the notation “\( \setminus \)” to indicate the combined operations of inversion and multiplication on the left; that is, \( B \setminus A \) is the same as \( B^{-1}A \). The solution given in equation (3.116) is also sometimes represented as \( A \setminus b \).

We discuss the solution of systems of equations in Chapter 6, but here we will point out that when we write an expression that involves computations to evaluate it, such as \( A^{-1}b \) or \( A \setminus b \), the form of the expression does not specify how to do the computations. This is an instance of a principle that we will encounter repeatedly: the form of a mathematical expression and the way the expression should be evaluated in actual practice may be quite different.
Nonsquare Full Rank Matrices; Right and Left Inverses

Suppose $A$ is $n \times m$ and $\text{rank}(A) = n$; that is, $n \leq m$ and $A$ is of full row rank. Then $\text{rank}([A \mid e_i]) = \text{rank}(A)$, where $e_i$ is the $i^{th}$ unit vector of length $n$; hence the system

$$Ax_i = e_i$$

is consistent for each $e_i$, and, as before, we can represent all $n$ such systems as

$$A \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} = \begin{bmatrix} e_1 & \cdots & e_n \end{bmatrix}$$

or

$$AX = I_n.$$

As above, there must be an $X$ such that $AX = I_n$, and we call $X$ a right inverse of $A$. The matrix $X$ must be $m \times n$ and it must be of rank $n$ (because $I$ is). This matrix is not necessarily the inverse of $A$, however, because $A$ and $X$ may not be square. We denote the right inverse of $A$ as

$$A^{-R}.$$

Furthermore, we could only have solved the system $AX$ if $A$ was of full row rank because $n \leq m$ and $n = \text{rank}(I) = \text{rank}(AX) \leq \text{rank}(A)$. To summarize, $A$ has a right inverse if and only if $A$ is of full row rank.

Now, suppose $A$ is $n \times m$ and $\text{rank}(A) = m$; that is, $m \leq n$ and $A$ is of full column rank. Writing $YA = I_m$ and reversing the roles of the coefficient matrix and the solution matrix in the argument above, we have that $Y$ exists and is a left inverse of $A$. We denote the left inverse of $A$ as

$$A^{-L}.$$

Also, using a similar argument as above, we see that the matrix $A$ has a left inverse if and only if $A$ is of full column rank.

We also note that if $AA^T$ is of full rank, the right inverse of $A$ is $A^T(AA^T)^{-1}$. Likewise, if $A^TA$ is of full rank, the left inverse of $A$ is $(A^TA)^{-1}A^T$.

3.3.4 Full Rank Factorization

For a given matrix $A$, it is often of interest to find matrices $A_1, \ldots, A_n$ such that $A_1, \ldots, A_n$ have some useful properties and $A = A_1 \cdots A_n$. This is called a factorization or decomposition of $A$. (We will use these two words interchangeably.) In most cases, the number of factors $n$ is either 2 or 3. In this chapter, we will discuss some factorizations as they arise naturally in the development, and then in Chapter 5 we will discuss factorizations in more detail.

The partitioning of an $n \times m$ matrix as in equation (3.105) on page 93 leads to an interesting factorization of a matrix. Recall that we had an $n \times m$ matrix $B$ partitioned as
B = \begin{bmatrix} W_{r \times r} & X_{r \times m - r} \\ Y_{n - r \times r} & Z_{n - r \times m - r} \end{bmatrix},

where \( r \) is the rank of \( B \), \( W \) is of full rank, the rows of \( R = [W|X] \) span the full row space of \( B \), and the columns of \( C = [W|Y] \) span the full column space of \( B \).

Therefore, for some \( T \), we have \( [Y|Z] = TR \), and for some \( S \), we have \( [X|Z] = CS \). From this, we have \( Y = TW \), \( Z = TX \), \( X = WS \), and \( Z = YS \), so \( Z = TWS \). Since \( W \) is nonsingular, we have \( T = YW^{-1} \) and \( S = W^{-1}X \), so \( Z = YW^{-1}X \).

We can therefore write the partitions as

\[
B = \begin{bmatrix} W & X \\ Y & YW^{-1}X \end{bmatrix} = \begin{bmatrix} I \\ YW^{-1} \end{bmatrix} W [I | W^{-1}X].
\] (3.117)

From this, we can form two equivalent factorizations of \( B \):

\[
B = \begin{bmatrix} W \\ Y \end{bmatrix} [I | W^{-1}X] = \begin{bmatrix} I \\ YW^{-1} \end{bmatrix} [W | X].
\]

The matrix \( B \) has a very special property: the full set of linearly independent rows are the first \( r \) rows, and the full set of linearly independent columns are the first \( r \) columns. We have seen, however, that any matrix \( A \) of rank \( r \) can be put in this form, and \( A = E_{\pi_2}BE_{\pi_1} \) for an \( n \times n \) permutation matrix \( E_{\pi_2} \) and an \( m \times m \) permutation matrix \( E_{\pi_1} \).

We therefore have, for the \( n \times m \) matrix \( A \) with rank \( r \), two equivalent factorizations,

\[
A = \begin{bmatrix} QW \\ QY \end{bmatrix} [P | W^{-1}XP] = \begin{bmatrix} Q \\ QYW^{-1} \end{bmatrix} [WP | XP],
\]
both of which are in the general form

\[
A_{n \times m} = L_{n \times r} R_{r \times m},
\] (3.118)

where \( L \) is of full column rank and \( R \) is of full row rank. This is called a full rank factorization of the matrix \( A \). We will use a full rank factorization in proving various properties of matrices. We will consider other factorizations later in this chapter and in Chapter 5 that have more practical uses in computations.
3.3 Matrix Rank and the Inverse of a Matrix

3.3.5 Equivalent Matrices

Matrices of the same order that have the same rank are said to be *equivalent matrices*.

**Equivalent Canonical Forms**

For any $n \times m$ matrix $A$ with $\text{rank}(A) = r > 0$, by combining the permutations that yield equation (3.105) with other operations, we have, for some matrices $P$ and $Q$ that are products of various elementary operator matrices,

$$PAQ = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}.$$  \hspace{1cm} (3.119)

This is called an *equivalent canonical form* of $A$, and it exists for any matrix $A$ that has at least one nonzero element (which is the same as requiring $\text{rank}(A) > 0$).

We can see by construction that an equivalent canonical form exists for any $n \times m$ matrix $A$ that has a nonzero element. First, assume $a_{ij} \neq 0$. By two successive permutations, we move $a_{ij}$ to the $(1,1)$ position; specifically, $(E_{i1}AE_{1j})_{11} = a_{ij}$. We then divide the first row by $a_{ij}$; that is, we form $E_1(1/a_{ij})E_{i1}AE_{1j}$. We then proceed with a sequence of $n-1$ premultiplications by axpy matrices to zero out the first column of the matrix, as in expression (3.53), followed by a sequence of $(m-1)$ postmultiplications by axpy matrices to zero out the first row. We then have a matrix of the form

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & X \end{bmatrix}.$$  \hspace{1cm} (3.120)

If $X = 0$, we are finished; otherwise, we perform the same kinds of operations on the $(n-1) \times (m-1)$ matrix $X$ and continue until we have the form of equation (3.119).

The matrices $P$ and $Q$ in equation (3.119) are not unique. The order in which they are built from elementary operator matrices can be very important in preserving the accuracy of the computations.

Although the matrices $P$ and $Q$ in equation (3.119) are not unique, the equivalent canonical form itself (the right-hand side) is obviously unique because the only thing that determines it, aside from the shape, is the $r$ in $I_r$, and that is just the rank of the matrix. There are two other, more general, equivalent forms that are often of interest. These equivalent forms, “row echelon form” and “Hermite form”, are not unique. A matrix $R$ is said to be in *row echelon form*, or just *echelon form*, if

- $r_{ij} = 0$ for $i > j$, and
A matrix in echelon form is upper triangular. An upper triangular matrix $H$ is said to be in Hermite form if

- $h_{ii} = 0$ or $1$,
- if $h_{ii} = 0$, then $h_{ij} = 0$ for all $j$, and
- if $h_{ii} = 1$, then $h_{ki} = 0$ for all $k \neq i$.

If $H$ is in Hermite form, then $H^2 = H$, as is easily verified. (A matrix $H$ such that $H^2 = H$ is said to be idempotent. We discuss idempotent matrices beginning on page 302.) Another, more specific, equivalent form, called the Jordan form, is a special row echelon form based on eigenvalues. Any of these equivalent forms is useful in determining the rank of a matrix. Each form may have special uses in proving properties of matrices. We will often make use of the equivalent canonical form in other sections of this chapter.

**Products with a Nonsingular Matrix**

It is easy to see that if $A$ is a square full rank matrix (that is, $A$ is nonsingular), and if $B$ and $C$ are conformable matrices for the multiplications $AB$ and $CA$, respectively, then

$$\text{rank}(AB) = \text{rank}(B)$$

(3.121)

and

$$\text{rank}(CA) = \text{rank}(C).$$

(3.122)

This is true because, for a given conformable matrix $B$, by the inequality (3.102), we have $\text{rank}(AB) \leq \text{rank}(B)$. Forming $B = A^{-1}AB$, and again applying the inequality, we have $\text{rank}(B) \leq \text{rank}(AB)$; hence, $\text{rank}(AB) = \text{rank}(B)$. Likewise, for a square full rank matrix $A$, we have $\text{rank}(CA) = \text{rank}(C)$. (Here, we should recall that all matrices are real.)

On page 101, we give a more general result for products with general full rank matrices.

**A Factorization Based on an Equivalent Canonical Form**

Elementary operator matrices and products of them are of full rank and thus have inverses. When we introduced the matrix operations that led to the definitions of the elementary operator matrices in Section 3.2.3, we mentioned the inverse operations, which would then define the inverses of the matrices.

The matrices $P$ and $Q$ in the equivalent canonical form of the matrix $A$, $PAQ$ in equation (3.119), have inverses. From an equivalent canonical form of a matrix $A$ with rank $r$, we therefore have the equivalent canonical factorization of $A$:

$$A = P^{-1} \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} Q^{-1}. \quad (3.123)$$
A factorization based on an equivalent canonical form is also a full rank factorization and could be written in the same form as equation (3.118).

**Equivalent Forms of Symmetric Matrices**

If $A$ is symmetric, the equivalent form in equation (3.119) can be written as $PAP^T = \text{diag}(I_r, 0)$ and the equivalent canonical factorization of $A$ in equation (3.123) can be written as

$$A = P^{-1} \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} P^{-T}. \quad (3.124)$$

These facts follow from the same process that yielded equation (3.119) for a general matrix.

Also a full rank factorization for a symmetric matrix, as in equation (3.118), can be given as

$$A = LL^T. \quad (3.125)$$

### 3.3.6 Multiplication by Full Rank Matrices

We have seen that a matrix has an inverse if it is square and of full rank. Conversely, it has an inverse only if it is square and of full rank. We see that a matrix that has an inverse must be square because $A^{-1}A = AA^{-1}$, and we see that it must be full rank by the inequality (3.102). In this section, we consider other properties of full rank matrices. In some cases, we require the matrices to be square, but in other cases, these properties hold whether or not they are square.

Using matrix inverses allows us to establish important properties of products of matrices in which at least one factor is a full rank matrix.

#### Products with a General Full Rank Matrix

If $A$ is a full column rank matrix and if $B$ is a matrix conformable for the multiplication $AB$, then

$$\text{rank}(AB) = \text{rank}(B). \quad (3.126)$$

If $A$ is a full row rank matrix and if $C$ is a matrix conformable for the multiplication $CA$, then

$$\text{rank}(CA) = \text{rank}(C). \quad (3.127)$$

Consider a full rank $n \times m$ matrix $A$ with $\text{rank}(A) = m$ (that is, $m \leq n$) and let $B$ be conformable for the multiplication $AB$. Because $A$ is of full column rank, it has a left inverse (see page 97); call it $A^{-L}$, and so $A^{-L}A = I_m$. From inequality (3.102), we have $\text{rank}(AB) \leq \text{rank}(B)$, and applying
the inequality again, we have \( \text{rank}(B) = \text{rank}(A^{-L}AB) \leq \text{rank}(AB) \); hence \( \text{rank}(AB) = \text{rank}(B) \).

Now consider a full rank \( n \times m \) matrix \( A \) with \( \text{rank}(A) = n \) (that is, \( n \leq m \)) and let \( C \) be conformable for the multiplication \( CA \). Because \( A \) is of full row rank, it has a right inverse; call it \( A^{-R} \), and so \( AA^{-R} = I_n \). From inequality (3.102), we have \( \text{rank}(CA) \leq \text{rank}(C) \), and applying the inequality again, we have \( \text{rank}(C) = \text{rank}(CAA^{-L}) \leq \text{rank}(CA) \); hence \( \text{rank}(CA) = \text{rank}(C) \).

To state this more simply:

- Premultiplication of a given matrix by a full column rank matrix does not change the rank of the given matrix, and postmultiplication of a given matrix by a full row rank matrix does not change the rank of the given matrix.

From this we see that \( A^T A \) is of full rank if (and only if) \( A \) is of full column rank, and \( AA^T \) is of full rank if (and only if) \( A \) is of full row rank. We will develop a stronger form of these statements in Section 3.3.7.

**Preservation of Positive Definiteness**

A certain type of product of a full rank matrix and a positive definite matrix preserves not only the rank, but also the positive definiteness: if \( C \) is \( n \times n \) and positive definite, and \( A \) is \( n \times m \) and of rank \( m \) (hence, \( m \leq n \)), then \( A^TCA \) is positive definite. (Recall from inequality (3.66) that a matrix \( C \) is positive definite if it is symmetric and for any \( x \neq 0 \), \( x^T C x > 0 \).)

To see this, assume matrices \( C \) and \( A \) as described. Let \( x \) be any \( m \)-vector such that \( x \neq 0 \), and let \( y = Ax \). Because \( A \) is of full column rank, \( y \neq 0 \). We have

\[
x^T (A^T CA) x = (Ax)^T C (Ax)
= y^T C y
> 0.
\] (3.128)

Therefore, since \( A^T CA \) is symmetric,

- if \( C \) is positive definite and \( A \) is of full column rank, then \( A^T CA \) is positive definite.

Furthermore, we have the converse:

- if \( A^T CA \) is positive definite, then \( A \) is of full column rank,

for otherwise there exists an \( x \neq 0 \) such that \( Ax = 0 \), and so \( x^T (A^T CA) x = 0 \).
3.3 Matrix Rank and the Inverse of a Matrix

The General Linear Group

Consider the set of all square $n \times n$ full rank matrices together with the usual (Cayley) multiplication. As we have seen, this set is closed under multiplication. (The product of two square matrices of full rank is of full rank, and of course the product is also square.) Furthermore, the (multiplicative) identity is a member of this set, and each matrix in the set has a (multiplicative) inverse in the set; therefore, the set together with the usual multiplication is a mathematical structure called a group. (See any text on modern algebra.) This group is called the general linear group and is denoted by $GL(n)$. General group-theoretic properties can be used in the derivation of properties of these full-rank matrices. Note that this group is not commutative.

As we mentioned earlier (before we had considered inverses in general), if $A$ is an $n \times n$ matrix and if $A^{-1}$ exists, we define $A^0$ to be $I_n$.

The $n \times n$ elementary operator matrices are members of the general linear group $GL(n)$.

The elements in the general linear group are matrices and, hence, can be viewed as transformations or operators on $n$-vectors. Another set of linear operators on $n$-vectors are the doubletons $(A, v)$, where $A$ is an $n \times n$ full-rank matrix and $v$ is an $n$-vector. As an operator on $x \in \mathbb{R}^n$, $(A, v)$ is the transformation $Ax + v$, which preserves affine spaces. Two such operators, $(A, v)$ and $(B, w)$, are combined by composition: $(A, v)(B, w)(x) = ABx + Aw + v$. The set of such doubletons together with composition forms a group, called the affine group. It is denoted by $AL(n)$. A subset of the elements of the affine group with the same first element, together with the axpy operator, constitute a quotient space.

3.3.7 Products of the Form $A^T A$

Given a real matrix $A$, an important matrix product is $A^T A$. (This is called a Gramian matrix. We will discuss this kind of matrix in more detail beginning on page 309.)

Matrices of this form have several interesting properties. First, for any $n \times m$ matrix $A$, we have the fact that $A^T A = 0$ if and only if $A = 0$. We see this by noting that if $A = 0$, then $\text{tr}(A^T A) = 0$. Conversely, if $\text{tr}(A^T A) = 0$, then $a_{ij}^2 = 0$ for all $i, j$, and so $a_{ij} = 0$, that is, $A = 0$. Summarizing, we have

$$\text{tr}(A^T A) = 0 \iff A = 0 \quad (3.129)$$

and

$$A^T A = 0 \iff A = 0. \quad (3.130)$$

Another useful fact about $A^T A$ is that it is nonnegative definite. This is because for any $y$, $y^T (A^T A) y = (Ay)^T (Ay) \geq 0$. In addition, we see that $A^T A$ is positive definite if and only if $A$ is of full column rank. This follows from (3.130), and if $A$ is of full column rank, $Ay = 0 \Rightarrow y = 0$. 
Now consider a generalization of the equation $A^T A = 0$:

$$A^T A (B - C) = 0.$$ 

Multiplying by $B^T - C^T$ and factoring $(B^T - C^T) A^T A (B - C)$, we have

$$(AB - AC)^T (AB - AC) = 0;$$

hence, from (3.130), we have $AB - AC = 0$. Furthermore, if $AB - AC = 0$, then clearly $A^T A (B - C) = 0$. We therefore conclude that

$$A^T A B = A^T A C \iff AB = AC. \quad (3.131)$$

By the same argument, we have

$$B A^T A = C A^T A \iff BA = CA^T.$$

Now, let us consider rank($A^T A$). We have seen that ($A^T A$) is of full rank if and only if $A$ is of full column rank. Next, preparatory to our main objective, we note from above that

$$\text{rank}(A^T A) = \text{rank}(AA^T). \quad (3.132)$$

Let $A$ be an $n \times m$ matrix, and let $r = \text{rank}(A)$. If $r = 0$, then $A = 0$ (hence, $A^T A = 0$) and rank($A^T A$) = 0. If $r > 0$, interchange columns of $A$ if necessary to obtain a partitioning similar to equation (3.105),

$$A = [A_1 A_2],$$

where $A_1$ is an $n \times r$ matrix of rank $r$. (Here, we are ignoring the fact that the columns might have been permuted. All properties of the rank are unaffected by these interchanges.) Now, because $A_1$ is of full column rank, there is an $r \times m - r$ matrix $B$ such that $A_2 = A_1 B$; hence we have $A = A_1 [I_r B]$ and

$$A^T A = \begin{bmatrix} I_r & B^T \\ B & A_1^T A_1 \end{bmatrix} [I_r B].$$

Because $A_1$ is of full rank, rank($A_1^T A_1$) = $r$. Now let

$$T = \begin{bmatrix} I_r & 0 \\ -B^T & I_{m-r} \end{bmatrix}.$$ 

It is clear that $T$ is of full rank, and so

$$\text{rank}(A^T A) = \text{rank}(T A_1^T A_1)$$

$$= \text{rank} \left( \begin{bmatrix} A_1^T A_1 & 0 \\ 0 & 0 \end{bmatrix} \right)$$

$$= \text{rank}(A_1^T A_1)$$

$$= r;$$
that is,
\[
\text{rank}(A^T A) = \text{rank}(A). \tag{3.133}
\]
From this equation, we have a useful fact for Gramian matrices. The system
\[
A^T A x = A^T b \tag{3.134}
\]
is consistent for any \( A \) and \( b \).

### 3.3.8 A Lower Bound on the Rank of a Matrix Product

Equation (3.102) gives an upper bound on the rank of the product of two matrices; the rank cannot be greater than the rank of either of the factors. Now, using equation (3.123), we develop a lower bound on the rank of the product of two matrices if one of them is square.

If \( A \) is \( n \times n \) (that is, square) and \( B \) is a matrix with \( n \) rows, then
\[
\text{rank}(AB) \geq \text{rank}(A) + \text{rank}(B) - n. \tag{3.135}
\]
We see this by first letting \( r = \text{rank}(A) \), letting \( P \) and \( Q \) be matrices that form an equivalent canonical form of \( A \) (see equation (3.123)), and then forming
\[
C = P^{-1} \begin{bmatrix} 0 & 0 \\ 0 & I_{n-r} \end{bmatrix} Q^{-1},
\]
so that \( A + C = P^{-1}Q^{-1} \). Because \( P^{-1} \) and \( Q^{-1} \) are of full rank, \( \text{rank}(C) = \text{rank}(I_{n-r}) = n - \text{rank}(A) \). We now develop an upper bound on \( \text{rank}(B) \),
\[
\text{rank}(B) = \text{rank}(P^{-1}Q^{-1}B)
\]
\[
= \text{rank}(AB + CB)
\]
\[
\leq \text{rank}(AB) + \text{rank}(CB), \text{ by equation } (3.103)
\]
\[
\leq \text{rank}(AB) + \text{rank}(C), \text{ by equation } (3.102)
\]
\[
= \text{rank}(AB) + n - \text{rank}(A),
\]
yielding (3.135), a lower bound on \( \text{rank}(AB) \).

The inequality (3.135) is called Sylvester’s law of nullity. It provides a lower bound on \( \text{rank}(AB) \) to go with the upper bound of inequality (3.102), \( \min(\text{rank}(A), \text{rank}(B)) \).

### 3.3.9 Determinants of Inverses

From the relationship \( \det(AB) = \det(A) \det(B) \) for square matrices mentioned earlier, it is easy to see that for nonsingular square \( A \),
\[
\det(A^{-1}) = (\det(A))^{-1}, \tag{3.136}
\]
and so
det(A) = 0 if and only if A is singular.

(From the definition of the determinant in equation (3.18), we see that the determinant of any finite-dimensional matrix with finite elements is finite, and we implicitly assume that the elements are finite.)

For an \( n \times n \) matrix with \( n \geq 2 \) whose determinant is nonzero, from equation (3.28) we have

\[
A^{-1} = \frac{1}{\det(A)} \text{adj}(A).
\]

(3.137)

If \( \det(A) = 1 \), this obviously implies

\[
A^{-1} = \text{adj}(A).
\]

See Exercise 3.12 on page 158 for an interesting consequence of this.

### 3.3.10 Inverses of Products and Sums of Nonsingular Matrices

In linear regression analysis and other applications, we sometimes need inverses of various sums or products of matrices. In regression analysis, this may be because we wish to update regression estimates based on additional data or because we wish to delete some observations.

There is no simple relationship between the inverses of factors in a Hadamard product and the product matrix, but there are simple relationships between the inverses of factors in Cayley and Kronecker products and the product matrices.

#### Inverses of Cayley Products of Matrices

The inverse of the Cayley product of two nonsingular matrices of the same size is particularly easy to form. If \( A \) and \( B \) are square full rank matrices of the same size,

\[
(AB)^{-1} = B^{-1}A^{-1}.
\]

(3.138)

We can see this by multiplying \( B^{-1}A^{-1} \) and \( (AB) \). This, of course, generalizes to

\[
(A_1 \cdots A_n)^{-1} = A_n^{-1} \cdots A_1^{-1}
\]

if \( A_1, \cdots, A_n \) are all full rank and conformable.

#### Inverses of Kronecker Products of Matrices

If \( A \) and \( B \) are square full rank matrices, then

\[
(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}.
\]

(3.139)

We can see this by multiplying \( A^{-1} \otimes B^{-1} \) and \( A \otimes B \).
Inverses of Sums of Matrices and Their Inverses

The inverse of the sum of two nonsingular matrices is somewhat more complicated. The first question of course is whether the sum is nonsingular. We can develop several useful relationships of inverses of sums and the sums and products of the individual matrices.

The simplest case to get started is $I + A$. Let $A$ and $I + A$ be nonsingular. Then it is easy to derive $(I + A)^{-1}$ by use of $I = AA^{-1}$ and equation (3.138). We get

$$(I + A)^{-1} = A^{-1}(I + A^{-1})^{-1}. \quad (3.140)$$

If $A$ and $B$ are full rank matrices of the same size and such sums as $I + A$, $A + B$, and so on, are full rank, the following relationships are easy to show (and are easily proven in the order given, using equations (3.138) and (3.140); see Exercise 3.13):

$$(A + A)^{-1} = (A + A^{-1})^{-1}, \quad (3.141)$$

$$(A + B)^{-1} = A^{-1} - A^{-1}(A^{-1} + B^{-1})^{-1} A^{-1}, \quad (3.142)$$

$$(A + BB^T)^{-1} B = A^{-1} B (I + B^T A^{-1} B)^{-1}, \quad (3.143)$$

$$(A^{-1} + B^{-1})^{-1} = A (A + B)^{-1} B, \quad (3.144)$$

$$A - A (A + B)^{-1} A = B - B (A + B)^{-1} B, \quad (3.145)$$

$$A^{-1} + B^{-1} = A^{-1} (A + B) B^{-1}, \quad (3.146)$$

$$(I + AB)^{-1} = I - A (I + BA)^{-1} B, \quad (3.147)$$

$$(I + AB)^{-1} A = A (I + BA)^{-1}. \quad (3.148)$$

When $A$ and/or $B$ are not of full rank, the inverses may not exist, but in that case these equations may or may not hold for a generalized inverse, which we will discuss in Section 3.6.

Another simple general result, this time involving some non-square matrices, is that if $A$ is a full-rank $n \times n$ matrix, $B$ is a full-rank $m \times m$ matrix, $C$ is any $n \times m$ matrix, and $D$ is any $m \times n$ matrix such that $A + CBD$ is full rank, then

$$(A + CBD)^{-1} = A^{-1} - A^{-1} C (B^{-1} + DA^{-1} C)^{-1} DA^{-1}. \quad (3.149)$$

This can be derived from equation (3.141), which is a special case of it. We can verify this by multiplication (Exercise 3.14).
From this it also follows that if $A$ is a full-rank $n \times n$ matrix and $b$ and $c$ are $n$-vectors such that $(A + bc^T)$ is full rank, then

$$
(A + bc^T)^{-1} = A^{-1} - \frac{A^{-1}bc^TA^{-1}}{1 + c^TA^{-1}b}.
$$

(3.150)

This fact has application in adding an observation to a least squares linear regression problem (page 361).

**An Expansion of a Matrix Inverse**

There is also an analogue to the expansion of the inverse of $(1 - a)$ for a scalar $a$:

$$(1 - a)^{-1} = 1 + a + a^2 + a^3 + \cdots, \quad \text{if } |a| < 1.$$  

This expansion for the scalar $a$ comes from a factorization of the binomial $1 - a^k$ and the fact that $a^k \to 0$ if $|a| < 1$.

To extend this to $(I + A)^{-1}$ for a matrix $A$, we need a similar condition on $A^k$ as $k$ increases without bound. In Section 3.9 on page 145, we will discuss conditions that ensure the convergence of $A^k$ for a square matrix $A$. We will define a norm $\|A\|$ on $A$ and show that if $\|A\| < 1$, then $A^k \to 0$. Then, analogous to the scalar series, using equation (3.44) on page 71 for a square matrix $A$, we have

$$
(I - A)^{-1} = I + A + A^2 + A^3 + \cdots, \quad \text{if } \|A\| < 1.
$$

(3.151)

We include this equation here because of its relation to equations (3.141) through (3.147). We will discuss it further on page 151, after we have introduced and discussed $\|A\|$ and other conditions that ensure convergence. This expression and the condition that determines it are very important in the analysis of time series and other stochastic processes.

Also, looking ahead, we have another expression similar to equations (3.141) through (3.147) and (3.151) for a special type of matrix. If $A^2 = A$, for any $a \neq -1$,

$$
(I + aA)^{-1} = I - \frac{a}{a + 1} A
$$

(see page 304).

### 3.3.11 Inverses of Matrices with Special Forms

Matrices with various special patterns may have inverses with similar patterns.

- The inverse of a nonsingular diagonal matrix with nonzero entries is a diagonal matrix consisting of the reciprocals of those elements.
- The inverse of a block diagonal matrix with nonsingular submatrices along the diagonal is a block diagonal matrix consisting of the inverses of the submatrices.
The inverse of a nonsingular triangular matrix is a triangular matrix with the same pattern; furthermore, the diagonal elements in the inverse are the reciprocals of the diagonal elements in the original matrix. Each of these statements can be easily proven by multiplication (using the fact that the inverse is unique).

The inverses of other matrices with special patterns, such as banded matrices, may not have those patterns.

In Chapter 8, we discuss inverses of various other special matrices that arise in applications in statistics.

### 3.3.12 Determining the Rank of a Matrix

Although the equivalent canonical form (3.119) immediately gives the rank of a matrix, in practice the numerical determination of the rank of a matrix is not an easy task. The problem is that rank is a mapping \( \mathbb{R}^{n \times m} \mapsto \mathbb{Z}_+ \), where \( \mathbb{Z}_+ \) represents the positive integers. Such a function is often difficult to compute because the domain is relatively dense and the range is sparse. Small changes in the domain may result in large discontinuous changes in the function value. The common way that the rank of a matrix is evaluated is by use of the QR decomposition; see page 208.

It is not even always clear whether a matrix is nonsingular. Because of rounding on the computer, a matrix that is mathematically nonsingular may appear to be singular. We sometimes use the phrase “nearly singular” or “algorithmically singular” to describe such a matrix. In Sections 6.1 and 11.4, we consider this kind of problem in more detail.

### 3.4 More on Partitioned Square Matrices: The Schur Complement

A square matrix \( A \) that can be partitioned as

\[
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix},
\]

(3.152)

where \( A_{11} \) is nonsingular, has interesting properties that depend on the matrix

\[
Z = A_{22} - A_{21}A_{11}^{-1}A_{12},
\]

(3.153)

which is called the Schur complement of \( A_{11} \) in \( A \).

We first observe from equation (3.117) that if equation (3.152) represents a full rank partitioning (that is, if the rank of \( A_{11} \) is the same as the rank of \( A \)), then

\[
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}^{-1}A_{11}A_{12}
\end{bmatrix},
\]

(3.154)
and $Z = 0$.

There are other useful properties, which we mention below. There are also some interesting properties of certain important random matrices partitioned in this way. For example, suppose $A_{22}$ is $k \times k$ and $A$ is an $m \times m$ Wishart matrix with parameters $n$ and $\Sigma$ partitioned like $A$ in equation (3.152). (This of course means $A$ is symmetrical, and so $A_{12} = A_{21}^T$.) Then $Z$ has a Wishart distribution with parameters $n - m + k$ and $\Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$, and is independent of $A_{21}$ and $A_{11}$. (See Exercise 4.8 on page 187 for the probability density function for a Wishart distribution.)

### 3.4.1 Inverses of Partitioned Matrices

Suppose $A$ is nonsingular and can be partitioned as above with both $A_{11}$ and $A_{22}$ nonsingular. It is easy to see (Exercise 3.16, page 159) that the inverse of $A$ is given by

$$A^{-1} = \begin{bmatrix} A_{11}^{-1} + A_{11}^{-1} A_{12} Z^{-1} A_{21} A_{11}^{-1} & -A_{11}^{-1} A_{12} Z^{-1} \\ -Z^{-1} A_{21} A_{11}^{-1} & Z^{-1} \end{bmatrix},$$

(3.155)

where $Z$ is the Schur complement of $A_{11}$.

If

$$A = [X\ y]^T [X\ y]$$

and is partitioned as in equation (3.46) on page 72 and $X$ is of full column rank, then the Schur complement of $X^T X$ in $[X\ y]^T [X\ y]$ is

$$y^T y - y^T X (X^T X)^{-1} X^T y.$$  

(3.156)

This particular partitioning is useful in linear regression analysis, where this Schur complement is the residual sum of squares and the more general Wishart distribution mentioned above reduces to a chi-squared one. (Although the expression is useful, this is an instance of a principle that we will encounter repeatedly: the form of a mathematical expression and the way the expression should be evaluated in actual practice may be quite different.)

### 3.4.2 Determinants of Partitioned Matrices

If the square matrix $A$ is partitioned as

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

and $A_{11}$ is square and nonsingular, then

$$\det(A) = \det(A_{11}) \det\left(A_{22} - A_{21} A_{11}^{-1} A_{12}\right);$$

(3.157)
3.5 Linear Systems of Equations

that is, the determinant is the product of the determinant of the principal submatrix and the determinant of its Schur complement.

This result is obtained by using equation (3.32) on page 65 and the factorization

\[
\begin{bmatrix}
    A_{11} & A_{12} \\
    A_{21} & A_{22}
\end{bmatrix}
= \begin{bmatrix}
    A_{11} & 0 \\
    A_{21} & A_{22} - A_{21}A_{11}^{-1}A_{12}
\end{bmatrix}
\begin{bmatrix}
    I & A_{11}^{-1}A_{12} \\
    0 & I
\end{bmatrix}.
\]

The factorization in equation (3.158) is often useful in other contexts as well.

3.5 Linear Systems of Equations

Some of the most important applications of matrices are in representing and solving systems of \( n \) linear equations in \( m \) unknowns,

\[ Ax = b, \]

where \( A \) is an \( n \times m \) matrix, \( x \) is an \( m \)-vector, and \( b \) is an \( n \)-vector. As we observed in equation (3.63), the product \( Ax \) in the linear system is a linear combination of the columns of \( A \); that is, if \( a_j \) is the \( j \)th column of \( A \), \( Ax = \sum_{j=1}^{m} x_j a_j \).

If \( b = 0 \), the system is said to be \textit{homogeneous}. In this case, unless \( x = 0 \), the columns of \( A \) must be linearly dependent.

3.5.1 Solutions of Linear Systems

When in the linear system \( Ax = b \), \( A \) is square and nonsingular, the solution is obviously \( x = A^{-1}b \). We will not discuss this simple but common case further here. Rather, we will discuss it in detail in Chapter 6 after we have discussed matrix factorizations later in this chapter and in Chapter 5.

When \( A \) is not square or is singular, the system may not have a solution or may have more than one solution. A consistent system (see equation (3.111)) has a solution. For consistent systems that are singular or not square, the \textit{generalized inverse} is an important concept. We introduce it in this section but defer its discussion to Section 3.6.

Underdetermined Systems

A consistent system in which \( \text{rank}(A) < m \) is said to be \textit{underdetermined}. An underdetermined system may have fewer equations than variables, or the coefficient matrix may just not be of full rank. For such a system there is more than one solution. In fact, there are infinitely many solutions because if the vectors \( x_1 \) and \( x_2 \) are solutions, the vector \( wx_1 + (1 - w)x_2 \) is likewise a solution for any scalar \( w \).
Underdetermined systems arise in analysis of variance in statistics, and it is useful to have a compact method of representing the solution to the system. It is also desirable to identify a unique solution that has some kind of optimal properties. Below, we will discuss types of solutions and the number of linearly independent solutions and then describe a unique solution of a particular type.

**Overdetermined Systems**

Often in mathematical modeling applications, the number of equations in the system $Ax = b$ is not equal to the number of variables; that is the coefficient matrix $A$ is $n \times m$ and $n \neq m$. If $n > m$ and rank($[A \mid b]$) > rank($A$), the system is said to be *overdetermined*. There is no $x$ that satisfies such a system, but approximate solutions are useful. We discuss approximate solutions of such systems in Section 6.7 on page 243 and in Section 9.2.2 on page 352.

**Generalized Inverses**

A matrix $G$ such that $AGA = A$ is called a *generalized inverse* and is denoted by $A^{-}$:

$$AA^{-}A = A.$$ (3.159)

Note that if $A$ is $n \times m$, then $A^{-}$ is $m \times n$. If $A$ is nonsingular (square and of full rank), then obviously $A^{-} = A^{-1}$.

Without additional restrictions on $A$, the generalized inverse is not unique. Various types of generalized inverses can be defined by adding restrictions to the definition of the inverse. In Section 3.6, we will discuss various types of generalized inverses and show that $A^{-}$ exists for any $n \times m$ matrix $A$. Here we will consider some properties of any generalized inverse.

From equation (3.159), we see that

$$A^{T}(A^{-})^{T}A^{T} = A^{T};$$

thus, if $A^{-}$ is a generalized inverse of $A$, then $(A^{-})^{T}$ is a generalized inverse of $A^{T}$.

The $m \times m$ square matrices $A^{-}A$ and $(I - A^{-}A)$ are often of interest. By using the definition (3.159), we see that

$$(A^{-}A)(A^{-}A) = A^{-}A.$$ (3.160)

(Such a matrix is said to be *idempotent*. We discuss idempotent matrices beginning on page 302.) From equation (3.102) together with the fact that $AA^{-}A = A$, we see that

$$\text{rank}(A^{-}A) = \text{rank}(A).$$ (3.161)

By multiplication as above, we see that
\[ A(I - A^-) = 0, \]  
that
\[ (I - A^-)(I - A^-) = 0, \]  
and that \( (I - A^-) \) is also idempotent:
\[ (I - A^-)(I - A^-) = (I - A^-). \]  
The fact that \( (A^-A)(A^-A) = A^-A \) yields the useful fact that
\[ \text{rank}(I - A^-) = m - \text{rank}(A). \]  
This follows from equations (3.163), (3.135), and (3.161), which yield
\[ 0 \geq \text{rank}(I - A^-) + \text{rank}(A) - m, \]  
and from equation (3.103), which gives
\[ m = \text{rank}(I) \leq \text{rank}(I - A^-) + \text{rank}(A). \]  
The two inequalities result in the equality of equation (3.165).

**Multiple Solutions in Consistent Systems**

Suppose the system \( Ax = b \) is consistent and \( A^- \) is a generalized inverse of \( A \); that is, it is any matrix such that \( AA^-A = A \). Then
\[ x = A^-b \]  
is a solution to the system because if \( AA^-A = A \), then \( AA^-Ax = Ax \) and since \( Ax = b \),
\[ AA^-b = b; \]  
that is, \( A^-b \) is a solution. Furthermore, if \( x = Gb \) is any solution, then \( AGA = A \); that is, \( G \) is a generalized inverse of \( A \). This can be seen by the following argument. Let \( a_j \) be the \( j^{th} \) column of \( A \). The \( m \) systems of \( n \) equations, \( Ax = a_j, j = 1, \ldots, m \), all have solutions. (Each solution is a vector with 0s in all positions except the \( j^{th} \) position, which is a 1.) Now, if \( Gb \) is a solution to the original system, then \( Ga_j \) is a solution to the system \( Ax = a_j \). So \( AGa_j = a_j \) for all \( j \); hence \( AGA = A \).

If \( Ax = b \) is consistent, not only is \( A^-b \) a solution but also, for any \( z \),
\[ A^-b + (I - A^-)z \]  
is a solution because \( A(A^-b + (I - A^-)z) = AA^-b + (A - AA^-A)z = b. \)  
Furthermore, any solution to \( Ax = b \) can be represented as \( A^-b + (I - A^-)z \) for some \( z \). This is because if \( y \) is any solution (that is, if \( Ay = b \), we have

The number of linearly independent solutions arising from \( (I - A^-A)z \) is just the rank of \( (I - A^-A) \), which from equation (3.165) is \( \text{rank}(I - A^-A) = m - \text{rank}(A) \).
3.5.2 Null Space: The Orthogonal Complement

The solutions of a consistent system $Ax = b$, which we characterized in equation (3.168) as $A^{-1}b + (I - A^{-1}A)z$ for any $z$, are formed as a given solution to $Ax = b$ plus all solutions to $Az = 0$.

For an $n \times m$ matrix $A$, the set of vectors generated by all solutions, $z$, of the homogeneous system

$$Az = 0$$

is called the null space of $A$. We denote the null space of $A$ by $N(A)$.

The null space is either the single 0 vector (in which case we say the null space is empty or null) or it is a vector space.

We see that the null space of $A$ is a vector space if it is not empty because the zero vector is in $N(A)$, and if $x$ and $y$ are in $N(A)$ and $a$ is any scalar, $ax + y$ is also a solution of $Az = 0$. We call the dimension of $N(A)$ the nullity of $A$. The nullity of $A$ is

$$\dim(N(A)) = \text{rank}(I - A^{-1}A) = m - \text{rank}(A) \quad (3.170)$$

from equation (3.165).

The order of $N(A)$ is $m$. (Recall that the order of $\mathcal{V}(A)$ is $n$. The order of $\mathcal{V}(A^T)$ is $m$.)

If $A$ is square, we have

$$N(A) \subset N(A^2) \subset N(A^3) \subset \cdots \quad (3.171)$$

and

$$\mathcal{V}(A) \supset \mathcal{V}(A^2) \supset \mathcal{V}(A^3) \supset \cdots \quad (3.172)$$

(We see this easily from the inequality (3.102).)

If $Ax = b$ is consistent, any solution can be represented as $A^{-1}b + z$, for some $z$ in the null space of $A$, because if $y$ is some solution, $Ay = b = AA^{-1}b$ from equation (3.167), and so $A(y - A^{-1}b) = 0$; that is, $z = y - A^{-1}b$ is in the null space of $A$. If $A$ is nonsingular, then there is no such $z$, and the solution is unique. The number of linearly independent solutions to $Ax = 0$, is the same as the nullity of $A$.

If $a$ is in $\mathcal{V}(A^T)$ and $b$ is in $N(A)$, we have $b^T a = b^T A^T x = 0$. In other words, the null space of $A$ is orthogonal to the row space of $A$; that is, $\mathcal{N}(A) \perp \mathcal{V}(A^T)$. This is because $A^T x = a$ for some $x$, and $Ab = 0$ or $b^T A^T = 0$. For any matrix $B$ whose columns are in $\mathcal{N}(A)$, $AB = 0$, and $B^T A^T = 0$.

Because $\dim(\mathcal{N}(A)) + \dim(\mathcal{V}(A^T)) = m$ and $\mathcal{N}(A) \perp \mathcal{V}(A^T)$, by equation (2.37) we have

$$\mathcal{N}(A) \oplus \mathcal{V}(A^T) = \mathbb{R}^m; \quad (3.173)$$

that is, the null space of $A$ is the orthogonal complement of $\mathcal{V}(A^T)$. All vectors in the null space of the matrix $A^T$ are orthogonal to all vectors in the column space of $A$. 
3.6 Generalized Inverses

On page 112, we defined a generalized inverse of a matrix \( A \) as a matrix \( A^\dagger \) such that \( AA^\dagger A = A \), and we observed several interesting properties of generalized inverses. We will now consider some additional properties, after quickly summarizing some we observed previously.

**Immediate Properties of Generalized Inverses**

Let \( A \) be an \( n \times m \) matrix, and let \( A^\dagger \) be a generalized inverse of \( A \). The properties of a generalized inverse \( A^\dagger \) derived in equations (3.160) through (3.168) include:

- \((A^\dagger)^T\) is a generalized inverse of \( A^T \).
- \( \text{rank}(A) = \text{rank}(A^\dagger) \).
- \( A^\dagger A \) is idempotent.
- \( I - A^\dagger A \) is idempotent.
- \( \text{rank}(I - A^\dagger A) = m - \text{rank}(A) \).

We note that if \( A \) is \( m \times m \) and nonsingular, then \( A^\dagger = A^{-1} \), and so all of these properties apply to ordinary inverses.

In this section, we will first consider some more properties of “general” generalized inverses, which are analogous to properties of inverses, and then we will discuss some additional requirements on the generalized inverse that make it unique.

3.6.1 Generalized Inverses of Products and Sums of Matrices

We often need to perform various operations on a matrix that is expressed as sums or products of various other matrices. Some operations are rather simple, for example, the transpose of the sum of two matrices is the sum of the transposes (equation (3.10)), and the transpose of the product is the product of the transposes in reverse order (equation (3.38)). Once we know the relationships for a single sum and a single product, we can extend those relationships to various sums and products of more than just two matrices.

In Section 3.3.10, beginning on page 106, we gave a number of relationships between inverses of sums and/or products and sums and/or products of sums. The two basic relationships were equations (3.138) and (3.140):

\[
(AB)^{-1} = B^{-1}A^{-1}
\]

and

\[
(I + A)^{-1} = A^{-1}(I + A^{-1})^{-1}.
\]

These same relations hold with the inverse replaced by generalized inverses.
3.6.2 Generalized Inverses of Partitioned Matrices

If \( A \) is partitioned as
\[
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix},
\]
then, similar to equation (3.155), a generalized inverse of \( A \) is given by
\[
A^\dagger = 
\begin{bmatrix}
A_{11}^{-1} + A_{11}^{-1}A_{12}Z^{-}A_{21}A_{11}^{-1} - A_{11}^{-1}A_{12}Z^{-}

-Z^{-}A_{21}A_{11}^{-1}
\end{bmatrix},
\]
where \( Z = A_{22} - A_{21}A_{11}^{-1}A_{12} \) (see Exercise 3.17, page 159).

If the partitioning in (3.174) happens to be such that \( A_{11} \) is of full rank and of the same rank as \( A \), a generalized inverse of \( A \) is given by
\[
A^\dagger = 
\begin{bmatrix}
A_{11}^{-1} & 0 \\
0 & 0
\end{bmatrix},
\]
where 0 represents matrices of the appropriate shapes. This is not necessarily the same generalized inverse as in equation (3.175). The fact that it is a generalized inverse is easy to establish by using the definition of generalized inverse and equation (3.154).

3.6.3 Pseudoinverse or Moore-Penrose Inverse

A generalized inverse is not unique in general. As we have seen, a generalized inverse determines a set of linearly independent solutions to a linear system \( Ax = b \). We may impose other conditions on the generalized inverse to arrive at a unique matrix that yields a solution that has some desirable properties. If we impose three more conditions, we have a unique matrix, denoted by \( A^+ \), that yields a solution \( A^+b \) that has the minimum length of any solution to \( Ax = b \). We define this matrix and discuss some of its properties below, and in Section 6.7 we discuss properties of the solution \( A^+b \).
Definition and Terminology

To the general requirement $AA^{-}A = A$, we successively add three requirements that define special generalized inverses, sometimes called respectively $g_2$ or $g_{12}$, $g_3$ or $g_{123}$, and $g_4$ or $g_{1234}$ inverses. The “general” generalized inverse is sometimes called a $g_1$ inverse. The $g_4$ inverse is called the Moore-Penrose inverse. As we will see below, it is unique. The terminology distinguishing the various types of generalized inverses is not used consistently in the literature. I will indicate some alternative terms in the definition below.

For a matrix $A$, a Moore-Penrose inverse, denoted by $A^+$, is a matrix that has the following four properties.

1. $AA^+A = A$. Any matrix that satisfies this condition is called a generalized inverse, and as we have seen above is denoted by $A^{-}$. For many applications, this is the only condition necessary. Such a matrix is also called a $g_1$ inverse, an inner pseudoinverse, or a conditional inverse.
2. $A^+AA^+ = A^+$. A matrix $A^+$ that satisfies this condition is called an outer pseudoinverse. A $g_1$ inverse that also satisfies this condition is called a $g_2$ inverse or reflexive generalized inverse, and is denoted by $A^*$.
3. $A^+A$ is symmetric.
4. $AA^+$ is symmetric.

The Moore-Penrose inverse is also called the pseudoinverse, the $p$-inverse, and the normalized generalized inverse. (My current preferred term is “Moore-Penrose inverse”, but out of habit, I often use the term “pseudoinverse” for this special generalized inverse. I generally avoid using any of the other alternative terms introduced above. I use the term “generalized inverse” to mean the “general generalized inverse”, the $g_1$.) The name Moore-Penrose derives from the preliminary work of Moore (1920) and the more thorough later work of Penrose (1955), who laid out the conditions above and proved existence and uniqueness.

Existence

We can see by construction that the Moore-Penrose inverse exists for any matrix $A$. First, if $A = 0$, note that $A^+ = 0$. If $A \neq 0$, it has a full rank factorization, $A = LR$, as in equation (3.118), so $L^TAR^T = L^T LRR^T$. Because the $n \times r$ matrix $L$ is of full column rank and the $r \times m$ matrix $R$ is of full row rank, $L^T L$ and $RR^T$ are both of full rank, and hence $L^T LRR^T$ is of full rank. Furthermore, $L^T AR^T = L^T LRR^T$, so it is of full rank, and $(L^T AR^T)^{-1}$ exists. Now, form $R^T(L^T AR^T)^{-1}L$. By checking properties 1 through 4 above, we see that

$$A^+ = R^T(L^T AR^T)^{-1}L$$

(3.177)
is a Moore-Penrose inverse of $A$. This expression for the Moore-Penrose inverse based on a full rank decomposition of $A$ is not as useful as another expression we will consider later, based on $QR$ decomposition (equation (5.37) on page 208).

**Uniqueness**

We can see that the Moore-Penrose inverse is unique by considering any matrix $G$ that satisfies the properties 1 through 4 for $A \neq 0$. (The Moore-Penrose inverse of $A = 0$ (that is, $A^+ = 0$) is clearly unique, as there could be no other matrix satisfying property 2.) By applying the properties and using $A^+$ given above, we have the following sequence of equations:

$$
G = \frac{GAG = (GA)^T G = A^T G T G = (A A^+ A)^T G T G = (A^+ A)^T A^T G T G =}
A^+ A A^T G T G = A^+ A (GA)^T G = A^+ A G A G = A^+ A A^+ A G = \frac{A^+ (A A^+)^T (AG)^T = A^+ (A^+)^T A^T G A T = A^+ (A^+)^T (AG A)^T =}
A^+ (A^+)^T A^T = A^+ (A A^+)^T = A^+ A A^+ = A^+.
$$

**Other Properties**

Similarly to the property for inverses expressed in equation 3.115, we have

$$(A^+)^T = (A^T)^+.$$  (3.178)

This is easily seen from the defining properties of the Moore-Penrose inverse.

If $A$ is nonsingular, then obviously $A^+ = A^{-1}$, just as for any generalized inverse.

Because $A^+$ is a generalized inverse, all of the properties for a generalized inverse $A^-$ discussed above hold; in particular, $A^+ b$ is a solution to the linear system $Ax = b$ (see equation (3.166)). In Section 6.7, we will show that this unique solution has a kind of optimality.

If the inverses on the right-hand side of equation (3.175) are pseudoinverses, then the result is the pseudoinverse of $A$.

The generalized inverse given in equation (3.176) is the same as the pseudoinverse given in equation (3.177).

Pseudoinverses also have a few additional interesting properties not shared by generalized inverses; for example

$$(I - A^+ A)A^+ = 0.$$  (3.179)
3.7 Orthogonality

In Section 2.1.8, we defined orthogonality and orthonormality of two or more vectors in terms of dot products. On page 88, in equation (3.87), we also defined the orthogonal binary relationship between two matrices. Now we define the orthogonal unary property of a matrix. This is the more important property and is what is commonly meant when we speak of orthogonality of matrices. We use the orthonormality property of vectors, which is a binary relationship, to define orthogonality of a single matrix.

Orthogonal Matrices; Definition and Simple Properties

A matrix whose rows or columns constitute a set of orthonormal vectors is said to be an *orthogonal* matrix. If \( Q \) is an \( n \times m \) orthogonal matrix, then \( QQ^T = I_n \) if \( n \leq m \), and \( Q^TQ = I_m \) if \( n \geq m \). If \( Q \) is a square orthogonal matrix, then \( QQ^T = Q^TQ = I \). An orthogonal matrix is also called a *unitary matrix*. (For matrices whose elements are complex numbers, a matrix is said to be *unitary* if the matrix times its conjugate transpose is the identity; that is, if \( QQ^H = I \).)

The determinant of a square orthogonal matrix is \( \pm 1 \) (because the determinant of the product is the product of the determinants and the determinant of \( I \) is 1).

When \( n \geq m \), the matrix inner product of an \( n \times m \) orthogonal matrix \( Q \) with itself is its number of columns:

\[
\langle Q, Q \rangle = m. \tag{3.180}
\]

This is because \( Q^TQ = I_m \). If \( n \leq m \), it is its number of rows. Recalling the definition of the orthogonal binary relationship from page 88, we note that if \( Q \) is an orthogonal matrix, then \( Q \) is not orthogonal to itself.

A permutation matrix (see page 74) is orthogonal. We can see this by building the permutation matrix as a product of elementary permutation matrices, and it is easy to see that they are all orthogonal.

One further property we see by simple multiplication is that if \( A \) and \( B \) are orthogonal, then \( A \otimes B \) is orthogonal.

The definition of orthogonality is sometimes made more restrictive to require that the matrix be square.

Orthogonal and Orthonormal Columns

The definition given above for orthogonal matrices is sometimes relaxed to require only that the columns or rows be orthogonal (rather than orthonormal). If orthonormality is not required, the determinant is not necessarily \( \pm 1 \). If \( Q \) is a matrix that is “orthogonal” in this weaker sense of the definition, and \( Q \) has more rows than columns, then
Unless stated otherwise, I use the term “orthogonal matrix” to refer to a matrix whose columns are orthonormal; that is, for which $Q^TQ = I$.

The Orthogonal Group

The set of $n \times m$ orthogonal matrices for which $n \geq m$ is called an $(n, m)$ Stiefel manifold, and an $(n, n)$ Stiefel manifold together with Cayley multiplication is a group, sometimes called the orthogonal group and denoted as $O(n)$. The orthogonal group $O(n)$ is a subgroup of the general linear group $GL(n)$, defined on page 103. The orthogonal group is useful in multivariate analysis because of the invariance of the so-called Haar measure over this group (see Section 4.5.1).

Because the Euclidean norm of any column of an $n \times m$ orthogonal matrix with $n \geq m$ is 1, no element in the matrix can be greater than 1 in absolute value. We therefore have an analogue of the Bolzano-Weierstrass theorem for sequences of orthogonal matrices. The standard Bolzano-Weierstrass theorem for real numbers states that if a sequence $a_i$ is bounded, then there exists a subsequence $a_{i_j}$ that converges. (See any text on real analysis.) From this, we conclude that if $Q_1, Q_2, \ldots$ is a sequence of $n \times n$ orthogonal matrices, then there exists a subsequence $Q_{i_1}, Q_{i_2}, \ldots$, such that

$$\lim_{j \to \infty} Q_{i_j} = Q,$$

(3.181)

where $Q$ is some fixed matrix. The limiting matrix $Q$ must also be orthogonal because $Q_{i_j}^TQ_{i_j} = I$, and so, taking limits, we have $Q^TQ = I$. The set of $n \times n$ orthogonal matrices is therefore compact.

Conjugate Vectors

Instead of defining orthogonality of vectors in terms of dot products as in Section 2.1.8, we could define it more generally in terms of a bilinear form as in Section 3.2.9. If the bilinear form $x^TAy = 0$, we say $x$ and $y$ are orthogonal with respect to the matrix $A$. We also often use a different term and say that the vectors are conjugate with respect to $A$, as in equation (3.71). The usual definition of orthogonality in terms of a dot product is equivalent to the definition in terms of a bilinear form in the identity matrix.

Likewise, but less often, orthogonality of matrices is generalized to conjugacy of two matrices with respect to a third matrix: $Q^TAQ = I$. 

$$Q^TQ = \begin{bmatrix} X & 0 & \cdots & 0 \\ 0 & X & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & X \end{bmatrix}.$$
3.8 Eigenanalysis; Canonical Factorizations

Multiplication of a given vector by a square matrix may result in a scalar multiple of the vector. Stating this more formally, and giving names to such a special vector and scalar, if \( A \) is an \( n \times n \) (square) matrix, \( v \) is a vector not equal to 0, and \( c \) is a scalar such that

\[
Av = cv, \tag{3.182}
\]

we say \( v \) is an \textit{eigenvector} of the matrix \( A \), and \( c \) is an \textit{eigenvalue} of the matrix \( A \). We refer to the pair \( c \) and \( v \) as an associated eigenvector and eigenvalue or as an \textit{eigenpair}. While we restrict an eigenvector to be nonzero (or else we would have 0 as an eigenvector associated with any number being an eigenvalue), an eigenvalue can be 0; in that case, of course, the matrix must be singular. (Some authors restrict the definition of an eigenvalue to real values that satisfy (3.182), and there is an important class of matrices for which it is known that all eigenvalues are real. In this book, we do not want to restrict ourselves to that class; hence, we do not require \( c \) or \( v \) in equation (3.182) to be real.)

We use the term “eigenanalysis” or “eigenproblem” to refer to the general theory, applications, or computations related to either eigenvectors or eigenvalues.

There are various other terms used for eigenvalues and eigenvectors. An eigenvalue is also called a \textit{characteristic value} (that is why I use a “\( e \)” to represent an eigenvalue), a \textit{latent root}, or a \textit{proper value}, and similar synonyms exist for an eigenvector. An eigenvalue is also sometimes called a \textit{singular value}, but the latter term has a different meaning that we will use in this book (see page 143; the absolute value of an eigenvalue is a singular value, and singular values are also defined for nonsquare matrices).

Although generally throughout this chapter we have assumed that vectors and matrices are real, in eigenanalysis, even if \( A \) is real, it may be the case that \( c \) and \( v \) are complex. Therefore, in this section, we must be careful about the nature of the eigenpairs, even though we will continue to assume the basic matrices are real.

Before proceeding to consider properties of eigenvalues and eigenvectors, we should note how remarkable the relationship \( Av = cv \) is: the effect of a matrix multiplication of an eigenvector is the same as a scalar multiplication of the eigenvector. The eigenvector is an \textit{invariant} of the transformation in the sense that its direction does not change. This would seem to indicate that the eigenvalue and eigenvector depend on some kind of deep properties of the matrix, and indeed this is the case, as we will see. Of course, the first question is whether such special vectors and scalars exist. The answer is yes, but before considering that and other more complicated issues, we will state some simple properties of any scalar and vector that satisfy \( Av = cv \) and introduce some additional terminology.
Left Eigenvectors

In the following, when we speak of an eigenvector or eigenpair without qualification, we will mean the objects defined by equation (3.182). There is another type of eigenvector for $A$, however, a left eigenvector, defined as a nonzero $w$ in

$$w^T A = cw^T.$$  \hspace{1cm} (3.183)

For emphasis, we sometimes refer to the eigenvector of equation (3.182), $Av = cv$, as a right eigenvector.

We see from the definition of a left eigenvector, that if a matrix is symmetric, each left eigenvector is an eigenvector (a right eigenvector).

If $v$ is an eigenvector of $A$ and $w$ is a left eigenvector of $A$ with a different associated eigenvalue, then $v$ and $w$ are orthogonal; that is, if $Av = c_1 v$, $w^T A = c_2 w^T$, and $c_1 \neq c_2$, then $w^T v = 0$. We see this by multiplying both sides of $w^T A = c_2 w^T$ by $v$ to get $w^T Av = c_2 w^T v$ and multiplying both sides of $Av = c_1 v$ by $w^T$ to get $w^T Av = c_1 w^T v$. Hence, we have $c_1 w^T v = c_2 w^T v$, and because $c_1 \neq c_2$, we have $w^T v = 0$.

3.8.1 Basic Properties of Eigenvalues and Eigenvectors

If $c$ is an eigenvalue and $v$ is a corresponding eigenvector for a real matrix $A$, we see immediately from the definition of eigenvector and eigenvalue in equation (3.182) the following properties. (In Exercise 3.19, you are asked to supply the simple proofs for these properties, or you can see the proofs in a text such as Harville, 1997, for example.)

Assume that $Av = cv$ and that all elements of $A$ are real.

1. $bv$ is an eigenvector of $A$, where $b$ is any nonzero scalar.
   It is often desirable to scale an eigenvector $v$ so that $v^T v = 1$. Such a normalized eigenvector is also called a **unit eigenvector**.
   For a given eigenvector, there is always a particular eigenvalue associated with it, but for a given eigenvalue there is a space of associated eigenvectors. (The space is a vector space if we consider the zero vector to be a member.) It is therefore not appropriate to speak of “the” eigenvector associated with a given eigenvalue — although we do use this term occasionally. (We could interpret it as referring to the normalized eigenvector.) There is, however, another sense in which an eigenvalue does not determine a unique eigenvector, as we discuss below.

2. $bc$ is an eigenvalue of $bA$, where $b$ is any nonzero scalar.
3. $1/c$ and $v$ are an eigenpair of $A^{-1}$ (if $A$ is nonsingular).
4. $1/c$ and $v$ are an eigenpair of $A^+$ if $A$ (and hence $A^+$) is square and $c$ is nonzero.
5. If $A$ is diagonal or triangular with elements $a_{ii}$, the eigenvalues are $a_{ii}$, and for diagonal $A$ the corresponding eigenvectors are $e_i$ (the unit vectors).
6. \( c^2 \) and \( v \) are an eigenpair of \( A^2 \). More generally, \( c^k \) and \( v \) are an eigenpair of \( A^k \) for \( k = 1, 2, \ldots \).

7. If \( A \) and \( B \) are conformable for the multiplications \( AB \) and \( BA \), the nonzero eigenvalues of \( AB \) are the same as the nonzero eigenvalues of \( BA \). (Note that \( A \) and \( B \) are not necessarily square.) The set of eigenvalues is the same if \( A \) and \( B \) are square. (Note, however, that if \( A \) and \( B \) are square and \( d \) is an eigenvalue of \( B \), \( d \) is not necessarily an eigenvalue of \( AB \).)

8. If \( A \) and \( B \) are square and of the same order and if \( B^{-1} \) exists, then the eigenvalues of \( BAB^{-1} \) are the same as the eigenvalues of \( A \). (This is called a similarity transformation; see page 129.)

### 3.8.2 The Characteristic Polynomial

From the equation \((A - cI)v = 0\) that defines eigenvalues and eigenvectors, we see that in order for \( v \) to be nonnull, \((A - cI)\) must be singular, and hence

\[
\det(A - cI) = \det(cI - A) = 0. \tag{3.184}
\]

Equation (3.184) is sometimes taken as the definition of an eigenvalue \( c \). It is definitely a fundamental relation, and, as we will see, allows us to identify a number of useful properties.

For the \( n \times n \) matrix \( A \), the determinant in equation (3.184) is a polynomial of degree \( n \) in \( c \), \( p_A(c) \), called the characteristic polynomial, and when it is equated to 0, it is called the characteristic equation:

\[
p_A(c) = s_0 + s_1c + \cdots + s_nc^n = 0. \tag{3.185}
\]

From the expansion of the determinant \( \det(cI - A) \), as in equation (3.35) on page 67, we see that \( s_0 = (-1)^n \det(A) \) and \( s_n = 1 \), and, in general, \( s_k = (-1)^{n-k} \) times the sums of all principal minors of \( A \) of order \( n - k \). (Note that the signs of the \( s_i \) are different depending on whether we use \( \det(cI - A) \) or \( \det(A - cI) \).)

An eigenvalue of \( A \) is a root of the characteristic polynomial. The existence of \( n \) roots of the polynomial (by the Fundamental Theorem of Algebra) allows the characteristic polynomial to be written in factored form as

\[
p_A(c) = (-1)^n (c - c_1) \cdots (c - c_n), \tag{3.186}
\]

and establishes the existence of \( n \) eigenvalues. Some may be complex, some may be zero, and some may be equal to others. We call the set of all eigenvalues the spectrum of the matrix. The “number of eigenvalues” must be distinguished from the cardinality of the spectrum, which is the number of unique values.

A real matrix may have complex eigenvalues (and, hence, eigenvectors), just as a polynomial with real coefficients can have complex roots. Clearly, the
eigenvalues of a real matrix must occur in conjugate pairs just as in the case of roots of polynomials with real coefficients. (As mentioned above, some authors restrict the definition of an eigenvalue to real values that satisfy (3.182). We will see below that the eigenvalues of a real symmetric matrix are always real, and this is a case that we will emphasize, but in this book we do not restrict the definition.)

The characteristic polynomial has many interesting properties. One, stated in the Cayley-Hamilton theorem, is that the matrix itself is a root of the matrix polynomial formed by the characteristic polynomial; that is,

\[ p_A(A) = s_0 I + s_1 A + \cdots + s_n A^n = 0_n. \]  

(3.187)

We see this by using equation (3.28) to write the matrix in equation (3.184) as

\[ (A - cI)\text{adj}(A - cI) = p_A(c)I. \]  

(3.188)

Hence \( \text{adj}(A - cI) \) is a polynomial in \( c \) of degree less than or equal to \( n - 1 \), so we can write it as

\[ \text{adj}(A - cI) = B_0 + B_1 c + \cdots + B_{n-1} c^{n-1}, \]

where the \( B_i \) are \( n \times n \) matrices. Now, equating the coefficients of \( c \) on the two sides of equation (3.188), we have

\[
\begin{align*}
AB_0 &= s_0 I \\
AB_1 - B_0 &= s_1 I \\
& \quad \vdots \\
AB_{n-1} - B_{n-2} &= s_{n-1} I \\
B_{n-1} &= s_n I.
\end{align*}
\]

Now, multiply the second equation by \( A \), the third equation by \( A^2 \), and the \( i^{th} \) equation by \( A^{i-1} \), and add all equations. We get the desired result: \( p_A(A) = 0 \).

See also Exercise 3.20.

Another interesting fact is that any given \( n^{th} \)-degree polynomial, \( p \), is the characteristic polynomial of an \( n \times n \) matrix, \( A \), of particularly simple form. Consider the polynomial

\[ p(c) = s_0 + s_1 c + \cdots + s_{n-1} c^{n-1} + c^n \]

and the matrix

\[
A = \begin{bmatrix}
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & \cdots & 0 \\
& & & \ddots & \\
0 & 0 & 0 & \cdots & 1 \\
-s_0 & -s_1 & -s_2 & \cdots & -s_{n-1}
\end{bmatrix}.
\]  

(3.189)
The matrix $A$ is called the *companion matrix* of the polynomial $p$, and it is easy to see (by a tedious expansion) that the characteristic polynomial of $A$ is $p$. This, of course, shows that a characteristic polynomial does not uniquely determine a matrix, although the converse is true (within signs).

### Additional Properties of Eigenvalues and Eigenvectors

Using the characteristic polynomial yields the following properties. This is a continuation of the list we began on page 122. We assume $A$ is a real matrix with eigenpair $(c, v)$.

10. $c$ is an eigenvalue of $A^T$ (because $\det(A^T - cI) = \det(A - cI)$ for any $c$). The eigenvectors of $A^T$, which are left eigenvectors of $A$, are not necessarily the same as the eigenvectors of $A$, however.

11. There is a left eigenvector such that $c$ is the associated eigenvalue.

12. $(\bar{c}, \bar{v})$ is an eigenpair of $A$, where $\bar{c}$ and $\bar{v}$ are the complex conjugates and $A$, as usual, consists of real elements. (If $c$ and $v$ are real, this is a tautology.)

13. $c\bar{c}$ is an eigenvalue of $A^TA$.

14. $c$ is real if $A$ is symmetric or if $A$ is triangular.

In Exercise 3.21, you are asked to supply the simple proofs for these properties, or you can see the proofs in a text such as Harville (1997), for example.

A further comment on property 12 may be worthwhile. Throughout this book, we assume we begin with real numbers. There are some times, however, when standard operations in the real domain carry us outside the reals. The simplest situations, which of course are related, are roots of polynomial equations with real coefficients and eigenpairs of matrices with real elements. In both of these situations, because sums must be real, the complex values occur in conjugate pairs.

### Eigenvalues and the Trace and Determinant

If the eigenvalues of the matrix $A$ are $c_1, \ldots, c_n$, because they are the roots of the characteristic polynomial, we can readily form that polynomial as

\[
p_A(c) = (c - c_1) \cdots (c - c_n) = (-1)^n \prod c_i + \cdots + (-1)^{n-1} \sum c_i c^{n-1} + c^n. \tag{3.190}
\]

Because this is the same polynomial as obtained by the expansion of the determinant in equation (3.185), the coefficients must be equal. In particular, by simply equating the corresponding coefficients of the constant terms and $(n-1)^{th}$-degree terms, we have the two very important facts:

\[
\det(A) = \prod c_i \tag{3.191}
\]
\[ \text{tr}(A) = \sum c_i. \]  

(3.192)

It might be worth recalling that we have assumed the \( A \) is real, and therefore \( \det(A) \) and \( \text{tr}(A) \) are real, but the eigenvalues \( c_i \) may not be real. Nonreal eigenvalues, however, occur in conjugate pairs (property 12 above); hence \( \prod c_i \) and \( \sum c_i \) are real.

### 3.8.3 The Spectrum

Although, for an \( n \times n \) matrix, from the characteristic polynomial we have \( n \) roots, and hence \( n \) eigenvalues, some of these roots may be the same. It may also be the case that more than one eigenvector corresponds to a given eigenvalue. As we mentioned above, the set of all the distinct eigenvalues of a matrix is called the *spectrum* of the matrix.

#### Notation

Sometimes it is convenient to refer to the distinct eigenvalues and sometimes we wish to refer to all eigenvalues, as in referring to the number of roots of the characteristic polynomial. To refer to the distinct eigenvalues in a way that allows us to be consistent in the subscripts, we will call the distinct eigenvalues \( \lambda_1, \ldots, \lambda_k \). The set of these constitutes the spectrum.

We denote the spectrum of the matrix \( A \) by \( \sigma(A) \):

\[ \sigma(A) = \{\lambda_1, \ldots, \lambda_k\}. \]  

(3.193)

In terms of the spectrum, equation (3.186) becomes

\[ p_A(c) = (-1)^n (c - \lambda_1)^{m_1} \cdots (c - \lambda_k)^{m_k}, \]  

for \( m_i \geq 1 \).

We label the \( c_i \) and \( v_i \) so that

\[ |c_1| \geq \cdots \geq |c_n|. \]  

(3.195)

We likewise label the \( \lambda_i \) so that

\[ |\lambda_1| > \cdots > |\lambda_k|. \]  

(3.196)

With this notation, we have

\[ |\lambda_1| = |c_1| \]

and

\[ |\lambda_k| = |c_n|, \]

but we cannot say anything about the other \( \lambda \)s and \( c \)s.
The Spectral Radius

For the matrix $A$ with these eigenvalues, $|c_1|$ is called the spectral radius and is denoted by $\rho(A)$:

$$\rho(A) = \max |c_i|.$$  

(3.197)

The set of complex numbers

$$\{x : |x| = \rho(A)\}$$

(3.198)

is called the spectral circle of $A$.

An eigenvalue corresponding to $\max |c_i|$ (that is, $c_1$) is called a dominant eigenvalue. We are more often interested in the absolute value (or modulus) of a dominant eigenvalue rather than the eigenvalue itself; that is, $\rho(A)$ (that is, $|c_1|$) is more often of interest than just $c_1$.

Interestingly, we have for all $i$

$$|c_i| \leq \max_j \sum_k |a_{kj}|$$

(3.199)

and

$$|c_i| \leq \max_k \sum_j |a_{kj}|.$$  

(3.200)

The inequalities of course also hold for $\rho(A)$ on the left-hand side. Rather than proving this here, we show this fact in a more general setting relating to matrix norms in inequality (3.259) on page 150. (These bounds relate to the $L_1$ and $L_\infty$ matrix norms, respectively.)

A matrix may have all eigenvalues equal to 0 but yet the matrix itself may not be 0. Any upper triangular matrix with all 0s on the diagonal is an example.

Because, as we saw on page 122, if $c$ is an eigenvalue of $A$, then $bc$ is an eigenvalue of $bA$ where $b$ is any nonzero scalar, we can scale a matrix with a nonzero eigenvalue so that its spectral radius is 1. The scaled matrix is simply $A/|c_1|$.

Linear Independence of Eigenvectors Associated with Distinct Eigenvalues

Suppose that $\{\lambda_1, \ldots, \lambda_k\}$ is a set of distinct eigenvalues of the matrix $A$ and $\{x_1, \ldots, x_k\}$ is a set of eigenvectors such that $(\lambda_i, x_i)$ is an eigenpair. Then $x_1, \ldots, x_k$ are linearly independent; that is, eigenvectors associated with distinct eigenvalues are linearly independent.

We can see that this must be the case by assuming that the eigenvectors are not linearly independent. In that case, let $\{y_1, \ldots, y_j\} \subset \{x_1, \ldots, x_k\}$, for some $j < k$, be a maximal linearly independent subset. Let the corresponding eigenvalues be $\{\mu_1, \ldots, \mu_j\} \subset \{\lambda_1, \ldots, \lambda_k\}$. Then, for some eigenvector $y_{j+1}$, we have
for some \( t_i \). Now, multiplying both sides of the equation by \( A - \mu_{j+1}I \), where \( \mu_{j+1} \) is the eigenvalue corresponding to \( y_{j+1} \), we have

\[
0 = \sum_{i=1}^{j} t_i (\mu_i - \mu_{j+1}) y_i.
\]

If the eigenvalues are unique (that is, for each \( i \leq j \)), we have \( \mu_i \neq \mu_{j+1} \), then the assumption that the eigenvalues are not linearly independent is contradicted because otherwise we would have a linear combination with nonzero coefficients equal to zero.

**The Eigenspace and Geometric Multiplicity**

Rewriting the definition (3.182) for the \( i \)th eigenvalue and associated eigenvector of the \( n \times n \) matrix \( A \) as

\[
(A - c_i I)v_i = 0,
\]

we see that the eigenvector \( v_i \) is in \( \mathcal{N}(A - c_i I) \), the null space of \( A - c_i I \). For such a nonnull vector to exist, of course, \( A - c_i I \) must be singular; that is, \( \text{rank}(A - c_i I) \) must be less than \( n \). This null space is called the *eigenspace* of the eigenvalue \( c_i \).

It is possible that a given eigenvalue may have more than one associated eigenvector that are linearly independent of each other. For example, we easily see that the identity matrix has only one unique eigenvalue, namely 1, but any vector is an eigenvector, and so the number of linearly independent eigenvectors is equal to the number of rows or columns of the identity. If \( u \) and \( v \) are eigenvectors corresponding to the same eigenvalue \( c \), then any linear combination of \( u \) and \( v \) is an eigenvector corresponding to \( c \); that is, if \( Au = cu \) and \( Av = cv \), for any scalars \( a \) and \( b \),

\[
A(au + bv) = c(au + bv).
\]

The dimension of the eigenspace corresponding to the eigenvalue \( c_i \) is called the *geometric multiplicity* of \( c_i \); that is, the geometric multiplicity of \( c_i \) is the nullity of \( A - c_i I \). If \( g_i \) is the geometric multiplicity of \( c_i \), an eigenvalue of the \( n \times n \) matrix \( A \), then we can see from equation (3.170) that \( \text{rank}(A - c_i I) + g_i = n \).

The multiplicity of 0 as an eigenvalue is just the nullity of \( A \). If \( A \) is of full rank, the multiplicity of 0 will be 0, but, in this case, we do not consider 0 to be an eigenvalue. If \( A \) is singular, however, we consider 0 to be an eigenvalue, and the multiplicity of the 0 eigenvalue is the rank deficiency of \( A \).
Multiple linearly independent eigenvectors corresponding to the same eigenvalue can be chosen to be orthogonal to each other using, for example, the Gram-Schmidt transformations, as in equation (2.47) on page 37. These orthogonal eigenvectors span the same eigenspace. They are not unique, of course, as any sequence of Gram-Schmidt transformations could be applied.

### Algebraic Multiplicity

A single value that occurs as a root of the characteristic equation \( m \) times is said to have **algebraic multiplicity** \( m \). Although we sometimes refer to this as just the multiplicity, algebraic multiplicity should be distinguished from geometric multiplicity, defined above. These are not the same, as we will see in an example later. An eigenvalue whose algebraic multiplicity and geometric multiplicity are the same is called a **semisimple** eigenvalue. An eigenvalue with algebraic multiplicity 1 is called a **simple** eigenvalue.

Because the determinant that defines the eigenvalues of an \( n \times n \) matrix is an \( n \)th-degree polynomial, we see that the sum of the multiplicities of distinct eigenvalues is \( n \).

Because most of the matrices in statistical applications are real, in the following we will generally restrict our attention to real matrices. It is important to note that the eigenvalues and eigenvectors of a real matrix are not necessarily real, but as we have observed, the eigenvalues of a symmetric real matrix are real. (The proof, which was stated as an exercise, follows by noting that if \( A \) is symmetric, the eigenvalues of \( A^T A \) are the eigenvalues of \( A^2 \), which from the definition are obviously nonnegative.)

### 3.8.4 Similarity Transformations

Two \( n \times n \) matrices, \( A \) and \( B \), are said to be **similar** if there exists a nonsingular matrix \( P \) such that

\[
B = P^{-1}AP. \tag{3.202}
\]

The transformation in equation (3.202) is called a **similarity transformation**. (Compare this with **equivalent matrices** on page 99. The matrices \( A \) and \( B \) in equation (3.202) are equivalent, as we see using equations (3.121) and (3.122).)

It is clear from the definition that the similarity relationship is both commutative and transitive.

If \( A \) and \( B \) are similar, as in equation (3.202), then for any scalar \( c \)

\[
\det(A - cI) = \det(P^{-1})\det(A - cI)\det(P) \\
= \det(P^{-1}AP - cP^{-1}I) \\
= \det(B - cI),
\]

and, hence, \( A \) and \( B \) have the same eigenvalues. (This simple fact was stated as property 8 on page 123.)
Orthogonally Similar Transformations

An important type of similarity transformation is based on an orthogonal matrix in equation (3.202). If \( Q \) is orthogonal and \( B = Q^T AQ \), (3.203)

\( A \) and \( B \) are said to be orthogonally similar.

If \( B \) in the equation \( B = Q^T AQ \) is a diagonal matrix, \( A \) is said to be orthogonally diagonalizable, and \( QBQ^T \) is called the orthogonally diagonal factorization or orthogonally similar factorization of \( A \). We will discuss characteristics of orthogonally diagonalizable matrices in Sections 3.8.5 and 3.8.6 below.

Schur Factorization

If \( B \) in equation (3.203) is an upper triangular matrix, \( QBQ^T \) is called the Schur factorization of \( A \).

For any square matrix, the Schur factorization exists; hence, it is one of the most useful similarity transformations. The Schur factorization clearly exists in the degenerate case of a \( 1 \times 1 \) matrix.

To see that it exists for any \( n \times n \) matrix \( A \), let \((c, v)\) be an arbitrary eigenpair of \( A \) with \( v \) normalized, and form an orthogonal matrix \( U \) with \( v \) as its first column. Let \( U_2 \) be the matrix consisting of the remaining columns; that is, \( U \) is partitioned as \([v \mid U_2]\).

\[
U^T AU = \begin{bmatrix}
v^T Av & v^T AU_2 \\
U_2^T Av & U_2^T AU_2
\end{bmatrix}
\]

\[
= \begin{bmatrix}
c & v^T AU_2 \\
0 & U_2^T AU_2
\end{bmatrix}
\]

\[
= B,
\]

where \( U_2^T AU_2 \) is an \((n - 1) \times (n - 1)\) matrix. Now the eigenvalues of \( U^T AU \) are the same as those of \( A \); hence, if \( n = 2 \), then \( U_2^T AU_2 \) is a scalar and must equal the other eigenvalue, and so the statement is proven.

We now use induction on \( n \) to establish the general case. Assume that the factorization exists for any \((n - 1) \times (n - 1)\) matrix, and let \( A \) be any \( n \times n \) matrix. We let \((c, v)\) be an arbitrary eigenpair of \( A \) (with \( v \) normalized), follow the same procedure as in the preceding paragraph, and get

\[
U^T AU = \begin{bmatrix}
c & v^T AU_2 \\
0 & U_2^T AU_2
\end{bmatrix}.
\]

Now, since \( U_2^T AU_2 \) is an \((n - 1) \times (n - 1)\) matrix, by the induction hypothesis there exists an \((n - 1) \times (n - 1)\) orthogonal matrix \( V \) such that \( V^T (U_2^T AU_2) V = T \), where \( T \) is upper triangular. Now let
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\[ Q = U \begin{bmatrix} 1 & 0 \\ 0 & V \end{bmatrix}. \]

By multiplication, we see that \( Q^T Q = I \) (that is, \( Q \) is orthogonal). Now form

\[ Q^T AQ = \begin{bmatrix} c & v^T AU_2 V \\ 0 & V^T U_2^T AU_2 V \end{bmatrix} = \begin{bmatrix} c & v^T AU_2 V \\ 0 & T \end{bmatrix} = B. \]

We see that \( B \) is upper triangular because \( T \) is, and so by induction the Schur factorization exists for any \( n \times n \) matrix.

Note that the Schur factorization is also based on orthogonally similar transformations, but the term “orthogonally similar factorization” is generally used only to refer to the diagonal factorization.

**Uses of Similarity Transformations**

Similarity transformations are very useful in establishing properties of matrices, such as convergence properties of sequences (see, for example, Section 3.9.5). Similarity transformations are also used in algorithms for computing eigenvalues (see, for example, Section 7.3). In an orthogonally similar factorization, the elements of the diagonal matrix are the eigenvalues. Although the diagonals in the upper triangular matrix of the Schur factorization are the eigenvalues, that particular factorization is rarely used in computations.

Although similar matrices have the same eigenvalues, they do not necessarily have the same eigenvectors. If \( A \) and \( B \) are similar, for some nonzero vector \( v \) and some scalar \( c \), \( Av = cv \) implies that there exists a nonzero vector \( u \) such that \( Bu = cu \), but it does not imply that \( u = v \) (see Exercise 3.22b).

**3.8.5 Similar Canonical Factorization; Diagonalizable Matrices**

If \( V \) is a matrix whose columns correspond to the eigenvectors of \( A \), and \( C \) is a diagonal matrix whose entries are the eigenvalues corresponding to the columns of \( V \), using the definition (equation (3.182)) we can write

\[ AV = VC. \]  

(3.204)

Now, if \( V \) is nonsingular, we have

\[ A = VCV^{-1}. \]  

(3.205)

Expression (3.205) represents a diagonal factorization of the matrix \( A \). We see that a matrix \( A \) with eigenvalues \( c_1, \ldots, c_n \) that can be factorized this way is similar to the matrix \( \text{diag}(c_1, \ldots, c_n) \), and this representation is sometimes called the similar canonical form of \( A \) or the similar canonical factorization of \( A \).
Not all matrices can be factored as in equation (3.205). It obviously depends on \( V \) being nonsingular; that is, that the eigenvectors are linearly independent. If a matrix can be factored as in (3.205), it is called a diagonalizable matrix, a simple matrix, or a regular matrix (the terms are synonymous, and we will generally use the term “diagonalizable”); a matrix that cannot be factored in that way is called a deficient matrix or a defective matrix (the terms are synonymous).

Any matrix all of whose eigenvalues are unique is diagonalizable (because, as we saw on page 127, in that case the eigenvectors are linearly independent), but uniqueness of the eigenvalues is not a necessary condition. A necessary and sufficient condition for a matrix to be diagonalizable can be stated in terms of the unique eigenvalues and their multiplicities: suppose for the \( n \times n \) matrix \( A \) that the distinct eigenvalues \( \lambda_1, \ldots, \lambda_k \) have algebraic multiplicities \( m_1, \ldots, m_k \). If, for \( l = 1, \ldots, k \),

\[
\text{rank}(A - \lambda_l I) = n - m_l \quad (3.206)
\]

(that is, if all eigenvalues are semisimple), then \( A \) is diagonalizable, and this condition is also necessary for \( A \) to be diagonalizable. This fact is called the “diagonalizability theorem”. Recall that \( A \) being diagonalizable is equivalent to \( V \) in \( AV = VC \) (equation (3.204)) being nonsingular.

To see that the condition is sufficient, assume, for each \( i \), \( \text{rank}(A - c_i I) = n - m_i \), and so the equation \( (A - c_i I)x = 0 \) has exactly \( n - (n - m_i) \) linearly independent solutions, which are by definition eigenvectors of \( A \) associated with \( c_i \). (Note the somewhat complicated notation. Each \( c_i \) is the same as some \( \lambda_l \), and for each \( \lambda_l \), we have \( \lambda_l = c_{i_l} = c_{m_l} \) for \( 1 \leq l_1 < \cdots < l_{m_l} \leq n \).)

Let \( w_1, \ldots, w_{m_i} \) be a set of linearly independent eigenvectors associated with \( c_i \), and let \( u \) be an eigenvector associated with \( c_j \) and \( c_j \neq c_i \). (The vectors \( w_1, \ldots, w_{m_i} \) and \( u \) are columns of \( V \).) We have already seen on page 127 that \( u \) must be linearly independent of the other eigenvectors, but we can also use a slightly different argument here. Now if \( u \) is not linearly independent of \( w_1, \ldots, w_{m_i} \), we write \( u = \sum b_kw_k \), and so \( Au = A \sum b_kw_k = c_i \sum b_kw_k = c_i u \), contradicting the assumption that \( u \) is not an eigenvector associated with \( c_i \). Therefore, the eigenvectors associated with different eigenvalues are linearly independent, and so \( V \) is nonsingular.

Now, to see that the condition is necessary, assume \( V \) is nonsingular; that is, \( V^{-1} \) exists. Because \( C \) is a diagonal matrix of all \( n \) eigenvalues, the matrix \( (C - c_i I) \) has exactly \( m_i \) zeros on the diagonal, and hence, \( \text{rank}(C - c_i I) = n - m_i \). Because \( V(C - c_i I)V^{-1} = (A - c_i I) \), and multiplication by a full rank matrix does not change the rank (see page 101), we have \( \text{rank}(A - c_i I) = n - m_i \).

**Symmetric Matrices**

A symmetric matrix is a diagonalizable matrix. We see this by first letting \( A \) be any \( n \times n \) symmetric matrix with eigenvalue \( c \) of multiplicity \( m \). We need
to show that \( \text{rank}(A - cI) = n - m \). Let \( B = A - cI \), which is symmetric because \( A \) and \( I \) are. First, we note that \( c \) is real, and therefore \( B \) is real. Let \( r = \text{rank}(B) \). From equation (3.133), we have

\[
\text{rank} \left( B^2 \right) = \text{rank} \left( B^T B \right) = \text{rank}(B) = r.
\]

In the full rank partitioning of \( B \), there is at least one \( r \times r \) principal submatrix of full rank. The \( r \)-order principal minor in \( B^2 \) corresponding to any full rank \( r \times r \) principal submatrix of \( B \) is therefore positive. Furthermore, any \( j \)-order principal minor in \( B^2 \) for \( j > r \) is zero. Now, rewriting the characteristic polynomial in equation (3.185) slightly by attaching the sign to the variable \( w \), we have

\[
p_{B^2}(w) = t_{n-r}(-w)^{n-r} + \cdots + t_{n-1}(-w)^{n-1} + (-w)^n = 0,
\]

where \( t_{n-j} \) is the sum of all \( j \)-order principal minors. Because \( t_{n-r} \neq 0 \), \( w = 0 \) is a root of multiplicity \( n - r \). It is likewise an eigenvalue of \( B \) with multiplicity \( n - r \). Because \( A = B + cI \), \( 0 + c \) is an eigenvalue of \( A \) with multiplicity \( n - r \); hence, \( m = n - r \). Therefore \( n - m = r = \text{rank}(A - cI) \).

**A Defective Matrix**

Although most matrices encountered in statistics applications are diagonalizable, it may be of interest to consider an example of a matrix that is not diagonalizable. Searle (1982) gives an example of a small matrix:

\[
A = \begin{bmatrix} 0 & 1 & 2 \\ 2 & 3 & 0 \\ 0 & 4 & 5 \end{bmatrix}.
\]

The three strategically placed 0s make this matrix easy to work with, and the determinant of \( (cI - A) \) yields the characteristic polynomial equation

\[
c^3 - 8c^2 + 13c - 6 = 0.
\]

This can be factored as \( (c - 6)(c - 1)^2 \), hence, we have eigenvalues \( c_1 = 6 \) with algebraic multiplicity \( m_1 = 1 \), and \( c_2 = 1 \) with algebraic multiplicity \( m_2 = 2 \). Now, consider \( A - c_2I \):

\[
A - I = \begin{bmatrix} -1 & 1 & 2 \\ 2 & 2 & 0 \\ 0 & 4 & 4 \end{bmatrix}.
\]

This is clearly of rank 2; hence the rank of the null space of \( A - c_2I \) (that is, the geometric multiplicity of \( c_2 \)) is \( 3 - 2 = 1 \). The matrix \( A \) is not diagonalizable.
3.8.6 Properties of Diagonalizable Matrices

If the matrix \( A \) has the similar canonical factorization \( VCV^{-1} \) of equation (3.205), some important properties are immediately apparent. First of all, this factorization implies that the eigenvectors of a diagonalizable matrix are linearly independent.

Other properties are easy to derive or to show because of this factorization. For example, the general equations (3.191) and (3.192) concerning the product and the sum of eigenvalues follow easily from

\[
\det(A) = \det(VCV^{-1}) = \det(V) \det(C) \det(V^{-1}) = \det(C)
\]

and

\[
\text{tr}(A) = \text{tr}(VCV^{-1}) = \text{tr}(V^{-1}VC) = \text{tr}(C).
\]

One important fact is that the number of nonzero eigenvalues of a diagonalizable matrix \( A \) is equal to the rank of \( A \). This must be the case because the rank of the diagonal matrix \( C \) is its number of nonzero elements and the rank of \( A \) must be the same as the rank of \( C \). Another way of saying this is that the sum of the multiplicities of the unique nonzero eigenvalues is equal to the rank of the matrix; that is, \( \sum_{i=1}^{k} m_{i} = \text{rank}(A) \), for the matrix \( A \) with \( k \) distinct eigenvalues with multiplicities \( m_{i} \).

3.8.7 Matrix Functions

There are various types of functions of matrices. Several that we have discussed, such as the trace, the rank, the determinant, and the different norms are all functions from \( \mathbb{R}^{n \times n} \) into the \( \mathbb{R} \) or the nonnegative reals, \( \mathbb{R}_{+} \).

Another type of functions of matrices are those defined by elementwise operations, such as \( \sin(A) = (\sin(a_{ij})) \) and \( \exp(A) = (\exp(a_{ij})) \). That is, a standard function that maps \( \mathbb{R} \) to \( \mathbb{R} \), when evaluated on \( \mathbb{R}^{n \times m} \) maps to \( \mathbb{R}^{n \times m} \) in a very direct way. Most of the mathematical software, such as R, Matlab, and Fortran 95 (and later), interpret builtin functions this way when a matrix if given as the argument.

We can also use the diagonal factorization (3.205) of the matrix \( A = VCV^{-1} \) to define a function of the matrix that corresponds to a function of a scalar, \( f(x) \),

\[
f(A) = V \text{diag}(f(c_{1}), \ldots, f(c_{n}))V^{-1}, \tag{3.207}
\]

if \( f(\cdot) \) is defined for each eigenvalue \( c_{i} \). (Notice the relationship of this definition to the Cayley-Hamilton theorem, page 124, and to Exercise 3.20.)

Another useful feature of the diagonal factorization of the matrix \( A \) in equation (3.205) is that it allows us to study functions of powers of \( A \) because \( A^{k} = VCV^{-1} \). In particular, we may assess the convergence of a function of a power of \( A \),

\[
\lim_{k \to \infty} g(k, A).
\]
Functions defined by elementwise operations have limited applications. Functions of real numbers that have power series expansions may be defined for matrices in terms of power series expansions in $A$, which are effectively power series in the diagonal elements of $C$. For example, using the power series expansion of $e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$, we can define the matrix exponential for the square matrix $A$ as the matrix

\[ e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}, \tag{3.208} \]

where $A^0/0!$ is defined as $I$. (Recall that we did not define $A^0$ if $A$ is singular.) If $A$ is represented as $VCV^{-1}$, this expansion becomes

\[ e^A = V \sum_{k=0}^{\infty} \frac{C^k}{k!} V^{-1} = V \text{diag} \left( (e^{c_1}, \ldots, e^{c_n}) \right) V^{-1}. \]

The expression $\exp(A)$ is generally interpreted as $\exp(A) = (\exp(a_{ij}))$, while the expression $e^A$ is interpreted as in equation (3.208), but often each expression is used in the opposite way. As mentioned above, the standard $\exp$ function in software systems, when evaluated for a matrix $A$, yields $(\exp(a_{ij}))$. Both R and Matlab have a function $\text{expm}$ for the matrix exponential. (In R, $\text{expm}$ is in the $\text{Matrix}$ package.)

An extensive coverage of matrix functions is given in Higham (2008).

### 3.8.8 Eigenanalysis of Symmetric Matrices

The eigenvalues and eigenvectors of symmetric matrices have some interesting properties. First of all, as we have already observed, for a real symmetric matrix, the eigenvalues are all real. We have also seen that symmetric matrices are diagonalizable; therefore all of the properties of diagonalizable matrices carry over to symmetric matrices.

**Orthogonality of Eigenvectors**

In the case of a symmetric matrix $A$, any eigenvectors corresponding to distinct eigenvalues are orthogonal. This is easily seen by assuming that $c_1$ and $c_2$ are unequal eigenvalues with corresponding eigenvectors $v_1$ and $v_2$. Now consider $v_1^T v_2$. Multiplying this by $c_2$, we get

\[ c_2 v_1^T v_2 = v_1^T A v_2 = v_2^T A v_1 = c_1 v_2^T v_1 = c_1 v_1^T v_2. \]

Because $c_1 \neq c_2$, we have $v_1^T v_2 = 0$.

Now, consider two eigenvalues $c_i = c_j$, that is, an eigenvalue of multiplicity greater than 1 and distinct associated eigenvectors $v_i$ and $v_j$. By what we
just saw, an eigenvector associated with \( c_k \neq c_i \) is orthogonal to the space spanned by \( v_i \) and \( v_j \). Assume \( v_i \) is normalized and apply a Gram-Schmidt transformation to form

\[
\tilde{v}_j = \frac{1}{\|v_j - \langle v_i, v_j \rangle v_i\|} (v_j - \langle v_i, v_j \rangle v_i),
\]
as in equation (2.47) on page 37, yielding a vector orthogonal to \( v_i \). Now, we have

\[
A\tilde{v}_j = \frac{1}{\|v_j - \langle v_i, v_j \rangle v_i\|} (Av_j - \langle v_i, v_j \rangle Av_i)
= \frac{1}{\|v_j - \langle v_i, v_j \rangle v_i\|} (c_j v_j - \langle v_i, v_j \rangle c_i v_i)
= c_j \frac{1}{\|v_j - \langle v_i, v_j \rangle v_i\|} (v_j - \langle v_i, v_j \rangle v_i)
= c_j \tilde{v}_j;
\]
hence, \( \tilde{v}_j \) is an eigenvector of \( A \) associated with \( c_j \). We conclude therefore that the eigenvectors of a symmetric matrix can be chosen to be orthogonal.

A symmetric matrix is orthogonally diagonalizable, because the \( V \) in equation (3.205) can be chosen to be orthogonal, and can be written as

\[
A = VCV^T, \tag{3.209}
\]
where \( VV^T = V^TV = I \), and so we also have

\[
V^TAV = C. \tag{3.210}
\]
Such a matrix is orthogonally similar to a diagonal matrix formed from its eigenvalues.

**Spectral Decomposition**

When \( A \) is symmetric and the eigenvectors \( v_i \) are chosen to be orthonormal,

\[
I = \sum_i v_i v_i^T, \tag{3.211}
\]
so

\[
A = A \sum_i v_i v_i^T
= \sum_i Av_i v_i^T
= \sum_i c_i v_i v_i^T. \tag{3.212}
\]
This representation is called the spectral decomposition of the symmetric matrix $A$. It is essentially the same as equation (3.209), so $A = VCV^T$ is also called the spectral decomposition.

The representation is unique except for the ordering and the choice of eigenvectors for eigenvalues with multiplicities greater than 1. If the rank of the matrix is $r$, we have $|c_1| \geq \cdots \geq |c_r| > 0$, and if $r < n$, then $c_{r+1} = \cdots = c_n = 0$.

Note that the matrices in the spectral decomposition are projection matrices that are orthogonal to each other (but they are not orthogonal matrices) and they sum to the identity. Let

$$P_i = v_i v_i^T.$$ (3.213)

Then we have

$$P_i P_i = P_i,$$ (3.214)

$$P_i P_j = 0 \text{ for } i \neq j,$$ (3.215)

$$\sum_i P_i = I,$$ (3.216)

and the spectral decomposition,

$$A = \sum_i c_i P_i.$$ (3.217)

The $P_i$ are called spectral projectors.

The spectral decomposition also applies to powers of $A$,

$$A^k = \sum_i c_i^k v_i v_i^T,$$ (3.218)

where $k$ is an integer. If $A$ is nonsingular, $k$ can be negative in the expression above.

The spectral decomposition is one of the most important tools in working with symmetric matrices.

Although we will not prove it here, all diagonalizable matrices have a spectral decomposition in the form of equation (3.217) with projection matrices that satisfy properties (3.214) through (3.216). These projection matrices cannot necessarily be expressed as outer products of eigenvectors, however. The eigenvalues and eigenvectors of a nonsymmetric matrix might not be real, the left and right eigenvectors might not be the same, and two eigenvectors might not be mutually orthogonal. In the spectral representation $A = \sum_i c_i P_i$, however, if $c_j$ is a simple eigenvalue with associated left and right eigenvectors $y_j$ and $x_j$, respectively, then the projection matrix $P_j$ is $x_j y_j^H / y_j^H x_j$. (Note that because the eigenvectors may not be real, we take the conjugate transpose.) This is Exercise 3.23.
Quadratic Forms and the Rayleigh Quotient

Equation (3.212) yields important facts about quadratic forms in $A$. Because $V$ is of full rank, an arbitrary vector $x$ can be written as $Vb$ for some vector $b$. Therefore, for the quadratic form $x^TAx$ we have

$$x^T Ax = x^T \sum_i c_i v_i v_i^T x = \sum_i b_i^T V^T v_i v_i^T V b_i = \sum_i b_i^2 c_i.$$ 

This immediately gives the inequality

$$x^T Ax \leq \max\{c_i\} b^T b.$$ 

(Notice that $\max\{c_i\}$ here is not necessarily $c_1$; in the important case when all of the eigenvalues are nonnegative, it is, however.) Furthermore, if $x \neq 0$, $b^T b = x^T x$, and we have the important inequality

$$\frac{x^T Ax}{x^T x} \leq \max\{c_i\}. \quad (3.219)$$

Equality is achieved if $x$ is the eigenvector corresponding to $\max\{c_i\}$, so we have

$$\max_{x \neq 0} \frac{x^T Ax}{x^T x} = \max\{c_i\}. \quad (3.220)$$

If $c_1 > 0$, this is the spectral radius, $\rho(A)$.

The expression on the left-hand side in (3.219) as a function of $x$ is called the Rayleigh quotient of the symmetric matrix $A$ and is denoted by $R_A(x)$:

$$R_A(x) = \frac{x^T Ax}{x^T x} = \frac{\langle x, Ax \rangle}{\langle x, x \rangle}. \quad (3.221)$$

Because if $x \neq 0$, $x^T x > 0$, it is clear that the Rayleigh quotient is nonnegative for all $x$ if and only if $A$ is nonnegative definite and is positive for all $x$ if and only if $A$ is positive definite.

The Fourier Expansion

The $v_i v_i^T$ matrices in equation (3.212) have the property that $\langle v_i v_i^T, v_j v_j^T \rangle = 0$ for $i \neq j$ and $\langle v_i v_i^T, v_i v_i^T \rangle = 1$, and so the spectral decomposition is a Fourier expansion as in equation (3.88) and the eigenvalues are Fourier coefficients.
From equation (3.89), we see that the eigenvalues can be represented as the inner product

\[ c_i = \langle A, v_i v_i^T \rangle. \]  

(3.222)

The eigenvalues \( c_i \) have the same properties as the Fourier coefficients in any orthonormal expansion. In particular, the best approximating matrices within the subspace of \( n \times n \) symmetric matrices spanned by \( \{v_1 v_1^T, \ldots, v_n v_n^T\} \) are partial sums of the form of equation (3.212). In Section 3.10, however, we will develop a stronger result for approximation of matrices that does not rely on the restriction to this subspace and which applies to general, nonsquare matrices.

**Powers of a Symmetric Matrix**

If \((c, v)\) is an eigenpair of the symmetric matrix \(A\) with \(v^T v = 1\), then for any \(k = 1, 2, \ldots,\)

\[ (A - cvv^T)^k = A^k - c^k vv^T. \]  

(3.223)

This follows from induction on \(k\), for it clearly is true for \(k = 1\), and if for a given \(k\) it is true that for \(k - 1\)

\[ (A - cvv^T)^{k-1} = A^{k-1} - c^{k-1} vv^T, \]

then by multiplying both sides by \((A - cvv^T)\), we see it is true for \(k\):

\[ (A - cvv^T)^k = (A^{k-1} - c^{k-1} vv^T)(A - cvv^T) \]

\[ = A^k - c^{k-1} vv^T A - cA^{k-1} vv^T + c^k vv^T \]

\[ = A^k - c^k vv^T + c^k vv^T \]

\[ = A^k - c^k vv^T. \]

There is a similar result for nonsymmetric square matrices, where \(w\) and \(v\) are left and right eigenvectors, respectively, associated with the same eigenvalue \(c\) that can be scaled so that \(w^T v = 1\). (Recall that an eigenvalue of \(A\) is also an eigenvalue of \(A^T\), and if \(w\) is a left eigenvector associated with the eigenvalue \(c\), then \(A^T w = cw\).) The only property of symmetry used above was that we could scale \(v^T v\) to be 1; hence, we just need \(w^T v \neq 0\). This is clearly true for a diagonalizable matrix (from the definition). It is also true if \(c\) is simple (which is somewhat harder to prove). It is thus true for the dominant eigenvalue, which is simple, in two important classes of matrices we will consider in Sections 8.7.1 and 8.7.2, positive matrices and irreducible nonnegative matrices.

If \(w\) and \(v\) are left and right eigenvectors of \(A\) associated with the same eigenvalue \(c\) and \(w^T v = 1\), then for \(k = 1, 2, \ldots,\)

\[ (A - cvw^T)^k = A^k - c^k vw^T. \]  

(3.224)

We can prove this by induction as above.
3 Basic Properties of Matrices

The Trace and Sums of Eigenvalues

For a general \( n \times n \) matrix \( A \) with eigenvalues \( c_1, \ldots, c_n \), we have \( \text{tr}(A) = \sum_{i=1}^{n} c_i \). (This is equation (3.192).) This is particularly easy to see for symmetric matrices because of equation (3.209), rewritten as \( V^TAV = C \), the diagonal matrix of the eigenvalues. For a symmetric matrix, however, we have a stronger result.

If \( A \) is an \( n \times n \) symmetric matrix with eigenvalues \( c_1 \geq \cdots \geq c_n \), and \( U \) is an \( n \times k \) orthogonal matrix, with \( k \leq n \), then

\[
\text{tr}(U^TAU) \leq \sum_{i=1}^{k} c_i.
\]

(3.225)

To see this, we represent \( U \) in terms of the columns of \( V \), which span \( \mathbb{R}^n \), as \( U = VX \). Hence,

\[
\text{tr}(U^TAU) = \text{tr}(X^TV^TAVX)
\]

\[
= \text{tr}(X^TCX)
\]

\[
= \sum_{i=1}^{n} x_i^T x_i c_i,
\]

(3.226)

where \( x_i^T \) is the \( i \)th row of \( X \).

Now \( X^T X = X^T V^T V X = U^T U = I_k \), so either \( x_i^T x_i = 0 \) or \( x_i^T x_i = 1 \), and \( \sum_{i=1}^{n} x_i^T x_i = k \). Because \( c_1 \geq \cdots \geq c_n \), therefore \( \sum_{i=1}^{n} x_i^T x_i c_i \leq \sum_{i=1}^{k} c_i \), and so from equation (3.226) we have \( \text{tr}(U^TAU) \leq \sum_{i=1}^{k} c_i \).

3.8.9 Positive Definite and Nonnegative Definite Matrices

The factorization of symmetric matrices in equation (3.209) yields some useful properties of positive definite and nonnegative definite matrices (introduced on page 82). We will briefly discuss these properties here and then return to the subject in Section 8.3 and discuss more properties of positive definite and nonnegative definite matrices.

Eigenvalues of Positive and Nonnegative Definite Matrices

In this book, we use the terms “nonnegative definite” and “positive definite” only for real symmetric matrices, so the eigenvalues of nonnegative definite or positive definite matrices are real.

Any real symmetric matrix is positive (nonnegative) definite if and only if all of its eigenvalues are positive (nonnegative). We can see this using the factorization (3.209) of a symmetric matrix. One factor is the diagonal matrix
$C$ of the eigenvalues, and the other factors are orthogonal. Hence, for any $x$, we have $x^T Ax = x^T V C V^T x = y^T C y$, where $y = V^T x$, and so

$$x^T Ax > (\geq) 0$$

if and only if

$$y^T C y > (\geq) 0.$$  

This, together with the resulting inequality (3.128) on page 102, implies that if $P$ is a nonsingular matrix and $D$ is a diagonal matrix, $P^T DP$ is positive (nonnegative) if and only if the elements of $D$ are positive (nonnegative).

A matrix (whether symmetric or not and whether real or not) all of whose eigenvalues have positive real parts is said to be positive stable. Positive stability is an important property in some applications, such as numerical solution of systems of nonlinear differential equations. Clearly, a positive definite matrix is positive stable.

**Inverse of Positive Definite Matrices**

If $A$ is positive definite and $A = V C V^T$ as in equation (3.209), then $A^{-1} = V C^{-1} V^T$ and $A^{-1}$ is positive definite because the elements of $C^{-1}$ are positive.

**Diagonalization of Positive Definite Matrices**

If $A$ is positive definite, the elements of the diagonal matrix $C$ in equation (3.209) are positive, and so their square roots can be absorbed into $V$ to form a nonsingular matrix $P$. The diagonalization in equation (3.210), $V^T A V = C$, can therefore be reexpressed as

$$P^T A P = I.$$  \hspace{1cm} (3.227)

**Square Roots of Positive and Nonnegative Definite Matrices**

The factorization (3.209) together with the nonnegativity of the eigenvalues of positive and nonnegative definite matrices allows us to define a square root of such a matrix.

Let $A$ be a nonnegative definite matrix and let $V$ and $C$ be as in equation (3.209): $A = V C V^T$. Now, let $S$ be a diagonal matrix whose elements are the square roots of the corresponding elements of $C$. Then $(V S V^T)^2 = A$; hence, we write

$$A^{\frac{1}{2}} = V S V^T$$ \hspace{1cm} (3.228)

and call this matrix the square root of $A$. This definition of the square root of a matrix is an instance of equation (3.207) with $f(x) = \sqrt{x}$. We also can similarly define $A^{\frac{1}{r}}$ for $r > 0$.

We see immediately that $A^{\frac{1}{2}}$ is symmetric because $A$ is symmetric.
If \( A \) is positive definite, \( A^{-1} \) exists and is positive definite. It therefore has a square root, which we denote as \( A^{\frac{1}{2}} \).

The square roots are nonnegative, and so \( A^{\frac{1}{2}} \) is nonnegative definite. Furthermore, \( A^{\frac{1}{2}} \) and \( A^{-\frac{1}{2}} \) are positive definite if \( A \) is positive definite.

In Section 5.9.1, we will show that this \( A^{\frac{1}{2}} \) is unique, so our reference to it as the square root is appropriate. (There is occasionally some ambiguity in the terms “square root” and “second root” and the symbols used to denote them. If \( x \) is a nonnegative scalar, the usual meaning of its square root, denoted by \( \sqrt{x} \), is a nonnegative number, while its second roots, which may be denoted by \( x^{\frac{1}{2}} \), are usually considered to be either of the numbers \( \pm \sqrt{x} \). In our notation \( A^{\frac{1}{2}} \), we mean the square root; that is, the nonnegative matrix, if it exists. Otherwise, we say the square root of the matrix does not exist. For example, \( I^{\frac{1}{2}} = I \), and while if \( J = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \), \( J^2 = I_2 \), we do not consider \( J \) to be a square root of \( I_2 \).)

3.8.10 The Generalized Eigenvalue Problem

The characterization of an eigenvalue as a root of the determinant equation (3.184) can be extended to define a \textit{generalized eigenvalue} of the square matrices \( A \) and \( B \) to be a root in \( c \) of the equation

\[
\det(A - cB) = 0
\]

if a root exists.

Equation (3.229) is equivalent to \( A - cB \) being singular; that is, for some \( c \) and some nonzero, finite \( v \),

\[
Av = cBv.
\]

Such a \( v \) (if it exists) is called the \textit{generalized eigenvector}. In contrast to the existence of eigenvalues of any square matrix with finite elements, the generalized eigenvalues may not exist; that is, they may be infinite.

If \( B \) is nonsingular and \( A \) and \( B \) are \( n \times n \), all \( n \) eigenvalues of \( A \) and \( B \) exist (and are finite). These generalized eigenvalues are the eigenvalues of \( AB^{-1} \) or \( B^{-1}A \). We see this because \( \det(B) \neq 0 \), and so if \( c_0 \) is any of the \( n \) (finite) eigenvalues of \( AB^{-1} \) or \( B^{-1}A \), then \( 0 = \det(AB^{-1} - c_0 I) = \det(B^{-1}A - c_0 I) = \det(A - c_0B) = 0 \). Likewise, we see that any eigenvector of \( AB^{-1} \) or \( B^{-1}A \) is a generalized eigenvector of \( A \) and \( B \).

In the case of ordinary eigenvalues, we have seen that symmetry of the matrix induces some simplifications. In the case of generalized eigenvalues, symmetry together with positive definiteness yields some useful properties, which we will discuss in Section 7.6.

Generalized eigenvalue problems often arise in multivariate statistical applications. Roy’s maximum root statistic, for example, is the largest generalized eigenvalue of two matrices that result from operations on a partitioned matrix of sums of squares.
Matrix Pencils

As \( c \) ranges over the reals (or, more generally, the complex numbers), the set of matrices of the form \( A - cB \) is called the matrix pencil, or just the pencil, generated by \( A \) and \( B \), denoted as

\[(A, B).\]

(In this definition, \( A \) and \( B \) do not need to be square.) A generalized eigenvalue of the square matrices \( A \) and \( B \) is called an eigenvalue of the pencil.

A pencil is said to be regular if \( \det(A - cB) \) is not identically 0 (assuming, of course, that \( \det(A - cB) \) is defined, meaning \( A \) and \( B \) are square). An interesting special case of a regular pencil is when \( B \) is nonsingular. As we have seen, in that case, eigenvalues of the pencil \((A, B)\) exist (and are finite) and are the same as the ordinary eigenvalues of \( AB^{-1} \) or \( B^{-1}A \), and the ordinary eigenvectors of \( AB^{-1} \) or \( B^{-1}A \) are eigenvectors of the pencil \((A, B)\).

3.8.11 Singular Values and the Singular Value Decomposition

An \( n \times m \) matrix \( A \) can be factored as

\[A = UDV^T, \tag{3.230}\]

where \( U \) is an \( n \times n \) orthogonal matrix, \( V \) is an \( m \times m \) orthogonal matrix, and \( D \) is an \( n \times m \) diagonal matrix with nonnegative entries. (An \( n \times m \) diagonal matrix has \( \min(n, m) \) elements on the diagonal, and all other entries are zero.)

The factorization \((3.230)\) is called the singular value decomposition (SVD) or the canonical singular value factorization of \( A \). The elements on the diagonal of \( D \), \( d_i \), are called the singular values of \( A \). We can rearrange the entries in \( D \) so that \( d_1 \geq d_2 \geq \cdots \), and by rearranging the columns of \( U \) correspondingly, nothing is changed.

We see that the factorization exists for any matrix by forming a square symmetric matrix and then using the decomposition in equation \((3.209)\) on page 136. We first form \( A^T A = VCV^T \). If \( n \geq m \), we have

\[
A^T A = VCV^T = V[I \ 0] \begin{bmatrix} C & 0 \end{bmatrix} V^T = \begin{bmatrix} V & 0 \end{bmatrix} \begin{bmatrix} C \\ 0 \end{bmatrix} V^T = UDV^T,
\]

as above. Note if \( n = m \), the 0 partitions in the matrices are nonexistent. If, on the other hand, \( n < m \), we form \( D = [C \ 0] \) and proceed as before.

From this development, we see that the squares of the singular values of \( A \) are the positive eigenvalues of \( A^T A \) and of \( AA^T \). Also, if \( A \) is symmetric,
we see that the singular values of $A$ are the absolute values of the eigenvalues of $A$.

The number of positive entries in $D$ is the same as the rank of $A$. (We see this by first recognizing that the number of nonzero entries of $D$ is obviously the rank of $D$, and multiplication by the full rank matrices $U$ and $V^T$ yields a product with the same rank from equations (3.126) and (3.127).)

If the rank of the matrix is $r$, we have $d_1 \geq \cdots \geq d_r > 0$, and if $r < \min(n, m)$, then $d_{r+1} = \cdots = d_{\min(n, m)} = 0$. In this case

$$D = \begin{bmatrix} D_r & 0 \\ 0 & 0 \end{bmatrix},$$

where $D_r = \text{diag}(d_1, \ldots, d_r)$.

From the factorization (3.230) defining the singular values, we see that the singular values of $A^T$ are the same as those of $A$.

For a matrix with more rows than columns, in an alternate definition of the singular value decomposition, the matrix $U$ is $n \times m$ with orthogonal columns, and $D$ is an $m \times m$ diagonal matrix with nonnegative entries. Likewise, for a matrix with more columns than rows, the singular value decomposition can be defined as above but with the matrix $V$ being $m \times n$ with orthogonal columns and $D$ being $n \times n$ and diagonal with nonnegative entries.

**The Fourier Expansion in Terms of the Singular Value Decomposition**

From equation (3.230), we see that the general matrix $A$ with rank $r$ also has a Fourier expansion, similar to equation (3.212), in terms of the singular values and outer products of the columns of the $U$ and $V$ matrices:

$$A = \sum_{i=1}^{r} d_i u_i v_i^T. \tag{3.231}$$

This is also called a spectral decomposition. The $u_i v_i^T$ matrices in equation (3.231) have the property that $\langle u_i v_i^T, u_j v_j^T \rangle = 0$ for $i \neq j$ and $\langle u_i v_i^T, u_i v_i^T \rangle = 1$, and so the spectral decomposition is a Fourier expansion as in equation (3.88), and the singular values are Fourier coefficients.

The singular values $d_i$ have the same properties as the Fourier coefficients in any orthonormal expansion. For example, from equation (3.89), we see that the singular values can be represented as the inner product

$$d_i = \langle A, u_i v_i^T \rangle.$$

After we have discussed matrix norms in the next section, we will formulate Parseval’s identity for this Fourier expansion.
3.9 Matrix Norms

Norms on matrices are scalar functions of matrices with the three properties on page 24 that define a norm in general. Matrix norms are often required to have another property, called the consistency property, in addition to the properties listed on page 24, which we repeat here for convenience. Assume $A$ and $B$ are matrices conformable for the operations shown.

1. Nonnegativity and mapping of the identity:
   if $A \neq 0$, then $\|A\| > 0$, and $\|0\| = 0$.
2. Relation of scalar multiplication to real multiplication:
   $\|aA\| = |a| \|A\|$ for real $a$.
3. Triangle inequality:
   $\|A + B\| \leq \|A\| + \|B\|$.
4. Consistency property:
   $\|AB\| \leq \|A\| \|B\|$.

Some people do not require the consistency property for a matrix norm. Most useful matrix norms have the property, however, and we will consider it to be a requirement in the definition. The consistency property for multiplication is similar to the triangular inequality for addition.

Any function from $\mathbb{R}^{n \times m}$ to $\mathbb{R}$ that satisfies these four properties is a matrix norm.

We note that the four properties of a matrix norm do not imply that it is invariant to transposition of a matrix, and in general, $\|A^T\| \neq \|A\|$. Some matrix norms are the same for the transpose of a matrix as for the original matrix. For instance, because of the property of the matrix inner product given in equation (3.85), we see that a norm defined by that inner product would be invariant to transposition.

For a square matrix $A$, the consistency property for a matrix norm yields

$$\|A^k\| \leq \|A\|^k$$

for any positive integer $k$.

A matrix norm $\|\cdot\|$ is orthogonal invariant if $A$ and $B$ being orthogonally similar implies $\|A\| = \|B\|$.

3.9.1 Matrix Norms Induced from Vector Norms

Some matrix norms are defined in terms of vector norms. For clarity, we will denote a vector norm as $\|\cdot\|_v$ and a matrix norm as $\|\cdot\|_M$. (This notation is meant to be generic; that is, $\|\cdot\|_v$ represents any vector norm.) The matrix norm $\|\cdot\|_M$ induced by $\|\cdot\|_v$ is defined by

$$\|A\|_M = \max_{x \neq 0} \frac{\|Ax\|_v}{\|x\|_v}.$$
It is easy to see that an induced norm is indeed a matrix norm. The first three properties of a norm are immediate, and the consistency property can be verified by applying the definition (3.233) to $AB$ and replacing $Bx$ with $y$; that is, using $Ay$.

We usually drop the $v$ or $M$ subscript, and the notation $\| \cdot \|$ is overloaded to mean either a vector or matrix norm. (Overloading of symbols occurs in many contexts, and we usually do not even recognize that the meaning is context-dependent. In computer language design, overloading must be recognized explicitly because the language specifications must be explicit.)

The induced norm of $A$ given in equation (3.233) is sometimes called the maximum magnification by $A$. The expression looks very similar to the maximum eigenvalue, and indeed it is in some cases.

For any vector norm and its induced matrix norm, we see from equation (3.233) that

$$\|Ax\| \leq \|A\| \|x\| \tag{3.234}$$

because $\|x\| \geq 0$.

**L_p Matrix Norms**

The matrix norms that correspond to the $L_p$ vector norms are defined for the $n \times m$ matrix $A$ as

$$\|A\|_p = \max_{\|x\|_p = 1} \|Ax\|_p. \tag{3.235}$$

(Notice that the restriction on $\|x\|_p$ makes this an induced norm as defined in equation (3.233). Notice also the overloading of the symbols; the norm on the left that is being defined is a matrix norm, whereas those on the right of the equation are vector norms.) It is clear that the $L_p$ matrix norms satisfy the consistency property, because they are induced norms.

The $L_1$ and $L_\infty$ norms have interesting simplifications of equation (3.233):

$$\|A\|_1 = \max_j \sum_i |a_{ij}|, \tag{3.236}$$

so the $L_1$ is also called the column-sum norm; and

$$\|A\|_\infty = \max_i \sum_j |a_{ij}|, \tag{3.237}$$

so the $L_\infty$ is also called the row-sum norm. We see these relationships by considering the $L_p$ norm of the vector

$$v = (a_{1,1}^T x, \ldots, a_{n,1}^T x),$$

where $a_{i,\ast}$ is the $i^{th}$ row of $A$, with the restriction that $\|x\|_p = 1$. The $L_p$ norm of this vector is based on the absolute values of the elements; that is, $|\sum_j a_{ij}x_j|$ for $i = 1, \ldots, n$. Because we are free to choose $x$ (subject to the
restriction that \( \|x\|_p = 1 \), for a given \( i \), we can choose the sign of each \( x_j \) to maximize the overall expression. For example, for a fixed \( i \), we can choose each \( x_j \) to have the same sign as \( a_{ij} \), and so \( \sum_j a_{ij} x_j \) is the same as \( \sum_j |a_{ij}| |x_j| \).

For the column-sum norm, the \( L_1 \) norm of \( v \) is \( \sum_i |a_i^T x| \). The elements of \( x \) are chosen to maximize this under the restriction that \( \sum |x_j| = 1 \). The maximum of the expression is attained by setting \( x_k = \text{sign}(\sum_i a_{ik}) \), where \( k \) is such that \( \sum_i |a_{ik}| \geq \sum_j |a_{ij}| \), for \( j = 1, \ldots, m \), and \( x_q = 0 \) for \( q = 1, \ldots, m \) and \( q \neq k \). (If there is no unique \( k \), any choice will yield the same result.) This yields equation (3.236).

For the row-sum norm, the \( L_\infty \) norm of \( v \) is \( \max_i |a_i^T x| = \max_i \sum_j |a_{ij}| |x_j| \) when the sign of \( x_j \) is chosen appropriately (for a given \( i \)). The elements of \( x \) must be chosen so that \( \max |x_j| = 1 \); hence, each \( x_j \) is chosen as \( \pm 1 \). The maximum \( |a_i^T x| \) is attained by setting \( x_j = \text{sign}(a_{kj}) \), for \( j = 1, \ldots, m \), where \( k \) is such that \( \sum_j |a_{kj}| \geq \sum_j |a_{ij}| \), for \( i = 1, \ldots, n \). This yields equation (3.237).

From equations (3.236) and (3.237), we see that \( \|A^T\|_\infty = \|A\|_1 \). (3.238)

Alternative formulations of the \( L_2 \) norm of a matrix are not so obvious from equation (3.235). It is related to the eigenvalues (or the singular values) of the matrix. The \( L_2 \) matrix norm is related to the spectral radius (page 127):

\[ \|A\|_2 = \sqrt{\rho(A^T A)}, \]  
(3.239)

(see Exercise 3.27, page 160). Because of this relationship, the \( L_2 \) matrix norm is also called the spectral norm.

From the invariance of the singular values to matrix transposition, we see that positive eigenvalues of \( A^T A \) are the same as those of \( AA^T \); hence, \( \|A^T\|_2 = \|A\|_2 \).

For \( Q \) orthogonal, the \( L_2 \) vector norm has the important property

\[ \|Qx\|_2 = \|x\|_2 \]  
(3.240)

(see Exercise 3.28a, page 160). For this reason, an orthogonal matrix is sometimes called an isometric matrix. By the proper choice of \( x \), it is easy to see from equation (3.240) that

\[ \|Q\|_2 = 1. \]  
(3.241)

Also from this we see that if \( A \) and \( B \) are orthogonally similar, then \( \|A\|_2 = \|B\|_2 \); hence, the spectral matrix norm is orthogonally invariant.

The \( L_2 \) matrix norm is a Euclidean-type norm since it is induced by the Euclidean vector norm (but it is not called the Euclidean matrix norm; see below).
L₁, L₂, and L∞ Norms of Symmetric Matrices

For a symmetric matrix \( A \), we have the obvious relationships

\[
\|A\|_1 = \|A\|_\infty \quad (3.242)
\]

and, from equation (3.239),

\[
\|A\|_2 = \rho(A). \quad (3.243)
\]

3.9.2 The Frobenius Norm — The “Usual” Norm

The Frobenius norm is defined as

\[
\|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2}. \quad (3.244)
\]

It is easy to see that this measure has the consistency property (Exercise 3.30), as a norm must. The Frobenius norm is sometimes called the Euclidean matrix norm and denoted by \( \| \cdot \|_E \), although the L₂ matrix norm is more directly based on the Euclidean vector norm, as we mentioned above. We will usually use the notation \( \| \cdot \|_F \) to denote the Frobenius norm. Occasionally we use \( \| \cdot \| \) without the subscript to denote the Frobenius norm, but usually the symbol without the subscript indicates that any norm could be used in the expression. The Frobenius norm is also often called the “usual norm”, which emphasizes the fact that it is one of the most useful matrix norms. Other names sometimes used to refer to the Frobenius norm are Hilbert-Schmidt norm and Schur norm.

From the definition, we have \( \|A^T\|_F = \|A\|_F \). We have seen that the L₂ matrix norm also has this property.

Another important property of the Frobenius norm that is obvious from the definition is

\[
\|A\|_F = \sqrt{\text{tr}(A^T A)} \quad (3.245)
\]

that is,

\[
\|A\|_F = \sqrt{\langle A, A \rangle} \quad (3.246)
\]

that is,

- the Frobenius norm is the norm that arises from the matrix inner product (see page 87).

The complete vector space \( \mathbb{R}^{n \times m} \) with the Frobenius norm is therefore a Hilbert space.

Another thing worth noting for a square \( A \) is the relationship of the Frobenius norm to the eigenvalues \( c_i \) of \( A \):

\[
\|A\|_F = \sqrt{\sum c_i \bar{c}_i}, \quad (3.247)
\]
and if $A$ is also symmetric,

$$\|A\|_F = \sqrt{\sum c_i^2},$$ (3.248)

These follow from equation (3.245) and equation (3.192) on page 126.

Similar to defining the angle between two vectors in terms of the inner product and the norm arising from the inner product, we define the angle between two matrices $A$ and $B$ of the same size and shape as

$$\text{angle}(A, B) = \cos^{-1} \left( \frac{\langle A, B \rangle}{\|A\|_F \|B\|_F} \right).$$ (3.249)

If $Q$ is an $n \times m$ orthogonal matrix, then

$$\|Q\|_F = \sqrt{m},$$ (3.250)

(see equation (3.180)).

If $A$ and $B$ are orthogonally similar (see equation (3.203)), then

$$\|A\|_F = \|B\|_F;$$

that is, the Frobenius norm is an orthogonally invariant norm. To see this, let $A = Q^T B Q$, where $Q$ is an orthogonal matrix. Then

$$\|A\|_F^2 = \text{tr}(A^T A)$$
$$= \text{tr}(Q^T B^T QQ^T B Q)$$
$$= \text{tr}(B^T B QQ^T)$$
$$= \text{tr}(B^T B)$$
$$= \|B\|_F^2.$$

(The norms are nonnegative, of course, and so equality of the squares is sufficient.)

**Parseval’s Identity**

Several important properties result because the Frobenius norm arises from an inner product. For example, following the Fourier expansion in terms of the singular value decomposition, equation (3.231), we mentioned that the singular values have the general properties of Fourier coefficients; for example, they satisfy Parseval’s identity, equation (2.51), on page 39. This identity states that the sum of the squares of the Fourier coefficients is equal to the square of the norm that arises from the inner product used in the Fourier expansion. Hence, we have the important property of the Frobenius norm that the square of the norm is the sum of squares of the singular values of the matrix:

$$\|A\|_F^2 = \sum d_i^2.$$ (3.251)
### 3.9.3 Matrix Norm Inequalities

There is an equivalence among any two matrix norms similar to that of expression (2.33) for vector norms (over finite-dimensional vector spaces). If $\| \cdot \|_a$ and $\| \cdot \|_b$ are matrix norms, then there are positive numbers $r$ and $s$ such that, for any matrix $A$,

$$r \| A \|_b \leq \| A \|_a \leq s \| A \|_b. \tag{3.252}$$

We will not prove this result in general but, in Exercise 3.31, ask the reader to do so for matrix norms induced by vector norms. These induced norms include the matrix $L_p$ norms of course.

If $A$ is an $n \times m$ real matrix, we have some specific instances of (3.252):

$$\| A \|_\infty \leq \sqrt{m} \| A \|_F, \tag{3.253}$$

$$\| A \|_F \leq \sqrt{\min(n,m)} \| A \|_2, \tag{3.254}$$

$$\| A \|_2 \leq \sqrt{m} \| A \|_1, \tag{3.255}$$

$$\| A \|_1 \leq \sqrt{n} \| A \|_2, \tag{3.256}$$

$$\| A \|_2 \leq \| A \|_F, \tag{3.257}$$

$$\| A \|_F \leq \sqrt{n} \| A \|_\infty. \tag{3.258}$$

See Exercises 3.32 and 3.33 on page 160. Compare these inequalities with those for $L_p$ vector norms on page 27. Recall specifically that for vector $L_p$ norms we had the useful fact that for a given $x$ and for $p \geq 1$, $\| x \|_p$ is a nonincreasing function of $p$; and specifically we had inequality (2.28):

$$\| x \|_\infty \leq \| x \|_2 \leq \| x \|_1.$$

### 3.9.4 The Spectral Radius

The spectral radius is the appropriate measure of the condition of a square matrix for certain iterative algorithms. Except in the case of symmetric matrices, as shown in equation (3.243), the spectral radius is not a norm (see Exercise 3.34a).

We have for any norm $\| \cdot \|$ and any square matrix $A$ that

$$\rho(A) \leq \| A \|. \tag{3.259}$$
To see this, we consider the associated eigenvalue and eigenvector \( c_i \) and \( v_i \) and form the matrix \( V = [v_i|0|\cdots|0] \), so \( c_iV = AV \), and by the consistency property of any matrix norm,

\[
|c_i|\|V\| = \|c_iV\| = \|AV\| \leq \|A\|\|V\|,
\]

or

\[
|c_i| \leq \|A\|,
\]

(see also Exercise 3.34b).

The inequality (3.259) and the \( L_1 \) and \( L_\infty \) norms yield useful bounds on the eigenvalues and the maximum absolute row and column sums of matrices: the modulus of any eigenvalue is no greater than the largest sum of absolute values of the elements in any row or column.

The inequality (3.259) and equation (3.243) also yield a minimum property of the \( L_2 \) norm of a symmetric matrix \( A \):

\[
\|A\|_2 \leq \|A\|.
\]

### 3.9.5 Convergence of a Matrix Power Series

We define the convergence of a sequence of matrices in terms of the convergence of a sequence of their norms, just as we did for a sequence of vectors (on page 31). We say that a sequence of matrices \( A_1, A_2, \ldots \) (of the same shape) converges to the matrix \( A \) with respect to the norm \( \| \cdot \| \) if the sequence of real numbers \( \|A_1 - A\|, \|A_2 - A\|, \ldots \) converges to 0. Because of the equivalence property of norms, the choice of the norm is irrelevant. Also, because of inequality (3.259), we see that the convergence of the sequence of spectral radii \( \rho(A_1 - A), \rho(A_2 - A), \ldots \) to 0 must imply the convergence of \( A_1, A_2, \ldots \) to \( A \).

#### Conditions for Convergence of a Sequence of Powers

For a square matrix \( A \), we have the important fact that

\[
A^k \to 0, \quad \text{if} \quad \|A\| < 1, \tag{3.260}
\]

where 0 is the square zero matrix of the same order as \( A \) and \( \| \cdot \| \) is any matrix norm. (The consistency property is required.) This convergence follows from inequality (3.232) because that yields \( \lim_{k \to \infty} \|A^k\| \leq \lim_{k \to \infty} \|A\|^k \), and so if \( \|A\| < 1 \), then \( \lim_{k \to \infty} \|A^k\| = 0 \).

Now consider the spectral radius. Because of the spectral decomposition, we would expect the spectral radius to be related to the convergence of a sequence of powers of a matrix. If \( A^k \to 0 \), then for any conformable vector
\[ x, \quad A^k x \to 0; \text{ in particular, for the eigenvector } v_1 \neq 0 \text{ corresponding to the dominant eigenvalue } c_1, \text{ we have } A^k v_1 = c_1^k v_1 \to 0. \] For \( c_1^k v_1 \) to converge to zero, we must have \( |c_1| < 1 \); that is, \( \rho(A) < 1 \). We can also show the converse:

\[ A^k \to 0 \quad \text{if } \rho(A) < 1. \quad (3.261) \]

We will do this by defining a norm \( \| \cdot \|_d \) in terms of the \( L_1 \) matrix norm in such a way that \( \rho(A) < 1 \) implies \( \|A\|_d < 1 \). Then we can use equation (3.260) to establish the convergence.

Let \( A = QTQ^T \) be the Schur factorization of the \( n \times n \) matrix \( A \), where \( Q \) is orthogonal and \( T \) is upper triangular with the same eigenvalues as \( A \), \( c_1, \ldots, c_n \). Now for any \( d > 0 \), form the diagonal matrix \( D = \text{diag}(d^1, \ldots, d^n) \).

Notice that \( DT^{-1} \) is an upper triangular matrix and its diagonal elements (which are its eigenvalues) are the same as the eigenvalues of \( T \) and \( A \). Consider the column sums of the absolute values of the elements of \( DT^{-1} \):

\[ |c_j| + \sum_{i=1}^{j-1} d^{-(j-i)} |t_{ij}|. \]

Now, because \( |c_j| \leq \rho(A) \) for given \( \epsilon > 0 \), by choosing \( d \) large enough, we have

\[ |c_j| + \sum_{i=1}^{j-1} d^{-(j-i)} |t_{ij}| < \rho(A) + \epsilon, \]

or

\[ \|DT^{-1}\|_1 = \max_j \left( |c_j| + \sum_{i=1}^{j-1} d^{-(j-i)} |t_{ij}| \right) < \rho(A) + \epsilon. \]

Now define \( \| \cdot \|_d \) for any \( n \times n \) matrix \( X \), where \( Q \) is the orthogonal matrix in the Schur factorization and \( D \) is as defined above, as

\[ \|X\|_d = \|(QD^{-1})^{-1} X (QD^{-1})\|_1. \quad (3.262) \]

Now \( \| \cdot \|_d \) is a norm (Exercise 3.35). Furthermore,

\[ \|A\|_d = \| (QD^{-1})^{-1} A (QD^{-1}) \|_1 \]
\[ = \| DT^{-1} \|_1 \]
\[ < \rho(A) + \epsilon, \]

and so if \( \rho(A) < 1 \), \( \epsilon \) and \( d \) can be chosen so that \( \|A\|_d < 1 \), and by equation (3.260) above, we have \( A^k \to 0 \); hence, we conclude that

\[ A^k \to 0 \quad \text{if and only if } \rho(A) < 1. \quad (3.263) \]

Informally, we see that \( A^k \) goes to 0 more rapidly the smaller is \( \rho(A) \).
Another Perspective on the Spectral Radius: Relation to Norms

From inequality (3.259) and the fact that \( \rho(A^k) = (\rho(A))^k \), we have

\[
\rho(A) \leq \|A^k\|^{1/k}, \tag{3.264}
\]

where \( \| \cdot \| \) is any matrix norm. Now, for any \( \epsilon > 0 \), \( \rho\left(\frac{A}{(\rho(A) + \epsilon)}\right) < 1 \) and so

\[
\lim_{k \to \infty} \left(\frac{A}{(\rho(A) + \epsilon)}\right)^k = 0
\]

from expression (3.263); hence,

\[
\lim_{k \to \infty} \frac{\|A^k\|}{(\rho(A) + \epsilon)^k} = 0.
\]

There is therefore a positive integer \( M_\epsilon \) such that \( \|A^k\|/(\rho(A) + \epsilon)^k < 1 \) for all \( k > M_\epsilon \), and hence \( \|A^k\|^{1/k} < (\rho(A) + \epsilon) \) for \( k > M_\epsilon \). We have therefore, for any \( \epsilon > 0 \),

\[
\rho(A) \leq \|A^k\|^{1/k} < \rho(A) + \epsilon \quad \text{for } k > M_\epsilon,
\]

and thus

\[
\lim_{k \to \infty} \|A^k\|^{1/k} = \rho(A). \tag{3.265}
\]

Convergence of a Power Series; Inverse of \( I - A \)

Consider the power series in an \( n \times n \) matrix such as in equation (3.151) on page 108,

\[
I + A + A^2 + A^3 + \cdots
\]

In the standard fashion for dealing with series, we form the partial sum

\[
S_k = I + A + A^2 + A^3 + \cdots A^k
\]

and consider \( \lim_{k \to \infty} S_k \). We first note that

\[
(I - A)S_k = I - A^{k+1}
\]

and observe that if \( A^{k+1} \to 0 \), then \( S_k \to (I - A)^{-1} \), which is equation (3.151). Therefore,

\[
(I - A)^{-1} = I + A + A^2 + A^3 + \cdots \quad \text{if } \|A\| < 1. \tag{3.266}
\]
Nilpotent Matrices

The condition in equation (3.252) is not necessary; that is, if $A^k \to 0$, it may be the case that, for some norm, $\|A\| > 1$. A simple example is

$$A = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}.$$  

For this matrix, $A^2 = 0$, yet $\|A\|_1 = \|A\|_2 = \|A\|_\infty = \|A\|_F = 2$.

A matrix like $A$ above such that its product with itself is $0$ is called nilpotent. More generally, for a square matrix $A$, if $A^k = 0$ for some positive integer $k$, but $A^{k-1} \neq 0$, $A$ is said to be nilpotent of index $k$. Strictly speaking, a nilpotent matrix is nilpotent of index 2, but often the term “nilpotent” without qualification is used to refer to a matrix that is nilpotent of any index. A simple example of a matrix that is nilpotent of index 3 is

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$  

It is easy to see that if $A_{m \times n}$ is nilpotent, then

$$\text{tr}(A) = 0,$$  

$$\det(A) = 0,$$  

$$\rho(A) = 0,$$  

(3.267, 3.268, 3.269)

(that is, all eigenvalues of $A$ are 0), and

$$\text{rank}(A) = n - 1.$$  

(3.270)

You are asked to supply the proofs of these statements in Exercise 3.36.

In applications, for example in time series or other stochastic processes, because of expression (3.263), the spectral radius is often the most useful. Stochastic processes may be characterized by whether the absolute value of the dominant eigenvalue (spectral radius) of a certain matrix is less than 1. Interesting special cases occur when the dominant eigenvalue is equal to 1.

3.10 Approximation of Matrices

In Section 2.2.6, we discussed the problem of approximating a given vector in terms of vectors from a lower dimensional space. Likewise, it is often of interest to approximate one matrix by another. In statistical applications, we may wish to find a matrix of smaller rank that contains a large portion of the information content of a matrix of larger rank (“dimension reduction” as on page 368; or variable selection as in Section 9.4.2, for example), or we may
want to impose conditions on an estimate that it have properties known to
be possessed by the estimand (positive definiteness of the correlation matrix,
for example, as in Section 9.4.6). In numerical linear algebra, we may wish
to find a matrix that is easier to compute or that has properties that ensure
more stable computations.

**Metric for the Difference of Two Matrices**

A natural way to assess the goodness of the approximation is by a norm of the
difference (that is, by a metric induced by a norm), as discussed on page 31.
If \( \tilde{A} \) is an approximation to \( A \), we measure the quality of the approximation
by \( \| A - \tilde{A} \| \) for some norm. In the following, we will measure the goodness
of the approximation using the norm that arises from the inner product (the
Frobenius norm).

**Best Approximation with a Matrix of Given Rank**

Suppose we want the best approximation to an \( n \times m \) matrix \( A \) of rank \( r \) by
a matrix \( \tilde{A} \in \mathbb{R}^{n \times m} \) but with smaller rank, say \( k \); that is, we want to find \( \tilde{A} \)
of rank \( k \) such that

\[
\| A - \tilde{A} \|_F
\]

is a minimum for all \( \tilde{A} \in \mathbb{R}^{n \times m} \) of rank \( k \).

We have an orthogonal basis in terms of the singular value decomposition,
equation (3.231), for some subspace of \( \mathbb{R}^{n \times m} \), and we know that the Fourier
coefficients provide the best approximation for any subset of \( k \) basis matrices,
as in equation (2.56). This Fourier fit would have rank \( k \) as required, but it
would be the best only within that set of expansions. (This is the limitation
imposed in equation (2.56).) Another approach to determine the best fit could
be developed by representing the columns of the approximating matrix as
linear combinations of the given matrix \( A \) and then expanding \( \| A - \tilde{A} \|_F^2 \).
Neither the Fourier expansion nor the restriction \( \mathcal{V}(A) \subset \mathcal{V}(A) \) permit us to
address the question of what is the overall best approximation of rank \( k \) within
\( \mathbb{R}^{n \times m} \). As we see below, however, there is a minimum of expression (3.271)
that occurs within \( \mathcal{V}(A) \), and a minimum is at the truncated Fourier expansion
in the singular values (equation (3.231)).

To state this more precisely, let \( A \) be an \( n \times m \) matrix of rank \( r \) with
singular value decomposition

\[
A = U \begin{bmatrix} D_r & 0 \\ 0 & 0 \end{bmatrix} V^T,
\]

where \( D_r = \text{diag}(d_1, \ldots, d_r) \), and the singular values are indexed so that
\( d_1 \geq \cdots \geq d_r > 0 \). Then, for all \( n \times m \) matrices \( X \) with rank \( k < r \),
\[ \| A - X \|_F^2 \geq \sum_{i=k+1}^{r} d_i^2, \]  
(3.272)

and this minimum occurs for \( X = \tilde{A} \), where
\[
\tilde{A} = U \begin{bmatrix} D_k & 0 \\ 0 & 0 \end{bmatrix} V^T.
\]  
(3.273)

To see this, for any \( X \), let \( Q \) be an \( n \times k \) matrix whose columns are an orthonormal basis for \( \mathcal{V}(X) \), and let \( X = QY \), where \( Y \) is a \( k \times n \) matrix, also of rank \( k \). The minimization problem now is
\[
\min_Y \| A - QY \|_F
\]
with the restriction \( \text{rank}(Y) = k \).

Now, expanding, completing the Gramian and using its nonnegative definiteness, and permuting the factors within a trace, we have
\[
\| A - QY \|_F^2 = \text{tr} ((A - QY)^T(A - QY)) \\
= \text{tr} (A^T A) + \text{tr} (Y^T Y - A^T QY - Y^T Q^T A) \\
= \text{tr} (A^T A) + \text{tr} ((Y - Q^T A)^T(Y - Q^T A)) - \text{tr} (A^T Q Q^T A) \\
\geq \text{tr} (A^T A) - \text{tr} (Q^T A A^T Q).
\]

The squares of the singular values of \( A \) are the eigenvalues of \( A^T A \), and so \( \text{tr}(A^T A) = \sum_{i=1}^{r} d_i^2 \). The eigenvalues of \( A^T A \) are also the eigenvalues of \( A A^T \), and so, from inequality (3.225), \( \text{tr}(Q^T A A^T Q) \leq \sum_{i=1}^{k} d_i^2 \), and so
\[
\| A - X \|_F^2 \geq \sum_{i=1}^{r} d_i^2 - \sum_{i=1}^{k} d_i^2;
\]

hence, we have inequality (3.272). (This technique of “completing the Gramian” when an orthogonal matrix is present in a sum is somewhat similar to the technique of completing the square; it results in the difference of two Gramian matrices, which are defined in Section 3.3.7.)

Direct expansion of \( \| A - \tilde{A} \|_F^2 \) yields
\[
\text{tr} (A^T A) - 2\text{tr} (A^T \tilde{A}) + \text{tr} (\tilde{A}^T \tilde{A}) = \sum_{i=1}^{r} d_i^2 - \sum_{i=1}^{k} d_i^2,
\]

and hence \( \tilde{A} \) is the best rank \( k \) approximation to \( A \) under the Frobenius norm.

Equation (3.273) can be stated another way: the best approximation of \( A \) of rank \( k \) is
\[
\tilde{A} = \sum_{i=1}^{k} d_i u_i v_i^T.
\]  
(3.274)
This result for the best approximation of a given matrix by one of lower rank was first shown by Eckart and Young (1936). On page 293, we will discuss a bound on the difference between two symmetric matrices whether of the same or different ranks.

In applications, the rank $k$ may be stated a priori or we examine a sequence $k = r - 1, r - 2, \ldots$, and determine the norm of the best fit at each rank. If $s_k$ is the norm of the best approximating matrix, the sequence $s_{r-1}, s_{r-2}, \ldots$ may suggest a value of $k$ for which the reduction in rank is sufficient for our purposes and the loss in closeness of the approximation is not too great. Principal components analysis is a special case of this process (see Section 9.3).

Exercises

   a) Exhibit a basis set for $\mathbb{R}^{n \times m}$ for $n \geq m$.
   b) Does the set of $n \times m$ diagonal matrices form a vector space? (The answer is yes.) Exhibit a basis set for this vector space (assuming $n \geq m$).
   c) Exhibit a basis set for the vector space of $n \times n$ symmetric matrices. (First, of course, we must ask is this a vector space. The answer is yes.)
   d) Show that the cardinality of any basis set for the vector space of $n \times n$ symmetric matrices is $n(n + 1)/2$.

3.2. By expanding the expression on the left-hand side, derive equation (3.70) on page 83.

3.3. Show that for any quadratic form $x^T Ax$ there is a symmetric matrix $A_s$ such that $x^T A_s x = x^T Ax$. (The proof is by construction, with $A_s = \frac{1}{2}(A + A^T)$, first showing $A_s$ is symmetric and then that $x^T A_s x = x^T Ax$.)

3.4. For $a, b, c \in \mathbb{R}$, give conditions on $a, b$, and $c$ for the matrix below to be positive definite.
   \[
   \begin{bmatrix}
   a & b \\
   b & c
   \end{bmatrix}
   \]

3.5. Show that the Mahalanobis distance defined in equation (3.73) is a metric (that is, show that it satisfies the properties listed on page 30).

3.6. Verify the relationships for Kronecker products shown in equations (3.75) through (3.79) on page 86. Make liberal use of equation (3.74) and previously verified equations.

3.7. Cauchy-Schwarz inequalities for matrices.
   a) Prove the Cauchy-Schwarz inequality for the dot product of matrices ((3.86), page 88), which can also be written as
   \[(\text{tr}(A^T B))^2 \leq \text{tr}(A^T A)\text{tr}(B^T B).\]
b) Prove the Cauchy-Schwarz inequality for determinants of matrices $A$ and $B$ of the same shape:

$$\det(AB)^2 \leq \det(A^T A) \det(B^T B).$$

Under what conditions is equality achieved?

c) Let $A$ and $B$ be matrices of the same shape, and define

$$p(A, B) = \det(A^T B).$$

Is $p(\cdot, \cdot)$ an inner product? Why or why not?

3.8. Prove that a square matrix that is either row or column (strictly) diagonally dominant is nonsingular.

3.9. Prove that a positive definite matrix is nonsingular.

3.10. Let $A$ be an $n \times m$ matrix.

a) Under what conditions does $A$ have a Hadamard multiplicative inverse?

b) If $A$ has a Hadamard multiplicative inverse, what is it?

3.11. The affine group $AL(n)$.

a) What is the identity in $AL(n)$?

b) Let $(A, v)$ be an element of $AL(n)$. What is the inverse of $(A, v)$?

3.12. In computational explorations involving matrices, it is often convenient to work with matrices whose elements are integers. If an inverse is involved, it would be nice to know that the elements of the inverse are also integers. Equation (3.137) on page 106 provides us a way of ensuring this.

Show that if the elements of the square matrix $A$ are integers and if $\det(A) = \pm 1$, then $(A^{-1})$ exists and the elements of $A^{-1}$ are integers.

3.13. Verify the relationships shown in equations (3.141) through (3.148) on page 107. Do this by multiplying the appropriate matrices. For example, equation (3.141) is verified by the equations

$$(I + A^{-1})A(I + A)^{-1} = (A + I)(I + A)^{-1} = (I + A)(I + A)^{-1} = I.$$  

Make liberal use of equation (3.138) and previously verified equations. Of course it is much more interesting to derive relationships such as these rather than merely to verify them. The verification, however, often gives an indication of how the relationship would arise naturally.


3.15. In equations (3.141) through (3.148) on page 107, drop the assumptions of nonsingularity of matrices, and assume only that the matrices are conformable for the operations in the expressions. Replace the inverse with the Moore-Penrose inverse.

Now, determine which of these relationships are true. For those that are true, show that they are (for general but conformable matrices). If the relationship does not hold, give a counterexample.
3.16. By writing $AA^{-1} = I$, derive the expression for the inverse of a partitioned matrix given in equation (3.155).

3.17. Show that the expression given for the generalized inverse in equation (3.175) on page 116 is correct.

3.18. Show that the expression given in equation (3.177) on page 117 is a Moore-Penrose inverse of $A$. (Show that properties 1 through 4 hold.)

3.19. Write formal proofs of the properties of eigenvalues/vectors listed on page 122.

3.20. Let $A$ be a square matrix with an eigenvalue $c$ and corresponding eigenvector $v$. Consider the matrix polynomial in $A$

\[ p(A) = b_0 I + b_1 A + \cdots + b_k A^k. \]

Show that if $(c, v)$ is an eigenpair of $A$, then $p(c)$, that is,

\[ b_0 + b_1 c + \cdots + b_k c^k, \]

is an eigenvalue of $p(A)$ with corresponding eigenvector $v$. (Technically, the symbol $p(\cdot)$ is overloaded in these two instances.)

3.21. Write formal proofs of the properties of eigenvalues/vectors listed on page 125.

3.22. a) Show that the unit vectors are eigenvectors of a diagonal matrix.

b) Give an example of two similar matrices whose eigenvectors are not the same.

*Hint:* In equation (3.202), let $A$ be a $2 \times 2$ diagonal matrix (so you know its eigenvalues and eigenvectors) with unequal values along the diagonal, and let $P$ be a $2 \times 2$ upper triangular matrix, so that you can invert it. Form $B$ and check the eigenvectors.

3.23. Let $A$ be a diagonalizable matrix (not necessarily symmetric) with a spectral decomposition of the form of equation (3.217), $A = \sum c_i P_i$. Let $c_j$ be a simple eigenvalue with associated left and right eigenvectors $y_j$ and $x_j$, respectively. (Note that because $A$ is not symmetric, it may have nonreal eigenvalues and eigenvectors.)

a) Show that $y_j^H x_j \neq 0$.

b) Show that the projection matrix $P_j$ is $x_j y_j^H / y_j^H x_j$.

3.24. If $A$ is nonsingular, show that for any (conformable) vector $x$

\[ (x^T A x)(x^T A^{-1} x) \geq (x^T x)^2. \]

*Hint:* Use the square roots and the Cauchy-Schwarz inequality.

3.25. Prove that the induced norm (page 145) is a matrix norm; that is, prove that it satisfies the consistency property.

3.26. Prove the inequality (3.234) for an induced matrix norm on page 146:

\[ \| Ax \| \leq \| A \| \| x \|. \]
3.27. Prove that, for the square matrix $A$,
\[ \|A\|_2^2 = \rho(A^T A). \]

*Hint:* Show that $\|A\|_2^2 = \max x^T A^T A x$ for any normalized vector $x$.

3.28. Let $Q$ be an $n \times n$ orthogonal matrix, and let $x$ be an $n$-vector.

a) Prove equation (3.240):
\[ \|Qx\|_2 = \|x\|_2. \]

*Hint:* Write $\|Qx\|_2$ as $\sqrt{(Qx)^T Qx}$.

b) Give examples to show that this does not hold for other norms.

3.29. The triangle inequality for matrix norms: $\|A + B\| \leq \|A\| + \|B\|$.

a) Prove the triangle inequality for the matrix $L_1$ norm.

b) Prove the triangle inequality for the matrix $L_\infty$ norm.

c) Prove the triangle inequality for the matrix Frobenius norm.

3.30. Prove that the Frobenius norm satisfies the consistency property.

3.31. If $\| \cdot \|_a$ and $\| \cdot \|_b$ are matrix norms induced respectively by the vector norms $\| \cdot \|_{v_a}$ and $\| \cdot \|_{v_b}$, prove inequality (3.252); that is, show that there are positive numbers $r$ and $s$ such that, for any $A$,
\[ r\|A\|_b \leq \|A\|_a \leq s\|A\|_b. \]

3.32. Use the Cauchy-Schwarz inequality to prove that for any square matrix $A$ with real elements,
\[ \|A\|_2 \leq \|A\|_F. \]

3.33. Prove inequalities (3.253) through (3.258), and show that the bounds are sharp by exhibiting instances of equality.

3.34. The spectral radius, $\rho(A)$.

a) We have seen by an example that $\rho(A) = 0$ does not imply $A = 0$. What about other properties of a matrix norm? For each, either show that the property holds for the spectral radius or, by means of an example, that it does not hold.

b) Use the outer product of an eigenvector and the one vector to show that for any norm $\| \cdot \|$ and any matrix $A$, $\rho(A) \leq \|A\|$. 

3.35. Show that the function $\| \cdot \|_a$ defined in equation (3.262) is a norm.
*Hint:* Just verify the properties on page 145 that define a norm.

3.36. Prove equations (3.267) through (3.270).

3.37. Prove equations (3.272) and (3.273) under the restriction that $\mathcal{V}(X) \subset \mathcal{V}(A)$; that is, where $X = BL$ for a matrix $B$ whose columns span $\mathcal{V}(A)$. 