3

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 Chap. 8, we will consider in more detail some special types of matrices that arise in regression analysis and multivariate data analysis, and then in Chap. 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

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

I make no distinction between these two notations. The notation $\mathcal{V}(\cdot)$ emphasizes that the result is a vector space. Note that if $A \in \mathbb{R}^{n \times m}$, then $\mathcal{V}(A) \subseteq \mathbb{R}^n$.

J.E. Gentle, *Matrix Algebra*, Springer Texts in Statistics,
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The argument of $\mathcal{V}(\cdot)$ or span$(\cdot)$ can also be a set of vectors instead of a matrix. Recall from Sect. 2.1.3 that if G is a set of vectors, the symbol 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.

Given an $n \times m$ matrix A with elements a_{ij}, the $m \times n$ matrix with elements a_{ji} is called the *transpose* of A. We use a superscript "T" to denote the transpose of a matrix; thus, if $A = (a_{ij})$, then

$$A^{\mathrm{T}} = (a_{ji}). \tag{3.1}$$

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

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*. Obviously, 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 with real elements on the diagonal, and, of course, a real symmetric matrix is Hermitian. A Hermitian matrix is also called a *self-adjoint* matrix.

3.1.1 Multiplication of a Matrix by a Scalar

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

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

3.1.2 Diagonal Elements: diag(·) and vecdiag(·)

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. This definition of principal diagonal applies whether or not the matrix is square.

We denote the principal diagonal of a matrix A by diag(A) or by vecdiag(A). The latter notation is sometimes used because, as we will see on page 60, diag$(\dot{)}$ is also used for an argument that is a vector (and the function produces a matrix). The diag or vecdiag function defined here is a mapping $\mathbb{R}^{n \times m} \to \mathbb{R}^{\min(n,m)}$.

If A is an $n \times m$ matrix, and $k = \min(n, m)$,

$$\text{diag}(A) = (a_{11}, \ldots, a_{kk}). \tag{3.2}$$

As noted above, we may also denote this as vecdiag(A), but I will generally use the notation "diag($\cdot$)".

Note from the definition that

$$\text{diag}(A^{\mathrm{T}}) = \text{diag}(A), \tag{3.3}$$

and this is true whether or not A is square.

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.

For $c = \pm 1, \ldots$, the elements $a_{i,i+c}$ are called "codiagonals" or "minor diagonals". The codiagonals $a_{i,i+1}$ are called "supradiagonals", and the codiagonals $a_{i,i-1}$ are called "infradiagonals" 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.

3.1.3 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

$$|a_{ii}| > \sum_{j \neq i}^{m} |a_{ij}| \quad \text{for each } i = 1, \ldots, n \tag{3.4}$$

is said to be row *diagonally dominant*; and a matrix A for which $|a_{jj}| > \sum_{i \neq j}^{n} |a_{ij}|$ 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.

3.1.4 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.

$$\begin{bmatrix} \mathtt{X} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{0} & \mathtt{X} \end{bmatrix} \quad \begin{bmatrix} \mathtt{X} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{0} & \mathtt{0} \end{bmatrix} \quad \begin{bmatrix} \mathtt{X} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{0} & \mathtt{X} \\ \mathtt{0} & \mathtt{0} & \mathtt{0} \end{bmatrix} \quad \begin{bmatrix} \mathtt{X} & \mathtt{X} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{X} & \mathtt{X} & \mathtt{X} \\ \mathtt{0} & \mathtt{0} & \mathtt{X} & \mathtt{X} \end{bmatrix}$$

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 390). 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 $a_{i,i\pm1}$ 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 385).

Using the intuitive notation of `X` and `0` as above, a band matrix may be written as

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

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 $i > j + 1$:

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

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

Hessenberg matrices arise in some methods for computing eigenvalues (see Chap. 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.

3.1.5 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.

3.1.5.1 Transpose

As defined above, 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 note immediately that

$$(A^{\mathrm{T}})^{\mathrm{T}} = A. \tag{3.5}$$

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

$$A^{\mathrm{H}} = (\bar{a}_{ji}). \tag{3.6}$$

We also use a similar notation for vectors. (The conjugate transpose is often denoted by an asterisk, as in $A^* = (\bar{a}_{ji}) = A^{\mathrm{H}}$. 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 128.) As with the transponse, $(A^{\mathrm{H}})^{\mathrm{H}} = A$. If (and only if) all of the elements of A are all real, then $A^{\mathrm{H}} = A^{\mathrm{T}}$.

If (and only if) A is symmetric, $A = A^{\mathrm{T}}$; if (and only if) A is skew symmetric, $A^{\mathrm{T}} = -A$; and if (and only if) A is Hermitian, $A = A^{\mathrm{H}}$ (and, in that case, all of the diagonal elements are real).

3.1.5.2 Diagonal Matrices and Diagonal Vectors: diag(·) (Again)

A square diagonal matrix can be specified by a constructor function that operates on a vector and forms a diagonal matrix with the elements of the vector along the diagonal. We denote that constructor function by diag(·), just as we used this name to denote a somewhat similar function on page 57.

$$\mathrm{diag}\big((d_1, d_2, \ldots, d_n)\big) = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ & & \ddots & \\ 0 & 0 & \cdots & d_n \end{bmatrix}. \tag{3.7}$$

(Notice that the argument of diag here 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 diag function defined here is a mapping $\mathbb{R}^n \to \mathbb{R}^{n\times n}$. 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 $I_n = \mathrm{diag}(1_n)$. 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.

Note that we have overloaded diag(·), which we defined on page 57 with a matrix argument, to allow its argument to be a vector. (Recall that vecdiag(·) is the same as diag(·) when the argument is a matrix.) Both the R and Matlab computing systems, for example, use this overloading; that is, they each provide a single function (called `diag` in each case).

Note further that over $\mathbb{R}^n$ and $\mathbb{R}^{n\times n}$, diag(·) is its own inverse; that is, if v is a vector,

$$\mathrm{diag}(\mathrm{diag}(v)) = v, \tag{3.8}$$

and if A is a square matrix,

$$\mathrm{diag}(\mathrm{diag}(A)) = A. \tag{3.9}$$

3.1.5.3 Forming a Vector from the Elements of a Matrix: vec(·) and vech(·)

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(·) function does this:

$$\text{vec}(A) = (a_1^{\mathrm{T}}, a_2^{\mathrm{T}}, \ldots, a_m^{\mathrm{T}}), \tag{3.10}$$

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 (3.10) is the notation for a column vector with elements a_i^{T}; see Chap. 1.) The vec function is a mapping $\mathbb{R}^{n\times m} \to \mathbb{R}^{nm}$.

For a symmetric matrix A with elements a_{ij}, the "vech" function stacks the unique elements into a vector:

$$\text{vech}(A) = (a_{11}, a_{21}, \ldots, a_{m1}, a_{22}, \ldots, a_{m2}, \ldots, a_{mm}). \tag{3.11}$$

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 548), but equation (3.11) is the standard definition of vech(·). The vech function is a mapping $\mathbb{R}^{n\times n} \to \mathbb{R}^{n(n+1)/2}$.

3.1.6 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

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{3.12}$$

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. A more precise notation specifies the rows and columns of the original matrix. For example, $A_{(i_1,\ldots,i_k)(j_1,\ldots,j_l)}$ denotes the submatrix of A formed by rows $i_1, \ldots, i_k$ and columns $j_1, \ldots, j_l$. When the entire rows are included, $A_{(i_1,\ldots,i_k)(*)}$ denotes the submatrix of A formed from rows $i_1, \ldots, i_k$; and $A_{(*)(j_1,\ldots,j_l)}$ denotes the submatrix formed from columns $j_1, \ldots, j_l$ with elements from all rows. Finally, a_{i*} denotes the vector whose elements correspond to those in the i^{th} row of the matrix A. We sometimes emphasize that it is a *vector* by writing it in the form a_{i*}^{T}. Likewise, a_{*j} denotes the vector whose elements correspond to those in the j^{th} column of A. See page 599 for a summary of this notation. 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

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

where $\mathtt{0}$ represents a submatrix with all zeros and $\mathtt{X}$ represents a general submatrix with at least some nonzeros.

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

$$\mathrm{diag}(A_1, A_2, \ldots, A_k)$$

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 $\oplus$:

$$A_1 \oplus \cdots \oplus A_k = \mathrm{diag}(A_1, \ldots, A_k). \tag{3.13}$$

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 diag(·).

3.1.6.1 Transposes of Partitioned Matrices

The transpose of a partitioned matrix is formed in the obvious way; for example,

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{bmatrix}^{\mathrm{T}} = \begin{bmatrix} A_{11}^{\mathrm{T}} & A_{21}^{\mathrm{T}} \\ A_{12}^{\mathrm{T}} & A_{22}^{\mathrm{T}} \\ A_{13}^{\mathrm{T}} & A_{23}^{\mathrm{T}} \end{bmatrix}. \tag{3.14}$$

3.1.7 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 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.

3.1.7.1 The Transpose of the Sum of Matrices

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

$$(A + B)^{\mathrm{T}} = A^{\mathrm{T}} + B^{\mathrm{T}}. \tag{3.15}$$

The sum of two symmetric matrices is therefore symmetric.

3.1.7.2 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

$$A > 0; \tag{3.16}$$

if all of the elements are nonnegative, we write

$$A \geq 0. \tag{3.17}$$

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 on page 92, and discuss further in Sect. 8.3.)

3.1.7.3 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 (2.13), which is different from the direct sum of matrices defined in terms of diag$(\cdot)$ as in equation (3.13)).

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).

3.1.8 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.

3.1.8.1 The Trace: tr(·)

The sum of the diagonal elements of a square matrix is called the *trace* of the matrix. We use the notation "$\mathrm{tr}(A)$" to denote the trace of the matrix A:

$$\mathrm{tr}(A) = \sum_i a_{ii}. \tag{3.18}$$

3.1.8.2 The Trace of the Transpose of Square Matrices

From the definition, we see

$$\mathrm{tr}(A) = \mathrm{tr}(A^{\mathrm{T}}). \tag{3.19}$$

3.1.8.3 The Trace of Scalar Products of Square Matrices

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

$$\mathrm{tr}(cA) = c\,\mathrm{tr}(A).$$

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

3.1.8.4 The Trace of Partitioned Square Matrices

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

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{3.20}$$

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

$$\mathrm{tr}(A) = \mathrm{tr}(A_{11}) + \mathrm{tr}(A_{22}). \tag{3.21}$$

3.1.8.5 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

$$\mathrm{tr}(A + B) = \mathrm{tr}(A) + \mathrm{tr}(B). \tag{3.22}$$

3.1.9 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.

3.1.9.1 The Determinant: det(·)

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, given the tuple $(1, 2, 3)$, then $(1, 3, 2)$ is an odd permutation, and $(3, 1, 2)$ and $(1, 2, 3)$ are even permutations. Let

$$\sigma(\pi) = \begin{cases} 1 \text{ if } \pi \text{ is an even permutation} \\ -1 \text{ otherwise.} \end{cases} \tag{3.23}$$

Then the *determinant* of A, denoted by $\det(A)$, is defined by

$$\det(A) = \sum_{\text{all permutations } \pi_j} \sigma(\pi_j) a_{1j_1} \cdots a_{nj_n}. \tag{3.24}$$

This simple function has many remarkable relationships to various properties of matrices.

3.1.9.2 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 (4.73)) that involve nonnegative definite matrices (see page 91 for the definition). The determinant of a matrix may be negative, and sometimes, as in measuring volumes (see page 74 for simple areas and page 215 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 ± 1, and it can be built up by elementary exchanges of adjacent elements. For example, consider $\sigma(3, 2, 1)$. There are two ways we can use three elementary exchanges, each beginning with the natural ordering:

$$(1, 2, 3) \to (2, 1, 3) \to (2, 3, 1) \to (3, 2, 1),$$

or

$$(1,2,3) \to (1,3,2) \to (3,1,2) \to (3,2,1);$$

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

If π_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 π_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:

$$\sigma(j_1,\ldots,j_n) = \sigma(j_1,\ldots,j_m)\sigma(j_{m+1},\ldots,j_n). \tag{3.25}$$

Furthermore, we see that the product $a_{1j_1}\cdots a_{nj_n}$ 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 (3.24) there is a 0, except in the term in which the subscripts on each factor are the same).

3.1.9.3 Minors, Cofactors, and Adjugate Matrices

Consider the 2×2 matrix

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

From the definition of the determinant, we see that

$$\det(A) = a_{11}a_{22} - a_{12}a_{21}. \tag{3.26}$$

Now let A be a 3×3 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

$$\begin{aligned}\det(A) = \; & a_{11}(-1)^{1+1}\det\left(\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}\right) \\ + \; & a_{12}(-1)^{1+2}\det\left(\begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{bmatrix}\right) \\ + \; & a_{13}(-1)^{1+3}\det\left(\begin{bmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}\right).\end{aligned} \tag{3.27}$$

Notice that this is the same form as in equation (3.26):

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

The manipulation in equation (3.27) of the terms in the determinant could be carried out with other rows of A.

The determinants of the 2×2 submatrices in equation (3.27) 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

$$\det\left(A_{-(i)(j)}\right), \tag{3.28}$$

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 $a_{(ij)}$:

$$a_{(ij)} = (-1)^{i+j}\det\left(A_{-(i)(j)}\right). \tag{3.29}$$

Notice that both minors and cofactors are scalars.

The manipulations leading to equation (3.27), though somewhat tedious, can be carried out for a square matrix of any size larger than 1×1, and minors and cofactors are defined as above. An expression such as in equation (3.27) is called an expansion in minors or an expansion in cofactors.

The extension of the expansion (3.27) 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

$$\begin{aligned}\det(A) &= \sum_{j=1}^{n} a_{ij}(-1)^{i+j}\det\left(A_{-(i)(j)}\right) \\ &= \sum_{j=1}^{n} a_{ij}a_{(ij)},\end{aligned} \tag{3.30}$$

or, over the rows,

$$\det(A) = \sum_{i=1}^{n} a_{ij} a_{(ij)}. \tag{3.31}$$

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

Expressions (3.30) and (3.31) 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 (3.30) or (3.31), 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 2×2 matrices consisting of a duplicated row. The determinant of such a matrix is 0, so the expansion is 0.

The expansion in equation (3.30) 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 $k \neq i$,

$$\begin{aligned} \sum_{j=1}^{n} a_{kj}(-1)^{i+j} \det\left(A_{-(i)(j)}\right) &= \sum_{j=1}^{n} a_{kj} a_{(ij)} \\ &= 0. \end{aligned} \tag{3.32}$$

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

$$\operatorname{adj}(A) = (a_{(ji)}), \tag{3.33}$$

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,

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

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

$$A\,\text{adj}(A) = \text{adj}(A)A = \det(A)I. \tag{3.34}$$

To see this, consider the $(i,j)^{\text{th}}$ 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 (3.33), and using equations (3.30) and (3.32), 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 (3.172).

3.1.9.4 The Determinant of the Transpose of Square Matrices

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

$$\det(A) = \det(A^{\mathrm{T}}). \tag{3.35}$$

3.1.9.5 The Determinant of Scalar Products of Square Matrices

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

$$\det(cA) = c^n \det(A). \tag{3.36}$$

This follows immediately from the definition because, for $\det(cA)$, each factor in each term of equation (3.24) is multiplied by c.

3.1.9.6 The Determinant of an Upper (or Lower) Triangular Matrix

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

$$\det(A) = \prod_{i=1}^{n} a_{ii}. \tag{3.37}$$

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

3.1.9.7 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:

$$\det(A) = \det\left(\begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix}\right) = \det\left(\begin{bmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{bmatrix}\right) = \det\left(\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}\right)$$
$$= \det(A_{11})\det(A_{22}). \tag{3.38}$$

We can see this by considering the individual terms in the determinant, equation (3.24). 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 (3.24), 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 $m+1, \ldots, n$,

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

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 (3.25), we therefore have for A of this special form

$$\begin{aligned} \det(A) &= \sum\sum \sigma(j_1, \ldots, j_m, j_{m+1}, \ldots, j_n) a_{1j_1} \cdots a_{mj_m} a_{m+1,j_{m+1}} \cdots a_{nj_n} \\ &= \sum \sigma(j_1, \ldots, j_m) a_{1j_1} \cdots a_{mj_m} \sum \sigma(j_{m+1}, \ldots, j_n) a_{m+1,j_{m+1}} \cdots a_{nj_n} \\ &= \det(A_{11})\det(A_{22}), \end{aligned}$$

which is equation (3.38). We use this result to give an expression for the determinant of more general partitioned matrices in Sect. 3.4.2.

Another useful partitioned matrix of the form of equation (3.20) has $A_{11} = 0$ and $A_{21} = -I$:

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

In this case, using equation (3.30), we get

$$\begin{aligned} \det(A) &= ((-1)^{n+1+1}(-1))^n \det(A_{12}) \\ &= (-1)^{n(n+3)} \det(A_{12}) \\ &= \det(A_{12}). \end{aligned} \tag{3.39}$$

We will consider determinants of a more general partitioning in Sect. 3.4.2, beginning on page 122.

3.1.9.8 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.

3.1.9.9 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 Sect. 3.8.4.)

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 (3.28)). In the current context, however, it is more convenient to adopt the notation $A_{(i_1,\ldots,i_k)}$ to represent the matrix formed from rows $i_1,\ldots,i_k$ and columns $i_1,\ldots,i_k$ from a given matrix A. That is, the notation $A_{(i_1,\ldots,i_k)}$ 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, $\det(A_{(i_1,\ldots,i_k)})$. Because the principal diagonal elements of this matrix are principal diagonal elements of A, we call $\det(A_{(i_1,\ldots,i_k)})$ a *principal minor* of A.

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

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

Expanding this, we have

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

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

$$= \det(A_{(1,2)}) + d_1 d_2 + a_{22} d_1 + a_{11} d_2.$$

Of course, $\det(A_{(1,2)}) = \det(A)$, but we are writing it this way to develop the pattern. Now, for the 3×3 case, we have

$$\begin{aligned} \det(A + D) = & \det(A_{(1,2,3)}) \\ & + \det(A_{(2,3)}) d_1 + \det(A_{(1,3)}) d_2 + \det(A_{(1,2)}) d_3 \\ & + a_{33} d_1 d_2 + a_{22} d_1 d_3 + a_{11} d_2 d_3 \\ & + d_1 d_2 d_3. \end{aligned} \tag{3.40}$$

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

$$\det(A + D) = \det(A_{(1,2,3)}) + \sum_{i \neq j} \det(A_{(i,j)}) d + \sum_i a_{i,i} d^2 + d^3. \tag{3.41}$$

Carefully continuing in this way for an $n \times n$ matrix, either as in equation (3.40) for n variables or as in equation (3.41) 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 $(n-1)^{\text{th}}$-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 Sect. 3.8.4.

3.1.9.10 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 Sect. 3.8).

3.1.9.11 A Geometrical Perspective of the Determinant

In Sect. 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 Fig. 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 θ. Thus, making use of equation (2.54) on page 37 for the cosine of the angle, we have

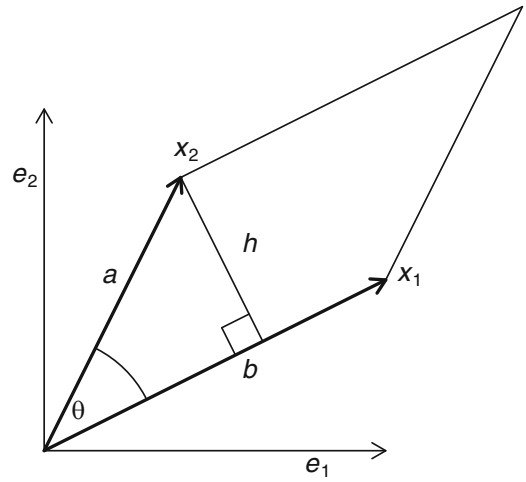

Figure 3.1. Volume (area) of region determined by x_1 and x_2

$$
\begin{aligned}
\text{area} &= bh \\
&= \|x_1\|\|x_2\| \sin(\theta) \\
&= \|x_1\|\|x_2\| \sqrt{1 - \left(\frac{\langle x_1, x_2 \rangle}{\|x_1\|\|x_2\|} \right)^2} \\
&= \sqrt{\|x_1\|^2 \|x_2\|^2 - (\langle x_1, x_2 \rangle)^2} \\
&= \sqrt{(x_{11}^2 + x_{12}^2)(x_{21}^2 + x_{22}^2) - (x_{11}x_{21} - x_{12}x_{22})^2}
\end{aligned}
$$

$$\begin{aligned} &= |x_{11}x_{22} - x_{12}x_{21}| \\ &= |\det(X)|, \end{aligned} \tag{3.42}$$

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

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

Although we will not go through the details here, this equivalence of a volume of a parallelotope 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 parallelotope extends to higher dimensions.

In making a change of variables in integrals, as in equation (4.62) on page 215, 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 368.

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

$$c_{ij} = \sum_k a_{ik} b_{kj}. \tag{3.43}$$

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 $n \times p$:

$$\begin{array}{ccc} C & = & A \qquad\qquad B \\ \left[\quad\right]_{n\times p} & = & \left[\quad\right]_{n\times m} \left[\quad\right]_{m\times p} \end{array}.$$

Cayley matrix multiplication is a mapping,

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

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 (3.43) that in general, even for square matrices, $AB \neq BA$. It is also obvious that if AB exists, then $B^{\mathrm{T}}A^{\mathrm{T}}$ exists and, in fact,

$$B^{\mathrm{T}}A^{\mathrm{T}} = (AB)^{\mathrm{T}}. \tag{3.44}$$

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

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,

$$A(BC) = (AB)C. \tag{3.45}$$

It is also *distributive* over addition; that is,

$$A(B + C) = AB + AC \tag{3.46}$$

and

$$(B + C)A = BA + CA. \tag{3.47}$$

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 *multiplicative identity* for the set of $n\times n$ matrices and Cayley multiplication. Such a matrix is called the *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

$$I_n A = A I_m = A.$$

Another matrix of interest is a *zero* matrix, which is any matrix consisting of all zeros. We denote a zero matrix as 0, with its shape being implied by the context. Two properties for any matrix A and a zero matrix of the appropriate shape are immediately obvious:

$$0A = 0$$

and

$$0 + A = A.$$

3.2.1.1 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 Sect. 3.3.6).

For an $n \times n$ matrix A, if A^k exists for negative integral values of k, we define A^0 by

$$A^0 = I_n. \tag{3.48}$$

For a diagonal matrix $D = \text{diag}\left((d_1, \ldots, d_n)\right)$, we have

$$D^k = \text{diag}\left((d_1^k, \ldots, d_n^k)\right). \tag{3.49}$$

3.2.1.2 Nilpotent Matrices

For an $n \times n$ matrix A, it may be the case for some positive integer k that $A^k = 0$. Such a matrix is said to be nilpotent; more generally, we define a *nilpotent matrix of index* k, for integer $k > 1$, as a square matrix A such that

$$A^k = 0, \qquad \text{but} \qquad A^{k-1} \neq 0. \tag{3.50}$$

We may use the term "nilpotent" without qualification to refer to a matrix that is nilpotent of any index; that is, strictly speaking, a nilpotent matrix is nilpotent of index 2.

A simple example of a matrix that is nilpotent of index 3 is

$$A = \left[\begin{array}{ccc|cc} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right], \tag{3.51}$$

in which I have indicated four submatrices of interest.

All nilpotent matrices have a certain relationship to matrices of the form of A in equation (3.51). We will identify that form here, but we will not discuss that form further. Notice two submatrices of A:

$$N_1 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad N_2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{3.52}$$

so

$$A = \begin{bmatrix} N_1 & 0 \\ 0 & N_2 \end{bmatrix}.$$

Matrices of the form of N_1 and N_2, consisting of all 0s except for 1s in the supradiagonal, are called *Jordan blocks* and the nilpotent matrix A is said be in *Jordan form*. An important property, which we will merely state without proof, is that the index of a nilpotent matrix in Jordan form is the number of 1s in the largest Jordan block.

A nilpotent matrix is necessarily singular. Nilpotent matrices have many other simple properties, some of which we will list on page 174.

3.2.1.3 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,

$$I - A^k = (I - A)(I + A + \cdots A^{k-1}), \tag{3.53}$$

and for an odd positive integer k,

$$I + A^k = (I + A)(I - A + \cdots A^{k-1}). \tag{3.54}$$

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 58 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 and the (i,i) element of AB is $a_{ii}b_{ii}$;
- if A and B are block diagonal with conformable blocks, AB is block diagonal;
- if A and B are upper triangular, AB is upper triangular and the (i,i) element of AB is $a_{ii}b_{ii}$;
- if A and B are lower triangular, AB is lower triangular and the (i,i) element of AB is $a_{ii}b_{ii}$;
- if A is upper triangular and B is lower triangular, in general, none of AB, BA, $A^{\mathrm{T}}A$, $B^{\mathrm{T}}B$, AA^{T}, and BB^{T} is triangular.

Each of these statements can be easily proven using the definition of multiplication in equation (3.43). An important special case of diagonal and triangular matrices is one in which all diagonal elements are 1. Such a diagonal matrix is the identity, of course, so it a very special multiplicative property. Triangular matrices with 1s on the diagonal are called "unit triangular" matrices, and they are often used in matrix factorizations, as we see later in this chapter and in Chap. 5.

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.

3.2.2.1 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

$$[X\ y]$$

or

$$[X \mid y],$$

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

$$[X\ y]^{\mathrm{T}}[X\ y] = \begin{bmatrix} X^{\mathrm{T}}X & X^{\mathrm{T}}y \\ y^{\mathrm{T}}X & y^{\mathrm{T}}y \end{bmatrix}. \tag{3.55}$$

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_p^{T}, 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*.

3.2.3.1 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 Chap. 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,

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

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

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

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:

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

Note that

$$A = E_{pq}E_{pq}A = AE_{pq}E_{pq}; \tag{3.56}$$

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, π.

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 permutation matrices in the opposite order; that is,

$$E_{(\pi)}^{\mathrm{T}}E_{(\pi)} = I.$$

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

$$B = E_{(\pi_1)}AE_{(\pi_2)}, \tag{3.57}$$

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 form a full rank partitioning as in equation (3.131) on page 104, to obtain an equivalent canonical form as in equation (3.151) on page 110 and LDU decomposition of a matrix as in equation (5.32) on page 246. 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.

3.2.3.2 The Vec-Permutation Matrix

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

$$\mathrm{vec}(A^{\mathrm{T}}) = K_{nm}\mathrm{vec}(A). \tag{3.58}$$

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

3.2.3.3 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

$$E_2(a) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

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 $a \neq 0$,

$$A = E_p(1/a)E_p(a)A, \tag{3.59}$$

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

3.2.3.4 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,

$$E_{pq}(a)A, \tag{3.60}$$

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

Given the 4×3 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

$$A = E_{pq}(-a)E_{pq}(a)A; \tag{3.61}$$

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

$$E_{ni}(-a_{nj}) \cdots E_{i+1,i}(-a_{i+1,j})E_i(1/a_{ij})A. \tag{3.62}$$

This process is called *Gaussian elimination*.

The matrix

$$G_{ij} = E_{ni}(-a_{nj}) \cdots E_{i+1,i}(-a_{i+1,j})E_i(1/a_{ij}) \tag{3.63}$$

is called a *Gaussian transformation* matrix. Notice that it is lower triangular, and its inverse, also lower triangular, is

$$G_{ij}^{-1} = E_i(a_{ij})E_{i+1,i}(a_{i+1,j}) \cdots E_{ni}(a_{nj}) \tag{3.64}$$

Gaussian elimination is often performed sequentially down the diagonal elements of a matrix (see its use in the LU factorization on page 244, for example).

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:

$$\widetilde{G}_{ij} = E_{ni}(-a_{nj}) \cdots E_{i+1,i}(-a_{i+1,j})E_{i-1,i}(-a_{i-1,j}) \cdots E_{1i}(-a_{1j})E_i(1/a_{ij}). \tag{3.65}$$

This is also called a Gaussian transformation matrix.

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

If at some point $a_{ii} = 0$, the operations of equation (3.62) 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 277 in Chap. 6.

As we mentioned above, 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.

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.*

These elementary transformations are the basic operations in Gaussian elimination, which is discussed in Sects. 5.7 and 6.2.1.

3.2.3.5 Elementary Operator Matrices: Summary of Notation and Properties

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 80, we have the various elementary operator matrices:

- E_{pq}: the interchange of rows p and q (E_{pq} is the same as E_{qp})

$$E_{pq} = E_{qp} = \begin{bmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 & 1 \end{bmatrix} \begin{matrix} \\ \\ \\ p \\ \\ q \\ \\ \\ \end{matrix} \tag{3.66}$$

  It is symmetric,

$$E_{pq}^{\mathrm{T}} = E_{pq}, \tag{3.67}$$

  and it is its own inverse,

$$E_{pq}^{-1} = E_{pq}, \tag{3.68}$$

  that is, it is orthogonal.

  $E_{(\pi)}$: a general permutation of rows, where π denotes a permutation. We have

$$E_{(\pi)} = E_{p_1 q_1} \cdots E_{p_k q_k}, \text{ for some } p_1, \ldots, p_k \text{ and } q_1, \ldots, q_k. \tag{3.69}$$

- $E_p(a)$: multiplication of row p by a.

$$E_p(a) = \begin{bmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & \cdots & 0 & 1 \end{bmatrix} \begin{matrix} \\ \\ \\ p \\ \\ \\ \\ \end{matrix} \tag{3.70}$$

Its inverse is

$$E_p^{-1}(a) = E_p(1/a). \tag{3.71}$$

- $E_{pq}(a)$: the replacement of row p by the sum of row p and a times row q. If $q > p$,

$$E_{pq}(a) = \begin{bmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & \cdots & a & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 & 1 \end{bmatrix} \begin{matrix} \\ \\ \\ p \\ \\ \\ q \\ \\ \end{matrix} \tag{3.72}$$

Its inverse is

$$E_{pq}^{-1}(a) = E_{pq}(-a). \tag{3.73}$$

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

3.2.3.6 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 (3.24), page 66), and that term is 1 times σ evaluated at the permutation that exchanges p and q. As we have seen (page 67), this is an odd permutation; hence, for an elementary permutation matrix E_{pq},

$$\det(E_{pq}) = -1. \tag{3.74}$$

Because a general permutation matrix $E_{(\pi)}$ can be formed as the product of elementary permutation matrices which together form the permutation π, we have from equation (3.74)

$$\det(E_\pi) = \sigma(\pi), \tag{3.75}$$

where $\sigma(\pi) = 1$ if π is an even permutation and -1 otherwise, as defined in equation (3.23).

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,

$$\begin{aligned}\det(E_{(\pi)}A) &= \det(E_{(\pi)})\det(A)\\ &= \sigma(\pi)\det(A).\end{aligned}$$

(In equation (3.81) below, we will see that this equation holds more generally.)

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

$$\det(E_p(a)) = a. \tag{3.76}$$

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 (3.24). (Again, this also follows from the general result in equation (3.81) below.)

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

$$\det(E_{pq}(a)) = 1, \tag{3.77}$$

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 (3.30)) along the p^{th} row yields

$$\begin{aligned}\det(E_{pq}(a)A) &= \sum_{j=1}^{n}(a_{pj} + aa_{qj})(-1)^{p+j}\det(A_{(ij)})\\ &= \sum_{j=1}^{n} a_{pj}(-1)^{p+j}\det(A_{(ij)}) + a\sum_{j=1}^{n} a_{qj}(-1)^{p+j}\det(A_{(ij)}).\end{aligned}$$

From equation (3.32) on page 69, we see that the second term is 0, and since the first term is just the determinant of A, we have

$$\det(E_{pq}(a)A) = \det(A). \tag{3.78}$$

(Again, this also follows from the general result in equation (3.81) below. I have shown the steps in the specific case because I think they help to see the effect of the elementary operator matrix.)

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

$$\mathrm{tr}(AB) = \mathrm{tr}(BA). \tag{3.79}$$

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

$$\mathrm{tr}(ABC) = \mathrm{tr}(BCA) = \mathrm{tr}(CAB) \tag{3.80}$$

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 (3.90).

3.2.5 The Determinant of a Cayley Product of Square Matrices

An important property of the determinant is

$$\det(AB) = \det(A)\det(B) \tag{3.81}$$

if A and B are square matrices conformable for multiplication. We see this by first forming

$$\det\left(\begin{bmatrix} I & A \\ 0 & I \end{bmatrix}\begin{bmatrix} A & 0 \\ -I & B \end{bmatrix}\right) = \det\left(\begin{bmatrix} 0 & AB \\ -I & B \end{bmatrix}\right) \tag{3.82}$$

and then observing from equation (3.39) 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:

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

Hence, applying equation (3.78) recursively, we have

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

and from equation (3.38) we have

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

and so finally we have equation (3.81).

From equation (3.81), we see that if A and B are square matrices conformable for multiplication, then

$$\det(AB) = \det(BA). \tag{3.83}$$

(Recall, in general, even in the case of square matrices, $AB \neq BA$.) This equation is to be contrasted with equation (3.79), $\mathrm{tr}(AB) = \mathrm{tr}(BA)$, which does not even require that the matrices be square. A simple counterexample for nonsquare matrices is $\det(xx^{\mathrm{T}}) \neq \det(x^{\mathrm{T}}x)$, 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 117, and observe that $\det(xx^{\mathrm{T}}) = 0$ 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 element 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 $x^{\mathrm{T}}A$ 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; in others, they are not. (R, for example sometimes does and sometimes does not; see the discussion beginning on page 572.) The alternative notation $x^{\mathrm{T}}y$ 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 $Z = \begin{bmatrix} z_{11} \\ \vdots \\ z_{m1} \end{bmatrix}$ or as $Z = [z_{11} \ldots z_{m1}]^{\mathrm{T}}$.

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

3.2.6.1 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:

$$Ax = \sum_{i=1}^{m} x_i a_i. \tag{3.84}$$

(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 $k \leq m$.

3.2.6.2 The Matrix as a Mapping on Vector Spaces

In this chapter we have considered matrices to be fundamental objects. Only after defining operations on matrices themselves have we defined an operation by a matrix on a vector. Another way of thinking about matrices is as a class of functions or mappings on vector spaces. In this approach, we give primacy to the vector spaces.

Let $\mathcal{V}_1$ and $\mathcal{V}_2$ be vector spaces of order m and n respectively. Then an $n \times m$ matrix A is a function from $\mathcal{V}_1$ to $\mathcal{V}_2$ defined for $x \in \mathcal{V}_1$ as

$$x \mapsto Ax. \tag{3.85}$$

Matrices are "transformations" of vectors. There is nothing essentially different in this development of concepts about matrices; it does, however, motivate terminology based in geometry that we will use from time to time ("rotations", "projections", and so on; see Sect. 5.3).

A matrix changes the "direction" of a vector. The cosine of the angle between the vector x and the vector Ax is the correlation

$$\text{Cor}(x, Ax) = \frac{(x - \bar{x})^{\mathrm{T}} A (x - \bar{x})}{(x - \bar{x})^{\mathrm{T}} (x - \bar{x})},$$

see page 51. (This expression is the Rayleigh quotient, $R_A(x - \bar{x})$, page 157.)

3.2.7 Outer Products

The *outer product* of the vectors x and y is the matrix

$$xy^{\mathrm{T}}. \tag{3.86}$$

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 $xy^{\mathrm{T}} = (yx^{\mathrm{T}})^{\mathrm{T}}$).

While the inner product is a mapping from $\mathbb{R}^n \times \mathbb{R}^n$ to $\mathbb{R}$, the outer product of two vectors is a mapping

$$\mathbb{R}^n \times \mathbb{R}^m \to \mathcal{M} \subseteq \mathbb{R}^{n \times m},$$

where $\mathcal{M}$ is the set of $n \times m$ matrices of rank one. (We will define and discuss matrix rank in Sect. 3.3, beginning on page 99. Also, see Exercise 3.14.)

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

$$xx^{\mathrm{T}}.$$

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 $A^{\mathrm{T}}B$ is a *matrix* even if both A and B are $n \times 1$ and so the result is 1×1. For the vectors x and y and matrix C, however, $x^{\mathrm{T}}y$ and $x^{\mathrm{T}}Cy$ 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

Given a matrix A of conformable shape, a variation of the vector dot product, $x^{\mathrm{T}}Ay$, is called a *bilinear form*, and the special bilinear form $x^{\mathrm{T}}Ax$ is called a *quadratic form*. Note

$$x^{\mathrm{T}}A^{\mathrm{T}}x = x^{\mathrm{T}}Ax \qquad \text{and} \qquad x^{\mathrm{T}}A^{\mathrm{T}}y = y^{\mathrm{T}}Ax \neq x^{\mathrm{T}}Ay \quad \text{in general.}$$

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 $x^{\mathrm{T}}Ax$ there is a unique symmetric matrix A_s such that $x^{\mathrm{T}}A_sx = x^{\mathrm{T}}Ax$—we generally work only with symmetric matrices in dealing with quadratic forms. (The matrix A_s is $\frac{1}{2}(A + A^{\mathrm{T}})$; see Exercise 3.3.) Quadratic forms correspond to sums of squares and hence play an important role in statistical applications.

3.2.8.1 Nonnegative Definite and Positive Definite Matrices

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

$$x^{\mathrm{T}}Ax \geq 0, \tag{3.87}$$

is called a *nonnegative definite matrix*. (There is another term, "positive semidefinite matrix" and its acronym PSD, that is often used to mean "nonnegative definite matrix", but the term is not used consistently in the literature. I will generally avoid the term "semidefinite".) 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

$$x^{\mathrm{T}}Ax > 0 \tag{3.88}$$

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.)

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 Sect. 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 (3.87) or (3.88).

3.2.8.2 Ordinal Relations among Symmetric Matrices

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 $A - B \succ 0$.

The $\succeq$ relationship is a *partial ordering* and the $\succ$ relationship is transitive; that is, if for conformable matrices, $A \succ B$ and $B \succ C$, then $A \succ C$ (See Exercise 8.2 on page 396; also compare ordinal relations among vectors, page 16.)

3.2.8.3 The Trace of Inner and Outer Products

The invariance of the trace to permutations of the factors in a product (equation (3.79)) 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 1×1 matrix), and because of the invariance, we have the very useful fact

$$\begin{aligned} x^{\mathrm{T}}Ay &= \mathrm{tr}(x^{\mathrm{T}}Ay) \\ &= \mathrm{tr}(Ayx^{\mathrm{T}}). \end{aligned} \tag{3.89}$$

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

$$x^{\mathrm{T}}Ax = \mathrm{tr}(Axx^{\mathrm{T}}). \tag{3.90}$$

In equation (3.90), 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,

$$x^{\mathrm{T}}x = \mathrm{tr}(xx^{\mathrm{T}}). \tag{3.91}$$

Also, by letting A be the identity in equation (3.90), we have an alternative way of showing that for a given vector x and any scalar a, the norm $\|x - a\|$ is minimized when $a = \bar{x}$:

$$(x-a)^{\mathrm{T}}(x-a) = \mathrm{tr}(x_{\mathrm{c}}x_{\mathrm{c}}^{\mathrm{T}}) + n(a-\bar{x})^2. \tag{3.92}$$

(Here, "$\bar{x}$" denotes the mean of the elements in x, and "x_{c}" is $x - \bar{x}$. Compare this with equation (2.71) on page 48.)

3.2.9 Anisometric Spaces

In Sect. 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 for real vectors the inner product is the bilinear form $x^{\mathrm{T}}Iy$, 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 $x^{\mathrm{T}}y$, we may use $x^{\mathrm{T}}Dy$, 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 367 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 $x^{\mathrm{T}}Ay$ may correspond more closely to the properties of the application than the standard inner product.

3.2.9.1 Conjugacy

We define orthogonality of two vectors real vectors x and y with respect to A by

$$x^{\mathrm{T}}Ay = 0. \tag{3.93}$$

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 $x^{\mathrm{T}}Ax$ for any symmetric positive definite matrix A. It is sometimes denoted by $\|x\|_A$:

$$\|x\|_A = \sqrt{x^{\mathrm{T}}Ax}. \tag{3.94}$$

It is easy to see that $\|x\|_A$ satisfies the definition of a norm given on page 25. If A is a diagonal matrix with elements $w_i \geq 0$, the elliptic norm is the weighted L_2 norm of equation (2.37).

The elliptic norm yields an *elliptic metric* in the usual way of defining a metric in terms of a norm. The distance between the real vectors x and y with respect to A is $\sqrt{(x-y)^{\mathrm{T}}A(x-y)}$. It is easy to see that this satisfies the definition of a metric given on page 32.

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 (8.67) on page 367.) If S is the covariance matrix, the Mahalanobis distance, with respect to that matrix, between the vectors x and y is

$$\sqrt{(x-y)^{\mathrm{T}}S^{-1}(x-y)}. \tag{3.95}$$

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*.

3.2.10.1 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 is often denoted by $\odot$; for two matrices $A_{n\times m}$ and $B_{n\times m}$ we have

$$A \odot B = \begin{bmatrix} a_{11}b_{11} & \dots & a_{1m}b_{1m} \\ \vdots & \dots & \vdots \\ a_{n1}b_{n1} & \dots & a_{nm}b_{nm} \end{bmatrix}.$$

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

$$\mathbb{R}^{n\times m} \times \mathbb{R}^{n\times m} \to \mathbb{R}^{n\times m}.$$

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

3.2.10.2 The Kronecker Product

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

$$A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1m}B \\ \vdots & \dots & \vdots \\ a_{n1}B & \dots & a_{nm}B \end{bmatrix}.$$

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

$$\mathbb{R}^{n\times m} \times \mathbb{R}^{p\times q} \to \mathbb{R}^{np\times mq}.$$

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 1×1 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,

$$(A \otimes B)_{i,j} = A_{\lfloor (i-1)/p \rfloor + 1,\ \lfloor (j-1)/q \rfloor + 1} B_{i - p\lfloor (i-1)/p \rfloor,\ j - q\lfloor (j-1)/q \rfloor}. \tag{3.96}$$

Some additional properties of Kronecker products that are immediate results of the definition are, assuming the matrices are conformable for the indicated operations,

$$\begin{aligned} (aA) \otimes (bB) &= ab(A \otimes B) \\ &= (abA) \otimes B \\ &= A \otimes (abB), \text{ for scalars } a, b, \end{aligned} \tag{3.97}$$

$$(A+B)\otimes(C) = A\otimes C + B\otimes C, \tag{3.98}$$

$$(A\otimes B)\otimes C = A\otimes(B\otimes C), \tag{3.99}$$

$$(A\otimes B)^{\mathrm{T}} = A^{\mathrm{T}}\otimes B^{\mathrm{T}}, \tag{3.100}$$

$$(A\otimes B)(C\otimes D) = AC\otimes BD. \tag{3.101}$$

$$I\otimes A = \mathrm{diag}(A,\ldots,A). \tag{3.102}$$

$$A\otimes I = (a_{ij}I)\,. \tag{3.103}$$

These properties are all easy to see by using equation (3.96) 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

$$aA_{[(i-1)/p]+1,\,[(j-1)/q]+1}bB_{i-p[(i-1)/p],\,j-q[(j-1)/q]}$$

and that on the right-hand side is

$$abA_{[(i-1)/p]+1,\,[(j-1)/q]+1}B_{i-p[(i-1)/p],\,j-q[(j-1)/q]}.$$

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:

$$\det(A\otimes B) = \det(A)^m\det(B)^n. \tag{3.104}$$

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.

From equation (3.100) we see that the Kronecker product of symmetric matrices is symmetric.

Another property of the Kronecker product of square matrices is

$$\mathrm{tr}(A\otimes B) = \mathrm{tr}(A)\mathrm{tr}(B). \tag{3.105}$$

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, Σ, and Ψ can be expressed in terms of an ordinary np-variate normal random variable $Y = \mathrm{vec}(X)$ with parameters $\mathrm{vec}(M)$ and $\Sigma \otimes \Psi$. (We discuss matrix random variables briefly on page 220. For a fuller discussion, the reader is referred to a text on matrix random variables such as Carmeli 1983, or Kollo and von Rosen 2005.)

A useful relationship between the vec function and Kronecker multiplication is

$$\mathrm{vec}(ABC) = (C^{\mathrm{T}} \otimes A)\mathrm{vec}(B) \tag{3.106}$$

for matrices A, B, and C that are conformable for the multiplication indicated. This is easy to show and is left as an exercise.

3.2.10.3 The Inner Product of Matrices

An inner 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

$$\langle A, B \rangle = \sum_{j=1}^{m} \langle a_j, b_j \rangle. \tag{3.107}$$

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 `dot` function, can refer either to $1 \times m$ matrix consisting of the individual terms in the sum in equation (3.107), 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 `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 (3.43) on page 75, 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 real matrices, equation (3.107) can be written as

$$\langle A, B \rangle = \sum_{j=1}^{m} a_j^{\mathrm{T}} b_j. \tag{3.108}$$

As in the case of the product of vectors, the product of matrices defined as in equation (3.108) over the complex field is not an inner product because the first property (on page 24 or as listed below) does not hold.

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 24:

- 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 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

$$\mathbb{R}^{n\times m} \times \mathbb{R}^{n\times m} \to \mathbb{R}.$$

We see from the definition above that the inner product of real matrices satisfies

$$\langle A, B\rangle = \mathrm{tr}(A^{\mathrm{T}}B), \tag{3.109}$$

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 for real matrices

$$\langle A, B\rangle = \langle A^{\mathrm{T}}, B^{\mathrm{T}}\rangle. \tag{3.110}$$

Like any inner product, inner products of matrices obey the Cauchy-Schwarz inequality (see inequality (2.26), page 24),

$$\langle A, B\rangle \leq \langle A, A\rangle^{\frac{1}{2}}\langle B, B\rangle^{\frac{1}{2}}, \tag{3.111}$$

with equality holding only if $A = 0$ or $B = sA$ for some scalar s.

3.2.10.4 Orthonormal Matrices

In Sect. 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

$$\langle A, B\rangle = 0. \tag{3.112}$$

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 Sect. 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. "Orthonormal", on the other hand, refers to the binary property.

3.2.10.5 Orthonormal Basis: Fourier Expansion

On page 64 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 $\mathcal{M} \subseteq \mathbb{R}^{n\times m}$ with the property that $\langle U_i, U_j\rangle = 0$ for $i \neq j$ and $\langle U_i, U_i\rangle = 1$, then the set is an orthonormal basis set.

If A is an $n \times m$ matrix, with the Fourier expansion

$$A = \sum_{i=1}^{k} c_i U_i, \tag{3.113}$$

we have, analogous to equation (2.59) on page 41,

$$c_i = \langle A, U_i \rangle. \tag{3.114}$$

The c_i have the same properties (such as the Parseval identity, equation (2.60), 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 (3.113) as in equation (2.63). The objective of course is to reduce the truncation error, and the optimality of the Fourier expansion in this regard discussed on page 42 holds in the matrix case as well. (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 Sect. 3.9 beginning on page 164.)

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

$$\text{rank}(aA) = \text{rank}(A). \tag{3.115}$$

From results developed in Sect. 2.1, we see that for the $n \times m$ matrix A,

$$\text{rank}(A) \leq \min(n, m). \tag{3.116}$$

The rank of the zero matrix is 0, and the rank of any nonzero matrix is positive.

3.3.1 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,

$$B = \begin{bmatrix} W_{p\times q} & X_{p\times m-q} \\ Y_{n-p\times q} & Z_{n-p\times m-q} \end{bmatrix}, \tag{3.117}$$

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 $a \neq 0$ such that $Wa = 0$. Now, since the rows of R are the full set of linearly independent rows, any row in $[Y|Z]$ 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

$$\text{rank}(A) = \dim(\mathcal{V}(A)), \tag{3.118}$$

$$\text{rank}(A^{\text{T}}) = \text{rank}(A), \tag{3.119}$$

$$\dim(\mathcal{V}(A^{\text{T}})) = \dim(\mathcal{V}(A)). \tag{3.120}$$

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

3.3.2 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 3.9. (It's easy!)

A positive definite matrix is nonsingular. The proof of this is Exercise 3.10.

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

3.3.3 Rank of Elementary Operator Matrices and Matrix Products Involving Them

Because within any set of rows of an elementary operator matrix (see Sect. 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 elementary 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; therefore, 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,

$$\operatorname{rank}(PAQ) = \operatorname{rank}(A). \tag{3.121}$$

On page 113, we will extend this result to products by any full rank matrices.

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

The partitioning in equation (3.117) leads us to consider partitioned matrices in more detail.

3.3.4.1 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 Sect. 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

$$\operatorname{rank}(A_{ij}) \leq \operatorname{rank}(A). \tag{3.122}$$

Furthermore, we see that

$$\operatorname{rank}(A) \leq \operatorname{rank}([A_{11}|A_{12}]) + \operatorname{rank}([A_{21}|A_{22}]) \tag{3.123}$$

because $\operatorname{rank}(A)$ 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

$$\operatorname{rank}(A) \leq \operatorname{rank}\left(\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}\right) + \operatorname{rank}\left(\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}\right). \tag{3.124}$$

In a similar manner, by merely counting the number of independent rows, we see that, if

$$\mathcal{V}\left([A_{11}|A_{12}]^{\mathrm{T}}\right) \perp \mathcal{V}\left([A_{21}|A_{22}]^{\mathrm{T}}\right),$$

then

$$\operatorname{rank}(A) = \operatorname{rank}([A_{11}|A_{12}]) + \operatorname{rank}([A_{21}|A_{22}]); \tag{3.125}$$

and, if

$$\mathcal{V}\left(\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}\right) \perp \mathcal{V}\left(\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}\right),$$

then

$$\operatorname{rank}(A) = \operatorname{rank}\left(\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}\right) + \operatorname{rank}\left(\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}\right). \tag{3.126}$$

3.3.4.2 An Upper Bound on the Rank of Products of Matrices

Because the columns of the product AB are linear combinations of the columns of A, it is clear that

$$\mathcal{V}(AB) \subseteq \mathcal{V}(A). \tag{3.127}$$

The rank of the product of two matrices is less than or equal to the lesser of the ranks of the two:

$$\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B)). \tag{3.128}$$

This follows from equation (3.127). We can also 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 inequality (3.128), we see that the rank of a nonzero outer product matrix (that is, a matrix formed as the outer product of two nonzero vectors) is 1.

The bound in inequality (3.128) is sharp, as we can see by exhibiting matrices A and B such that $\text{rank}(AB) = \min(\text{rank}(A), \text{rank}(B))$, as you are asked to do in Exercise 3.12a.

Inequality (3.128) provides a useful upper bound on $\text{rank}(AB)$. In Sect. 3.3.11, we will develop a lower bound on $\text{rank}(AB)$.

3.3.4.3 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,

$$\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B). \tag{3.129}$$

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 (3.128), which in turn is $\leq \text{rank}(A) + \text{rank}(B)$ by equation (3.124).

The bound in inequality (3.129) is sharp, as we can see by exhibiting matrices A and B such that $\text{rank}(A + B) = \text{rank}(A) + \text{rank}(B)$, as you are asked to do in Exercise 3.12c.

Using inequality (3.129) 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 (3.129) 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

$$\text{rank}(A+B) \geq |\text{rank}(A) - \text{rank}(B)|. \tag{3.130}$$

The bound in inequality (3.130) is sharp, as we can see by exhibiting matrices A and B such that $\text{rank}(A+B) = |\text{rank}(A) - \text{rank}(B)|$, as you are asked to do in Exercise 3.12d.

3.3.5 Full Rank Partitioning

As we saw above, the matrix W in the partitioned B in equation (3.117) is square; in fact, it is $r \times r$, where r is the rank of B:

$$B = \begin{bmatrix} W_{r\times r} & X_{r\times m-r} \\ Y_{n-r\times r} & Z_{n-r\times m-r} \end{bmatrix}. \tag{3.131}$$

This is called a *full rank partitioning* of B.

The matrix B in equation (3.131) 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 (3.131) by using permutation matrices as in equation (3.57), 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 $E_{(\pi_2)}$,

$$B = E_{(\pi_1)} A E_{(\pi_2)}. \tag{3.132}$$

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.

The partitioning in equation (3.131) is of general interest, and we will use this type of partitioning often. We express an equivalent partitioning of a transformed matrix in equation (3.151) 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

$$E_{(\pi_r)} A E_{(\pi_c)} = \begin{bmatrix} S_{q\times q} & T_{q\times m-q} \\ U_{n-q\times r} & V_{n-q\times m-q} \end{bmatrix}, \tag{3.133}$$

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.)

3.3.6 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.

3.3.6.1 Solutions of Linear Equations

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

$$\begin{array}{ccc} a_{11}x_1 + \cdots + a_{1m}x_m \stackrel{?}{=} b_1 \\ \vdots \qquad\qquad \vdots \qquad \vdots \\ a_{n1}x_1 + \cdots + a_{nm}x_m \stackrel{?}{=} b_n \end{array} \tag{3.134}$$

or

$$Ax \stackrel{?}{=} b. \tag{3.135}$$

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 (3.84), 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,

$$y^{\mathrm{T}}Ax = 0 \Longleftrightarrow y^{\mathrm{T}}b = 0. \tag{3.136}$$

3.3.6.2 Consistent Systems

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

$$\mathrm{rank}([A \mid b]) = \mathrm{rank}(A). \tag{3.137}$$

We can see this following the argument above that $b \in \mathcal{V}(A)$; that is, 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, and furthermore, the linear combination is a solution to the system $Ax = b$. (Note, of course, that it is not necessary that it be a unique linear combination.)

Equation (3.137) implies the equivalence of the conditions

$$[A \mid b]y = 0 \text{ for some } y \neq 0 \quad \Leftrightarrow \quad Ax = 0 \text{ for some } x \neq 0. \tag{3.138}$$

A special case that yields equation (3.137) for any b is

$$\operatorname{rank}(A_{n\times m}) = n, \tag{3.139}$$

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 (3.116)). A square system in which A is nonsingular is clearly consistent. (The condition of consistency is also called "compatibility" of the system; that is, the linear system $Ax = b$ is said to be *compatible* if it is 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, and in that case the system is also said to be compatible.

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 $c^{\mathrm{T}}A = 0$, then $c^{\mathrm{T}}B = 0$. To see this, let c be such that $c^{\mathrm{T}}A = 0$. We then have $c^{\mathrm{T}}AX = c^{\mathrm{T}}B = 0$, and so the same linear relationship that exists among the rows of A exists among the rows of B.

As above for $Ax = b$, we also see that the system $AX = B$ is consistent if and only if any of the following conditions hold:

$$\mathcal{V}(B) \subseteq \mathcal{V}(A) \tag{3.140}$$

$$\mathcal{V}([A \mid B]) = \mathcal{V}(A) \tag{3.141}$$

$$\operatorname{rank}([A \mid B]) = \operatorname{rank}(A). \tag{3.142}$$

These relations imply that if $AX = B$ is consistent, then for any conformable vector c,

$$c^{\mathrm{T}}A = 0 \iff c^{\mathrm{T}}B = 0. \tag{3.143}$$

It is clear that this condition also implies that $AX = B$ is consistent (because right-hand implication of the condition implies the relationship (3.140)).

We discuss methods for solving linear systems in Sect. 3.5 and in Chap. 6. In the next section, we consider a special case of $n \times n$ (square) A when equation (3.139) is satisfied (that is, when A is nonsingular).

3.3.6.3 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 (3.137).

We can represent all n such systems as

$$A\left[x_1|\cdots|x_n\right] = \left[e_1|\cdots|e_n\right]$$

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

$$A^{-1}A = AA^{-1} = I_n. \tag{3.144}$$

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

$$(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}, \tag{3.145}$$

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

$$A^{-\mathrm{T}}$$

to denote the inverse of the transpose.

In the linear system (3.135), if $n = m$ and A is nonsingular, the solution is

$$x = A^{-1}b. \tag{3.146}$$

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 "\" to indicate the combined operations of inversion and multiplication on the left; that is, $B\backslash A$ is the same as $B^{-1}A$. The solution given in equation (3.146) is also sometimes represented as $A\backslash b$.

We discuss the solution of systems of equations in Chap. 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 $A\backslash b$, 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.*

3.3.6.4 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 $\text{rank}([A \,|\, e_i]) = \text{rank}(A)$, 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

$$A\left[x_1|\cdots|x_n\right] = \left[e_1|\cdots|e_n\right]$$

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

$$A^{-\text{R}}.$$

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

$$A^{-\text{L}}.$$

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

$$A^{-\text{R}} = A^{\text{T}}(AA^{\text{T}})^{-1}. \tag{3.147}$$

Likewise, if $A^{\text{T}}A$ is of full rank, the left inverse of A is

$$A^{-\text{L}} = (A^{\text{T}}A)^{-1}A^{\text{T}}. \tag{3.148}$$

3.3.7 Full Rank Factorization

For a given matrix A, it is often of interest to find matrices $A_1, \ldots, A_k$ such that $A_1, \ldots, A_k$ have some useful properties and $A = A_1 \cdots A_k$. This is called a *factorization* or *decomposition* of A. (We will usually use these two words interchangeably; that is, by "decomposition", we will usually mean "multiplicative decomposition". Occasionally we will be interested in an additive decomposition of a matrix, as in Cochran's theorem, discussed on page 401 and later in Sect. 9.2.3.)

In most cases, the number of factors in $A = A_1 \cdots A_k$ is either 2 or 3. In this chapter, we will discuss some factorizations as they arise naturally in the development, and then in Chap. 5 we will discuss factorizations in more detail.

The partitioning of an $n \times m$ matrix as in equation (3.131) on page 104 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 $C = \begin{bmatrix} W \\ Y \end{bmatrix}$ span the full column space of B.

Therefore, for some T, we have $[Y|Z] = TR$, and for some S, we have $\begin{bmatrix} X \\ Z \end{bmatrix} = CS$. 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

$$\begin{aligned} B &= \begin{bmatrix} W & X \\ Y & YW^{-1}X \end{bmatrix} \\ &= \begin{bmatrix} I \\ YW^{-1} \end{bmatrix} W \begin{bmatrix} I \mid W^{-1}X \end{bmatrix}. \end{aligned} \tag{3.149}$$

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

$$B = \begin{bmatrix} W \\ Y \end{bmatrix} \begin{bmatrix} I \mid W^{-1}X \end{bmatrix} = \begin{bmatrix} I \\ YW^{-1} \end{bmatrix} \begin{bmatrix} W \mid X \end{bmatrix}.$$

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,

$$A = \begin{bmatrix} Q_1 W \\ Q_2 Y \end{bmatrix} \left[P_1 \mid W^{-1} X P_2 \right]$$
$$= \begin{bmatrix} Q_1 \\ Q_2 Y W^{-1} \end{bmatrix} \left[W P_1 \mid X P_2 \right],$$

both of which are in the general form

$$A_{n\times m} = L_{n\times r}\, R_{r\times m}, \tag{3.150}$$

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 Chap. 5 that have more practical uses in computations.

3.3.8 Equivalent Matrices

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

3.3.8.1 Equivalent Canonical Forms

For any $n\times m$ matrix A with $\text{rank}(A) = r > 0$, by combining the permutations that yield equation (3.131) with other operations, we have, for some matrices P and Q that are products of various elementary operator matrices,

$$PAQ = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}. \tag{3.151}$$

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, $(E_{i1} A E_{1j})_{11} = a_{ij}$. 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 (3.62), 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

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & X & \\ 0 & & & \end{bmatrix}. \tag{3.152}$$

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 (3.151).

The matrices P and Q in equation (3.151) 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 (3.151) 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
- if k is such that $r_{ik} \neq 0$ and $r_{il} = 0$ for $l < k$, then $r_{i+1,j} = 0$ for $j \leq k$.

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 352.) Another, more specific, equivalent form, called the *Jordan form*, is a special row echelon form based on eigenvalues, which we show on page 151.

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.

3.3.8.2 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

$$\text{rank}(AB) = \text{rank}(B) \tag{3.153}$$

and

$$\text{rank}(CA) = \text{rank}(C). \tag{3.154}$$

This is true because, for a given conformable matrix B, by the inequality (3.128), 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, $\text{rank}(AB) =$

rank(B). Likewise, for a square full rank matrix A, we have rank(CA) = rank(C). (Here, we should recall that all matrices are real.)

On page 113, we give a more general result for products with general full rank matrices.

3.3.8.3 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 Sect. 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 (3.151), have inverses. From an equivalent canonical form of a matrix A with rank r, we therefore have the equivalent canonical factorization of A:

$$A = P^{-1} \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} Q^{-1}. \tag{3.155}$$

A factorization based on an equivalent canonical form is also a full rank factorization and could be written in the same form as equation (3.150).

3.3.8.4 Equivalent Forms of Symmetric Matrices

If A is symmetric, the equivalent form in equation (3.151) can be written as $PAP^{\mathrm{T}} = \mathrm{diag}(I_r, 0)$ and the equivalent canonical factorization of A in equation (3.155) can be written as

$$A = P^{-1} \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} P^{-\mathrm{T}}. \tag{3.156}$$

These facts follow from the same process that yielded equation (3.151) for a general matrix.

Also a full rank factorization for a symmetric matrix, as in equation (3.150), can be given as

$$A = LL^{\mathrm{T}}. \tag{3.157}$$

3.3.9 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 (3.128). 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.

3.3.9.1 Products with a General Full Rank Matrix

If C is a full column rank matrix and if B is a matrix conformable for the multiplication CB, then

$$\text{rank}(CB) = \text{rank}(B). \tag{3.158}$$

To see this, consider a full rank $n \times m$ matrix C with $\text{rank}(C) = m$ (that is, $m \leq n$) and let B be conformable for the multiplication CB. Because C is of full column rank, it has a left inverse (see page 108); call it $C^{-\text{L}}$, and so $C^{-\text{L}}C = I_m$. From inequality (3.128), we have $\text{rank}(CB) \leq \text{rank}(B)$, and applying the inequality again, we have $\text{rank}(B) = \text{rank}(C^{-\text{L}}CB) \leq \text{rank}(CB)$; hence $\text{rank}(CB) = \text{rank}(B)$.

If R is a full row rank matrix and if B is a matrix conformable for the multiplication BR, then

$$\text{rank}(BR) = \text{rank}(B). \tag{3.159}$$

To see this, consider a full rank $n \times m$ matrix R with $\text{rank}(R) = n$ (that is, $n \leq m$) and let B be conformable for the multiplication BR. Because R is of full row rank, it has a right inverse; call it $R^{-\text{R}}$, and so $RR^{-\text{R}} = I_n$. From inequality (3.128), we have $\text{rank}(BR) \leq \text{rank}(B)$, and applying the inequality again, we have $\text{rank}(B) = \text{rank}(BRR^{-\text{L}}) \leq \text{rank}(BR)$; hence $\text{rank}(BR) = \text{rank}(B)$.

To state this more simply:

- Premultiplication of a given matrix by a full column rank matrix yields a product with the same rank as the given matrix, and postmultiplication of a given matrix by a full row rank matrix yields a product with the same rank as the given matrix.

From this we see that, given any matrix B, if A is a square matrix of full rank that is compatible for the multiplication $AB = D$, then B and D are equivalent matrices. (And, of course, a similar statement for postmultiplication by a full-rank matrix holds.)

Furthermore, if the matrix B is square and A is a square matrix of the same order that is full rank, then

$$\text{rank}(AB) = \text{rank}(BA) = \text{rank}(B). \tag{3.160}$$

3.3.9.2 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 A is $n \times n$ and positive definite, and C is $n \times m$ and of rank m (hence, $m \leq n$), then $C^{\text{T}}AC$ is positive definite. (Recall from inequality (3.88) that a matrix A is positive definite if it is symmetric and for any $x \neq 0$, $x^{\text{T}}Ax > 0$.)

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

$$\begin{aligned} x^{\mathrm{T}}(C^{\mathrm{T}}AC)x &= (Cx)^{\mathrm{T}}A(Cx) \\ &= y^{\mathrm{T}}Ay \\ &> 0. \end{aligned} \tag{3.161}$$

Therefore, since $C^{\mathrm{T}}AC$ is symmetric,

- if A is positive definite and C is of full column rank, then $C^{\mathrm{T}}AC$ is positive definite.

Furthermore, we have the converse:

- if $C^{\mathrm{T}}AC$ is positive definite, then C is of full column rank,

for otherwise there exists an $x \neq 0$ such that $Cx = 0$, and so $x^{\mathrm{T}}(C^{\mathrm{T}}AC)x = 0$.

3.3.9.3 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 $\mathcal{G}L(n)$. The *order* of the group is n, the order of the square matrices in the group. General group-theoretic properties can be used in the derivation of properties of these full-rank matrices. Note that this group is not commutative.

We note that all matrices in the general linear group of order n are equivalent.

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 (otherwise, A^0 does not exist).

The $n \times n$ elementary operator matrices are members of the general linear group $\mathcal{G}L(n)$.

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 $\mathcal{A}L(n)$. A subset of the elements of

the affine group with the same first element, together with the axpy operator, constitute a *quotient space*.

3.3.10 Gramian Matrices: Products of the Form $A^{\mathrm{T}}A$

Given a real matrix A, an important matrix product is $A^{\mathrm{T}}A$. (This is called a *Gramian matrix*, or just a *Gram matrix*. We will discuss this kind of matrix in more detail beginning on page 359. I should note here that this is not a definition of "Gramian" or "Gram"; these terms have more general meanings, but they do include any matrix expressible as $A^{\mathrm{T}}A$.)

We first note that AA^{T} is a Gramian matrix, and has the same properties as $A^{\mathrm{T}}A$ with any dependencies on A being replaced with dependencies on A^{T}.

3.3.10.1 General Properties of Gramian Matrices

Gramian matrices have several interesting properties. First of all, we note that for any A, because

$$(A^{\mathrm{T}}A)_{ij} = a_{*i}^{\mathrm{T}}a_{*j} = a_{*j}^{\mathrm{T}}a_{*i} = (A^{\mathrm{T}}A)_{ji} \quad \text{(recall notation, page 600)},$$

$A^{\mathrm{T}}A$ is symmetric, and hence has all of the useful properties of symmetric matrices. (These properties are shown in various places in this book, but are summarized conveniently in Sect. 8.2 beginning on page 340.) Furthermore, $A^{\mathrm{T}}A$ is nonnegative definite, as we see by observing that for any y, $y^{\mathrm{T}}(A^{\mathrm{T}}A)y = (Ay)^{\mathrm{T}}(Ay) \geq 0$.

Another interesting property of a Gramian matrix is that, for any matrices C and D (that are conformable for the operations indicated),

$$CA^{\mathrm{T}}A = DA^{\mathrm{T}}A \iff CA^{\mathrm{T}} = DA^{\mathrm{T}}. \tag{3.162}$$

The implication from right to left is obvious, and we can see the left to right implication by writing

$$(CA^{\mathrm{T}}A - DA^{\mathrm{T}}A)(C^{\mathrm{T}} - D^{\mathrm{T}}) = (CA^{\mathrm{T}} - DA^{\mathrm{T}})(CA^{\mathrm{T}} - DA^{\mathrm{T}})^{\mathrm{T}},$$

and then observing that if the left-hand side is null, then so is the right-hand side, and if the right-hand side is null, then $CA^{\mathrm{T}} - DA^{\mathrm{T}} = 0$ because $A^{\mathrm{T}}A = 0 \implies A = 0$, as above.

Similarly, we have

$$A^{\mathrm{T}}AC = A^{\mathrm{T}}AD \iff AC = AD. \tag{3.163}$$

3.3.10.2 Rank of $A^{\mathrm{T}}A$

Consider the linear system $A^{\mathrm{T}}AX = A^{\mathrm{T}}B$. Suppose that c is such that $c^{\mathrm{T}}A^{\mathrm{T}}A = 0$. Then by (3.162), $c^{\mathrm{T}}A^{\mathrm{T}} = 0$, which by (3.143) on page 106, implies

that $A^{\mathrm{T}}AX = A^{\mathrm{T}}B$ is consistent. Letting $B = I$, we have that $A^{\mathrm{T}}AX = A^{\mathrm{T}}$ is consistent.

Now if $A^{\mathrm{T}}AX = A^{\mathrm{T}}$, for any conformable matrix K,

$$\mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}}) = \mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}}AX).$$

By (3.127) on page 103, $\mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}}AX) \subseteq \mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}}A)$ and $\mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}}A) \subseteq \mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}})$; hence $\mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}}A) = \mathcal{V}(K^{\mathrm{T}}A^{\mathrm{T}})$. By similar arguments applied to the transposes we have $\mathcal{V}(A^{\mathrm{T}}AK) = \mathcal{V}(AK)$.

With $K = I$, this yields

$$\operatorname{rank}(A^{\mathrm{T}}A) = \operatorname{rank}(A). \tag{3.164}$$

In a similar manner, we have $\operatorname{rank}(AA^{\mathrm{T}}) = \operatorname{rank}(A)$, and hence,

$$\operatorname{rank}(A^{\mathrm{T}}A) = \operatorname{rank}(AA^{\mathrm{T}}). \tag{3.165}$$

It is clear from the statements above that $(A^{\mathrm{T}}A)$ is of full rank if and only if A is of full column rank.

We also see that $A^{\mathrm{T}}A$ is positive definite, that is, for any $y \neq 0$ $y^{\mathrm{T}}A^{\mathrm{T}}Ay > 0$, if and only if A is of full column rank. This follows from (3.167), and if A is of full column rank, $Ay = 0 \Rightarrow y = 0$.

3.3.10.3 Zero Matrices and Equations Involving Gramians

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

$$\operatorname{tr}(A^{\mathrm{T}}A) = 0 \;\Leftrightarrow\; A = 0 \tag{3.166}$$

and

$$A^{\mathrm{T}}A = 0 \;\Leftrightarrow\; A = 0. \tag{3.167}$$

Now consider the equation $A^{\mathrm{T}}A = 0$. We have for any conformable B and C

$$A^{\mathrm{T}}A(B - C) = 0.$$

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

$$(AB - AC)^{\mathrm{T}}(AB - AC) = 0;$$

hence, from (3.167), we have $AB - AC = 0$. Furthermore, if $AB - AC = 0$, then clearly $A^{\mathrm{T}}A(B - C) = 0$. We therefore conclude that

$$A^{\mathrm{T}}AB = A^{\mathrm{T}}AC \;\Leftrightarrow\; AB = AC. \tag{3.168}$$

By the same argument, we have

$$BA^{\mathrm{T}}A = CA^{\mathrm{T}}A \;\Leftrightarrow\; BA^{\mathrm{T}} = CA^{\mathrm{T}}.$$

From equation (3.164), we have another useful fact for Gramian matrices. The system

$$A^{\mathrm{T}}Ax = A^{\mathrm{T}}b \tag{3.169}$$

is consistent for any A and b.

3.3.11 A Lower Bound on the Rank of a Matrix Product

Equation (3.128) 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 (3.155), 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

$$\operatorname{rank}(AB) \geq \operatorname{rank}(A) + \operatorname{rank}(B) - n. \tag{3.170}$$

We see this by first letting $r = \operatorname{rank}(A)$, letting P and Q be matrices that form an equivalent canonical form of A (see equation (3.155)), 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, $\operatorname{rank}(C) = \operatorname{rank}(I_{n-r}) = n - \operatorname{rank}(A)$. We now develop an upper bound on $\operatorname{rank}(B)$,

$$\begin{aligned}
\operatorname{rank}(B) &= \operatorname{rank}(P^{-1}Q^{-1}B) \\
&= \operatorname{rank}(AB + CB) \\
&\leq \operatorname{rank}(AB) + \operatorname{rank}(CB), \text{ by equation (3.129)} \\
&\leq \operatorname{rank}(AB) + \operatorname{rank}(C), \text{ by equation (3.128)} \\
&= \operatorname{rank}(AB) + n - \operatorname{rank}(A),
\end{aligned}$$

yielding (3.170), a lower bound on $\operatorname{rank}(AB)$.

The inequality (3.170) is called *Sylvester's law of nullity*. It provides a lower bound on $\operatorname{rank}(AB)$ to go with the upper bound of inequality (3.128), $\min(\operatorname{rank}(A), \operatorname{rank}(B))$. The bound in inequality (3.170) is also sharp, as we can see by exhibiting matrices A and B such that $\operatorname{rank}(AB) = \operatorname{rank}(A) + \operatorname{rank}(B) - n$, as you are asked to do in Exercise 3.12b.

3.3.12 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,

$$\det(A^{-1}) = (\det(A))^{-1}, \tag{3.171}$$

and so

- $\det(A) = 0$ if and only if A is singular.

(From the definition of the determinant in equation (3.24), we see that the determinant of any finite-dimensional matrix with finite elements is finite. We implicitly assume that the elements are finite.)

For an $n \times n$ matrix with $n \geq 2$ whose determinant is nonzero, from equation (3.34) we have

$$A^{-1} = \frac{1}{\det(A)}\text{adj}(A). \tag{3.172}$$

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

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

See Exercise 3.15 on page 179 for an interesting consequence of this.

3.3.13 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.

3.3.13.1 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,

$$(AB)^{-1} = B^{-1}A^{-1}. \tag{3.173}$$

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.

3.3.13.2 Inverses of Kronecker Products of Matrices

If A and B are square full rank matrices, then

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}. \tag{3.174}$$

We can see this by multiplying $A^{-1} \otimes B^{-1}$ and $A \otimes B$ using equation (3.101) on page 96.

3.3.13.3 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 (3.173). We get

$$(I + A)^{-1} = A^{-1}(I + A^{-1})^{-1}. \tag{3.175}$$

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 (3.173) and (3.175); see Exercise 3.16):

$$A(I + A)^{-1} = (I + A^{-1})^{-1}, \tag{3.176}$$

$$(A + B)^{-1} = A^{-1} - A^{-1}(A^{-1} + B^{-1})^{-1}A^{-1}, \tag{3.177}$$

$$(A + BB^{\mathrm{T}})^{-1}B = A^{-1}B(I + B^{\mathrm{T}}A^{-1}B)^{-1}, \tag{3.178}$$

$$(A^{-1} + B^{-1})^{-1} = A(A + B)^{-1}B, \tag{3.179}$$

$$A - A(A + B)^{-1}A = B - B(A + B)^{-1}B, \tag{3.180}$$

$$A^{-1} + B^{-1} = A^{-1}(A + B)B^{-1}, \tag{3.181}$$

$$(I + AB)^{-1} = I - A(I + BA)^{-1}B, \tag{3.182}$$

$$(I + AB)^{-1}A = A(I + BA)^{-1}. \tag{3.183}$$

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 Sect. 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

$$(A + CBD)^{-1} = A^{-1} - A^{-1}C(B^{-1} + DA^{-1}C)^{-1}DA^{-1}. \tag{3.184}$$

This can be derived from equation (3.176), which is a special case of it. We can verify this by multiplication (Exercise 3.17).

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 $(A + bc^{\mathrm{T}})$ is full rank, then

$$(A + bc^{\mathrm{T}})^{-1} = A^{-1} - \frac{A^{-1}bc^{\mathrm{T}}A^{-1}}{1 + c^{\mathrm{T}}A^{-1}b}. \tag{3.185}$$

This fact has application in adding an observation to a least squares linear regression problem (page 418).

3.3.13.4 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 Sect. 3.9 on page 164, 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 (3.53) on page 78 for a square matrix A, we have

$$(I - A)^{-1} = I + A + A^2 + A^3 + \cdots, \quad \text{if } \|A\| < 1. \tag{3.186}$$

We include this equation here because of its relation to equations (3.176) through (3.182). We will discuss it further on page 171, 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 (3.176) through (3.182) and (3.186) 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 354).

3.3.14 Inverses of Matrices with Special Forms

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

- The inverse of a nonsingular symmetric matrix is symmetric.
- The inverse of a 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). See also Exercise 3.19 (and the hint).

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

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

3.3.15 Determining the Rank of a Matrix

Although the equivalent canonical form (3.151) 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 $\mathbb{R}^{n\times m} \to \mathbb{Z}_+$, where $\mathbb{Z}_+$ represents the positive integers. Such a function is often difficult to compute because the domain is dense and the range is sparse. Small changes in the domain may result in large discontinuous changes in the function value. (In Hadamard's sense, the problem is *ill-posed*.) The common way that the rank of a matrix is evaluated is by use of the QR decomposition; see page 252.

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 Sects. 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

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{3.187}$$

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

$$Z = A_{22} - A_{21}A_{11}^{-1}A_{12}, \tag{3.188}$$

which is called the *Schur complement* of A_{11} in A.

We first observe from equation (3.149) that if equation (3.187) represents a full rank partitioning (that is, if the rank of A_{11} is the same as the rank of A), then

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{21}A_{11}^{-1}A_{12} \end{bmatrix}, \tag{3.189}$$

and $Z = 0$.

There are other useful properties of the Schur complement, 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 Σ partitioned like A in equation (3.187). (This of course means A is symmetrical, and so $A_{12} = A_{21}^{\mathrm{T}}$.) 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 4.12 on page 224 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 3.20, page 180) that the inverse of A is given by

$$A^{-1} = \begin{bmatrix} A_{11}^{-1} + A_{11}^{-1}A_{12}Z^{-1}A_{21}A_{11}^{-1} & -A_{11}^{-1}A_{12}Z^{-1} \\ -Z^{-1}A_{21}A_{11}^{-1} & Z^{-1} \end{bmatrix}, \tag{3.190}$$

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

If

$$A = [X\ y]^{\mathrm{T}}[X\ y]$$

and is partitioned as in equation (3.55) on page 79 and X is of full column rank, then the Schur complement of $X^{\mathrm{T}}X$ in $[X\ y]^{\mathrm{T}}[X\ y]$ is

$$y^{\mathrm{T}}y - y^{\mathrm{T}}X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y. \tag{3.191}$$

This particular partitioning is useful in linear regression analysis (see, for example, page 363), where this Schur complement is the residual sum of squares and the more general Wishart distribution mentioned above reduces to a chi-squared distribution. (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

$$\det(A) = \det(A_{11}) \det\left(A_{22} - A_{21}A_{11}^{-1}A_{12}\right); \tag{3.192}$$

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 (3.38) on page 71 and the factorization

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & 0 \\ A_{21} & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{bmatrix} \begin{bmatrix} I & A_{11}^{-1}A_{12} \\ 0 & I \end{bmatrix}. \tag{3.193}$$

The factorization in equation (3.193) 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 (3.84), 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 *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 Chap. 6 after we have discussed matrix factorizations later in this chapter and in Chap. 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 (3.137)) has a solution. For consistent systems that are singular or not square, the *generalized inverse* is an important concept. We introduce it in this section but defer its discussion to Sect. 3.6.

3.5.1.1 Underdetermined Systems

A consistent system in which $\text{rank}(A) < m$ is said to be *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.

3.5.1.2 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 $\text{rank}([A \mid b]) > \text{rank}(A)$, 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 Sect. 6.6 on page 289 and in Sect. 9.3.2 on page 408.

3.5.1.3 Generalized Inverses

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

$$AA^-A = A. \tag{3.194}$$

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 Sect. 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 (3.194), we see that

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

thus, if A^- is a generalized inverse of A, then $(A^-)^{\mathrm{T}}$ 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 (3.194), we see that

$$(A^-A)(A^-A) = A^-A. \tag{3.195}$$

(Such a matrix is said to be *idempotent*. We discuss idempotent matrices beginning on page 352.) From equation (3.128) together with the fact that $AA^-A = A$, we see that

$$\text{rank}(A^-A) = \text{rank}(A). \tag{3.196}$$

By multiplication as above, we see that

$$A(I - A^{-}A) = 0, \tag{3.197}$$

that

$$(I - A^{-}A)(A^{-}A) = 0, \tag{3.198}$$

and that $(I - A^{-}A)$ is also idempotent:

$$(I - A^{-}A)(I - A^{-}A) = (I - A^{-}A). \tag{3.199}$$

The fact that $(A^{-}A)(A^{-}A) = A^{-}A$ yields the useful fact that

$$\text{rank}(I - A^{-}A) = m - \text{rank}(A). \tag{3.200}$$

This follows from equations (3.198), (3.170), and (3.196), which yield

$$0 \geq \text{rank}(I - A^{-}A) + \text{rank}(A) - m,$$

and from equation (3.129), which gives

$$m = \text{rank}(I) \leq \text{rank}(I - A^{-}A) + \text{rank}(A).$$

The two inequalities result in the equality of equation (3.200).

3.5.1.4 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

$$x = A^{-}b \tag{3.201}$$

is a solution to the system because if $AA^{-}A = A$, then $AA^{-}Ax = Ax$ and since $Ax = b$,

$$AA^{-}b = b; \tag{3.202}$$

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,

$$A^{-}b + (I - A^{-}A)z \tag{3.203}$$

is a solution because $A(A^{-}b + (I - A^{-}A)z) = AA^{-}b + (A - AA^{-}A)z = b$. Furthermore, any solution to $Ax = b$ can be represented as $A^{-}b + (I - A^{-}A)z$ for some z. This is because if y is any solution (that is, if $Ay = b$), we have

$$y = A^{-}b - A^{-}Ay + y = A^{-}b - (A^{-}A - I)y = A^{-}b + (I - A^{-}A)z.$$

The number of linearly independent solutions arising from $(I - A^{-}A)z$ is just the rank of $(I - A^{-}A)$, which from equation (3.200) is $m - \text{rank}(A)$.

3.5.2 Null Space: The Orthogonal Complement

The solutions of a consistent system $Ax = b$, which we characterized in equation (3.203) as $A^-b + (I - A^-A)z$ 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

$$Az = 0 \tag{3.204}$$

is called the *null space* of A. We denote the null space of A by

$$\mathcal{N}(A).$$

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. (It is actually a vector space in either case, but recall our ambiguity about the null vector space, page 13.)

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

$$\begin{aligned} \dim(\mathcal{N}(A)) &= \operatorname{rank}(I - A^-A) \\ &= m - \operatorname{rank}(A) \end{aligned} \tag{3.205}$$

from equation (3.200).

If $Ax = b$ is consistent, any solution can be represented as $A^-b + z$, for some z in the null space of A, because if y is some solution, $Ay = b = AA^-b$ from equation (3.202), and so $A(y - A^-b) = 0$; that is, $z = y - A^-b$ 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 $Az = 0$, is the same as the nullity of A.

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

If A is square, we have

$$\mathcal{N}(A) \subseteq \mathcal{N}(A^2) \subseteq \mathcal{N}(A^3) \subseteq \cdots \tag{3.206}$$

and

$$\mathcal{V}(A) \supseteq \mathcal{V}(A^2) \supseteq \mathcal{V}(A^3) \supseteq \cdots . \tag{3.207}$$

(We see this easily from the inequality (3.128) on page 103.)

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

Because $\dim(\mathcal{N}(A)) + \dim(\mathcal{V}(A^{\mathrm{T}})) = m$ and $\mathcal{N}(A) \perp \mathcal{V}(A^{\mathrm{T}})$, by equation (2.44) we have

$$\mathcal{N}(A) \oplus \mathcal{V}(A^{\mathrm{T}}) = \mathbb{R}^m; \tag{3.208}$$

that is, the null space of A is the *orthogonal complement* of $\mathcal{V}(A^{\mathrm{T}})$. 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 124, we defined a generalized inverse of a matrix A as a matrix A^- such that $AA^-A = A$, and we observed several interesting properties of generalized inverses. We will now consider some additional properties, after quickly summarizing some we observed previously.

3.6.1 Immediate Properties of Generalized Inverses

Let A be an $n \times m$ matrix, and let A^- be a generalized inverse of A. The properties of a generalized inverse A^- derived in equations (3.195) through (3.203) include:

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

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

In this section, we will first consider some special types of generalized inverses. Two of these special types of generalized inverses are unique. We will then discuss some more properties of "general" generalized inverses, which are analogous to properties of inverses. (We will call general generalized inverses "g_1 inverses".)

3.6.2 Special Generalized Inverses: The Moore-Penrose Inverse

A generalized inverse is not unique in general. As we have seen on page 125, 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 Sect. 6.6 we discuss properties of the solution A^+b.

3.6.2.1 Definitions 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.

3.6.2.2 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 (3.150), so $L^{\mathrm{T}}AR^{\mathrm{T}} = L^{\mathrm{T}}LRR^{\mathrm{T}}$. Because the $n \times r$ matrix L is of full column rank and the $r \times m$ matrix R is of full row rank, $L^{\mathrm{T}}L$ and RR^{T} are both of full rank, and hence $L^{\mathrm{T}}LRR^{\mathrm{T}}$ is of full rank. Furthermore, $L^{\mathrm{T}}AR^{\mathrm{T}} = L^{\mathrm{T}}LRR^{\mathrm{T}}$, so it is of full rank, and $(L^{\mathrm{T}}AR^{\mathrm{T}})^{-1}$ exists. Now, form $R^{\mathrm{T}}(L^{\mathrm{T}}AR^{\mathrm{T}})^{-1}L^{\mathrm{T}}$. By checking properties 1 through 4 above, we see that

$$A^+ = R^{\mathrm{T}}(L^{\mathrm{T}}AR^{\mathrm{T}})^{-1}L^{\mathrm{T}} \tag{3.209}$$

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 (5.45) on page 251).

3.6.2.3 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:

$$\begin{gathered} G = \\ GAG = (GA)^{\mathrm{T}}G = A^{\mathrm{T}}G^{\mathrm{T}}G = (AA^+A)^{\mathrm{T}}G^{\mathrm{T}}G = (A^+A)^{\mathrm{T}}A^{\mathrm{T}}G^{\mathrm{T}}G = \\ A^+AA^{\mathrm{T}}G^{\mathrm{T}}G = A^+A(GA)^{\mathrm{T}}G = A^+AGAG = A^+AG = A^+AA^+AG = \\ A^+(AA^+)^{\mathrm{T}}(AG)^{\mathrm{T}} = A^+(A^+)^{\mathrm{T}}A^{\mathrm{T}}G^{\mathrm{T}}A^{\mathrm{T}} = A^+(A^+)^{\mathrm{T}}(AGA)^{\mathrm{T}} = \\ A^+(A^+)^{\mathrm{T}}A^{\mathrm{T}} = A^+(AA^+)^{\mathrm{T}} = A^+AA^+ \\ = A^+. \end{gathered}$$

3.6.2.4 Other Properties

Similarly to the property for inverses expressed in equation (3.145), we have

$$(A^+)^{\mathrm{T}} = (A^{\mathrm{T}})^+. \tag{3.210}$$

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 (3.201)). In Sect. 6.6, we will show that this unique solution has a kind of optimality.

Moore-Penrose inverses also have a few additional interesting properties not shared by generalized inverses; for example

$$(I - A^+A)A^+ = 0. \tag{3.211}$$

3.6.2.5 Drazin Inverses

A *Drazin inverse* of a square matrix A is a matrix, which we will denote as A^{D}, such that

1. $A^{\mathrm{D}}AA^{\mathrm{D}} = A^{\mathrm{D}}$; that is, it is an outer pseudoinverse,
2. $AA^{\mathrm{D}} = A^{\mathrm{D}}A$, and
3. $A^{k+1}A^{\mathrm{D}} = A^k$ for any positive integer k.

Notice that these conditions together imply that a Drazin inverse is a g_1 inverse (that is, $AA^{\mathrm{D}}A = A$; see the conditions for the Moore-Penrose inverse on page 128). Because of this, a Drazin inverse satisfies most of the properties

listed for any generalized inverse on page 127; for example, $A^{\mathrm{D}}A$ is idempotent. The first property listed there is also satisfied; that is, $(A^{\mathrm{D}})^{\mathrm{T}}$ is the Drazin inverse of A^{T}. (This does not follow just because the Drazin inverse is a generalized inverse, however.)

Other important properties of Drazin inverses include

- $A^{\mathrm{D}} = A^{-1}$ if A is nonsingular.
- $(A^{\mathrm{D}})^{\mathrm{D}} = A$.
- For any square matrix, the Drazin inverse is unique.

These are left as exercises.

There is an interesting relationship between Drazin inverses and Moore-Penrose inverses. If A is any square matrix, for any positive integer k, its Drazin inverse is the matrix

$$A^{\mathrm{D}} = A^k(A^{2k+1})^+A^k. \tag{3.212}$$

Drazin inverses arise in the solutions of linear systems of differential equations. See Campbell and Meyer (1991) for further discussions of properties and applications of Drazin inverses and of their relationship to Moore-Penrose inverses.

3.6.3 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 (3.15)), and the transpose of the product is the product of the transposes in reverse order (equation (3.44)). 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 Sect. 3.3.13, beginning on page 118, 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 (3.173) and (3.175):

$$(AB)^{-1} = B^{-1}A^{-1}$$

and

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

These same relations hold with the inverse replaced by generalized inverses.

We can relax the conditions on nonsingularity of A, B, $I + A$ and so on, but because of the nonuniqueness of generalized inverses, in some cases we must interpret the equations as "holding for some generalized inverse".

With the relaxation on the nonsingularity of constituent matrices, equations (3.176) through (3.182) do not necessarily hold for generalized inverses of general matrices, but some do. For example,

$$A(I+A)^- = (I+A^-)^-.$$

(Again, the true relationships are easily proven if taken in the order given on page 119, and in Exercise 3.18 you are asked to determine which are true for generalized inverses of general matrices and to prove that those are.)

3.6.4 Generalized Inverses of Partitioned Matrices

If A is partitioned as

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{3.213}$$

then, similar to equation (3.190), a generalized inverse of A is given by

$$A^- = \begin{bmatrix} A_{11}^- + A_{11}^- A_{12} Z^- A_{21} A_{11}^- & -A_{11}^- A_{12} Z^- \\ -Z^- A_{21} A_{11}^- & Z^- \end{bmatrix}, \tag{3.214}$$

where $Z = A_{22} - A_{21}A_{11}^- A_{12}$ (see Exercise 3.23, page 180).

If the inverses on the right-hand side of equation (3.214) are Moore-Penrose inverses, then the result is the Moore-Penrose inverse of A.

If the partitioning in (3.213) 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

$$A^- = \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix}, \tag{3.215}$$

where 0 represents matrices of the appropriate shapes. The generalized inverse given in equation (3.215) is the same as the Moore-Penrose inverse given in equation (3.209), but it is not necessarily the same generalized inverse as in equation (3.214). The fact that it is a generalized inverse is easy to establish by using the definition of generalized inverse and equation (3.189).

3.7 Orthogonality

In Sect. 2.1.8, we defined orthogonality and orthonormality of two or more vectors in terms of dot products. On page 98, in equation (3.112), 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.

3.7.1 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 $QQ^{\mathrm{T}} = I_n$ if $n \leq m$, and $Q^{\mathrm{T}}Q = I_m$ if $n \geq m$. If Q is a square orthogonal matrix, then $QQ^{\mathrm{T}} = Q^{\mathrm{T}}Q = I$.

The determinant of a square orthogonal matrix is ± 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:

$$\langle Q, Q \rangle = m. \tag{3.216}$$

This is because $Q^{\mathrm{T}}Q = I_m$. If $n \leq m$, the matrix inner product of Q with itself is its number of rows.

Recalling the definition of the orthogonal binary relationship from page 98, we note that if Q is an orthogonal matrix, then Q is not orthogonal to itself in that sense.

A permutation matrix (see page 81) 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.

An Aside: Unitary Matrices

For square 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 $UU^{\mathrm{H}} = U^{\mathrm{H}}U = I$. Transformations using unitary matrices are analogous in many ways to transformations using orthogonal matrices, but there are important differences.

An orthogonal matrix with real elements is also a unitary matrix.

The definition of orthogonality of vectors is the same for complex vectors as it is for real vectors; in both cases, it is that the inner product is 0. Because of our emphasis on real vectors and matrices, we often think of orthogonality of vectors in terms of $x^{\mathrm{T}}y$, but this only applies to real vectors. In general, x and y are orthogonal if $x^{\mathrm{H}}y = 0$, which is the inner product. The corresponding binary relationship of orthogonality for matrices, as defined in equation (3.112) on page 98, likewise depends on an inner product, which is given in equation (3.107). The relationship in equation (3.108) may not be correct if the elements are not real.

For matrices, orthogonality is both a type of binary relationship and a unary property. The unary property of orthogonality is defined in terms of a transpose. A matrix that is orthogonal is also unitary only if it is real.

3.7.2 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 ± 1. If Q is a matrix that is "orthogonal" in this weaker sense of the definition, and Q has more rows than columns, then

$$Q^{\mathrm{T}}Q = \begin{bmatrix} \mathtt{X} & \mathtt{0} & \cdots & \mathtt{0} \\ \mathtt{0} & \mathtt{X} & \cdots & \mathtt{0} \\ & & \ddots & \\ \mathtt{0} & \mathtt{0} & \cdots & \mathtt{X} \end{bmatrix}.$$

Unless stated otherwise, I use the term "orthogonal matrix" to refer to a matrix whose columns are orthonormal; that is, for which $Q^{\mathrm{T}}Q = I$.

3.7.3 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 $\mathcal{O}(n)$. The orthogonal group $\mathcal{O}(n)$ is a subgroup of the general linear group $\mathcal{G}L(n)$, defined on page 114. The orthogonal group is useful in multivariate analysis because of the invariance of the so-called Haar measure over this group (see Sect. 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

$$\lim_{j \to \infty} Q_{i_j} = Q, \tag{3.217}$$

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

3.7.4 Conjugacy

Instead of defining orthogonality of vectors in terms of dot products as in Sect. 2.1.8, we could define it more generally in terms of a bilinear form as in Sect. 3.2.9. If the bilinear form $x^{\mathrm{T}}Ay = 0$, 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 (3.93). 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: $Q^{\mathrm{T}}AQ = I$.

3.8 Eigenanalysis: Canonical Factorizations

Throughout this section on eigenanalysis, we will generally implicitly assume that the matrices we discuss are square, unless we state otherwise.

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

$$Av = cv, \tag{3.218}$$

we say v is an *eigenvector* of the matrix A, and c is an *eigenvalue* of the matrix A. We refer to the pair c and v as an associated eigenvector and eigenvalue or as an *eigenpair*.

We immediately note that if v is an eigenvector of A, then for any scalar, b, because $A(bv) = c(bv)$, bv is also an eigenvector of A. (We will exclude the case $b = 0$, so that we do not consider the 0 vector to be an eigenvector of A.) That is, any vector in the double cone generated by an eigenvector, except the 0 vector, is an eigenvector (see discussion of cones, beginning on page 43).

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 (3.218), 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 (3.218) 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 *characteristic value* (that is why I use a "c" to represent an eigenvalue), a *latent root* (that is why I also might use a "λ" to

represent an eigenvalue), or a *proper value*, and similar synonyms exist for an eigenvector. An eigenvalue is also sometimes called a *singular value*, but the latter term has a different meaning that we will use in this book (see page 161; 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.

3.8.1 Eigenvalues and Eigenvectors Are Remarkable

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 *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, for a given matrix, do such special vectors and scalars exist?

> The answer is yes.

The next question is, for a given matrix, what is the formula for the eigenvalues (or what is a finite sequence of steps to compute the eigenvalues)?

> The answer is a formula does not exist and there is no finite sequence of steps, in general, for determining the eigenvalues (if the matrix is bigger than 4×4).

Before considering these 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.

3.8.2 Left Eigenvectors

In the following, when we speak of an eigenvector or eigenpair without qualification, we will mean the objects defined by equation (3.218). There is another type of eigenvector for A, however, a *left eigenvector*, defined as a nonzero w in

$$w^{\mathrm{T}}A = cw^{\mathrm{T}}. \tag{3.219}$$

For emphasis, we sometimes refer to the eigenvector of equation (3.218), $Av = cv$, 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 $Av = c_1v$, $w^{\mathrm{T}}A = c_2w^{\mathrm{T}}$, and $c_1 \neq c_2$, then $w^{\mathrm{T}}v = 0$. We see this by multiplying both sides of $w^{\mathrm{T}}A = c_2w^{\mathrm{T}}$ by v to get $w^{\mathrm{T}}Av = c_2w^{\mathrm{T}}v$ and multiplying both sides of $Av = c_1v$ by w^{T} to get $w^{\mathrm{T}}Av = c_1w^{\mathrm{T}}v$. Hence, we have $c_1w^{\mathrm{T}}v = c_2w^{\mathrm{T}}v$, and because $c_1 \neq c_2$, we have $w^{\mathrm{T}}v = 0$.

3.8.3 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 (3.218) the following properties. (In Exercise 3.25, 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 $v^{\mathrm{T}}v = 1$. Such an eigenvector is also called a "unit eigenvector", but I prefer the term "normalized eigenvector" because of the use of the phrase "unit vector" to refer to the special vectors e_i.
   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. $c - d$ and v are an eigenpair of $A - dI$. This obvious fact is useful in computing eigenvalues (see Sect. 7.1.5).
8. 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.) All of eigenvalues are 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.)

9. 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 146.)

List continued on page 140.

3.8.3.1 Eigenvalues of Elementary Operator Matrices

For a matrix with a very simple pattern, such as a disagonal matrix, whose determinant is just the product of the elements, we can determine the eigenvalues by inspection. For example, it is clear immediately that all eigenvalues of the identity matrix are 1s. (Although they are all the same, we still say there are n of them, if n is the order of the identity. Multiplicity of eigenvalues is an important property, which we will discuss beginning on page 143.)

Because of their simple patterns, we can also easily determine the eigenvalues of elementary operator matrices, possibly by considering one or two adjugates that arise from submatrices that are identity matrices.

The eigenvalues of the 2×2 permutation

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

are just the two square roots of 1; that is, 1 and -1. From this, using partitions of an elementary permutation matrix E_{pq} of order n to form adjugates that are identities, we see that the eigenvalues of an elementary permutation matrix E_{pq} are $n-1$ 1s and one -1.

With a little more effort we can determine the eigenvalues of general permutation matrices. Following the preceding approach, we immediately see that the eigenvalues of the matrix

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

are the three cube roots of 1, two of which contain imaginary components. In Chap. 8, on page 388, we describe the full set of eigenvalues for a permutation matrix in which all rows are moved.

By inspection of the determinant, we see that the eigenvalues of an elementary row-multiplication matrix $E_p(a)$ of order n are $n-1$ 1s and one a.

Again by inspection of the determinant, we see that the eigenvalues of an elementary axpy matrix $E_{pq}(a)$ of order n are n 1s, the same as the identity itself.

3.8.4 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

$$\det(A - cI) = \det(cI - A) = 0. \tag{3.220}$$

Equation (3.220) 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 (3.220) 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*:

$$p_A(c) = s_0 + s_1 c + \cdots + s_n c^n = 0. \tag{3.221}$$

From the expansion of the determinant $\det(cI - A)$, as in equation (3.41) on page 73, 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

$$p_A(c) = (-1)^n (c - c_1) \cdots (c - c_n), \tag{3.222}$$

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 (3.218). 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,

$$p_A(A) = s_0 I + s_1 A + \cdots + s_n A^n = 0_n. \tag{3.223}$$

We see this by using equation (3.34) to write the matrix in equation (3.220) as

$$(A - cI)\text{adj}(A - cI) = p_A(c)I. \tag{3.224}$$

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 (3.224), we have

$$\begin{aligned} AB_0 &= s_0 I \\ AB_1 - B_0 &= s_1 I \\ &\vdots \\ AB_{n-1} - B_{n-2} &= s_{n-1} I \\ B_{n-1} &= s_n I. \end{aligned}$$

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 3.26.

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

$$A = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1 \\ -s_0 & -s_1 & -s_2 & \cdots & -s_{n-1} \end{bmatrix}. \tag{3.225}$$

(Note that this matrix is the same as the Jordan block (see page 78), except that the last row of 0s is replaced with the row of coefficients of the characteristic equation.) 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).

3.8.4.1 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 136. We assume A is a real matrix with eigenpair (c, v).

10. c is an eigenvalue of A^{T} (because $\det(A^{\mathrm{T}}-cI) = \det(A-cI)$ 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 the Gramian matrix $A^{\mathrm{T}}A$.
14. The nonzero eigenvalues of the Gramian matrix $A^{\mathrm{T}}A$ are the same as the nonzero eigenvalues of the Gramian matrix AA^{T}. (This is actually property 8 on page 136.)
15. c is real if A is symmetric or if A is triangular (the elements of A are assumed to be real, of course).

In Exercise 3.27, 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.

There are many additional interesting properties of eigenvalues and eigenvectors that we will encounter in later sections, but there is one more that I want to list here with these very basic and important properties:

16. $|c| \leq \|A\|$, where $\|\cdot\|$ is any consistent matrix norm.

(We will discuss matrix norms in Sect. 3.9 beginning on page 164, and this particular bound is given in equation (3.310) in that section. In my definition of matrix norm, all norms are required to be consistent.)

3.8.4.2 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

$$\begin{aligned} p_A(c) &= (c-c_1)\cdots(c-c_n) \\ &= (-1)^n \prod c_i + \cdots + (-1)^{n-1} \sum c_i c^{n-1} + c^n. \end{aligned} \tag{3.226}$$

Because this is the same polynomial as obtained by the expansion of the determinant in equation (3.221), the coefficients must be equal. In particular, by simply equating the corresponding coefficients of the constant terms and $(n-1)^{\text{th}}$-degree terms, we have the two very important facts:

$$\det(A) = \prod c_i \tag{3.227}$$

and

$$\mathrm{tr}(A) = \sum c_i. \tag{3.228}$$

It might be worth recalling that we have assumed that A is real, and therefore $\det(A)$ and $\mathrm{tr}(A)$ 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 even though the individual elements may not be.

3.8.5 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.

3.8.5.1 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 $\sigma(A)$:

$$\sigma(A) = \{\lambda_1, \ldots, \lambda_k\}. \tag{3.229}$$

We see immediately that $\sigma(A^{\mathrm{T}}) = \sigma(A)$ (property 10 above).

In terms of the spectrum, equation (3.222) becomes

$$p_A(c) = (-1)^n (c - \lambda_1)^{m_1} \cdots (c - \lambda_k)^{m_k}, \tag{3.230}$$

for $m_i \geq 1$.

We label the c_i and v_i so that

$$|c_1| \geq \cdots \geq |c_n|. \tag{3.231}$$

We likewise label the λ_i so that

$$|\lambda_1| > \cdots > |\lambda_k|. \tag{3.232}$$

With this notation, we have

$$|\lambda_1| = |c_1|$$

and

$$|\lambda_k| = |c_n|,$$

but we cannot say anything about the other λs and cs.

3.8.5.2 The Spectral Radius

For the matrix A with these eigenvalues, $|c_1|$ is called the *spectral radius* and is denoted by $\rho(A)$:

$$\rho(A) = \max |c_i| = |c_1| = |\lambda_1|. \tag{3.233}$$

We immediately note that $\rho(A^{\mathrm{T}}) = \rho(A)$.

The set of complex numbers

$$\{z : |z| = \rho(A)\} \tag{3.234}$$

is called the *spectral circle* of A.

An eigenvalue equal to $\pm \max |c_i|$ (that is, equal to $\pm c_1$) 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, $\rho(A)$ (or $|c_1|$) is more often of interest than c_1.

Interestingly, we have for all i

$$|c_i| \leq \max_j \sum_k |a_{kj}| \tag{3.235}$$

and

$$|c_i| \leq \max_k \sum_j |a_{kj}|. \tag{3.236}$$

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 (3.310) on page 171. (The two bounds above relate to the L_1 and L_∞ matrix norms, respectively, as we will see.)

The spectral radius gives a very simple indication of the region in the complex plane in which the entire spectrum lies. Consider, for example, the matrix

$$A = \begin{bmatrix} 9 & -6 & 1 \\ -2 & 9 & -5 \\ 10 & -2 & 4 \end{bmatrix}. \tag{3.237}$$

(See Exercise 3.24 for comments on the origins of this matrix.)

From equation (3.235), we see that all eigenvalues are less than or equal to 16 in modulus. In fact, the eigenvalues are $\sigma(A) = \{16, 3 + 4\mathrm{i}, 3 - 4\mathrm{i}\}$, and $\rho(A) = 16$.

On page 145, we will discuss other regions of the complex plane in which all eigenvalues necessarily lie.

A matrix may have all eigenvalues equal to 0 but yet the matrix itself may not be 0. (The matrix must be singular, however.) A nilpotent matrix (see page 77), as well as any upper triangular matrix with all 0s on the diagonal are examples.

Because, as we saw on page 136, 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 $S = A/|c_1|$, and $\rho(S) = 1$.

The spectral radius, is one of the most important properties of a matrix. As we will see in Sect. 3.9.1, it is the the L_p norm for a symmetric matrix. From equations (3.235) and (3.236), we have seen in any event that it is bounded from above by the L_1 and L_∞ matrix norms (which we will define formally in Sect. 3.9.1), and, in fact, in equation (3.310) we will see that the spectral radius is bounded from above by any matrix norm. We will discuss the spectral radius further in Sects. 3.9.5 and 3.9.6. In Sect. 3.9.6 we will see that the spectral radius determines the convergence of a matrix power series (and this fact is related to the behavior of autoregressive processes).

3.8.5.3 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 (λ_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

$$y_{j+1} = \sum_{i=1}^{j} t_i y_i$$

for some t_i. Now, multiplying both sides of the equation by $A - \mu_{j+1} I$, where μ_{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 distinct (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.

3.8.5.4 The Eigenspace and Geometric Multiplicity

Rewriting the definition (3.218) for the i^{th} eigenvalue and associated eigenvector of the $n \times n$ matrix A as

$$(A - c_i I)v_i = 0, \tag{3.238}$$

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 distinct 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 λ, then any linear combination of u and v is an eigenvector corresponding to λ; that is, if $Au = \lambda u$ and $Av = \lambda v$, for any scalars a and b,

$$A(au + bv) = \lambda(au + bv).$$

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 (3.205) 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 (2.56) on page 38. These orthogonal eigenvectors span the same eigenspace. They are not unique, of course, as any sequence of Gram-Schmidt transformations could be applied.

3.8.5.5 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 (page 150). The algebraic multiplicity of a given eigenvalue is at least as great as its geometric multiplicity (exercise).

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 (hence, a simple eigenvalue semisimple 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.

3.8.5.6 Gershgorin Disks

In addition to the spectral circle, there is a another specification of regions in the complex plane that regions in the complex plane that contain the spectrum of an $n \times n$ matrix A. This is the union of the n *Gershgorin disks*, where for $i = 1, \ldots, n$, the i^{th} of which is the disk

$$|z - a_{ii}| \leq r_i \quad \text{where } r_i = \sum_{1 \leq j \leq n;\ j \neq i} |a_{ij}|. \tag{3.239}$$

("Gershgorin" is often spelled as "Gerschgorin" or "Gersgorin" or even "Geršgorin"; he was Russian.)

To see that this is the case, let (c, v) be an arbitrary eigenpair of A with v normalized by the L_∞ norm (that is, $\max(v) = 1$). Let k be such that $|v_k| = 1$. Then

$$cv_k = (Av)_k = \sum_{j=1}^{n} a_{kj} v_j;$$

hence

$$(c - a_{kk})v_k = \sum_{1 \leq j \leq n;\ j \neq k} a_{kj} v_j.$$

Now introduce the modulus, and we get the desired inequality:

$$\begin{aligned} |c - a_{kk}| &= |c - a_{kk}||v_k| \\ &= \left| \sum_{1 \leq j \leq n;\ j \neq k} a_{kj} v_j \right| \\ &\leq \sum_{1 \leq j \leq n;\ j \neq k} |a_{kj}||v_j| \\ &\leq \sum_{1 \leq j \leq n;\ j \neq k} |a_{kj}| \\ &= r_k. \end{aligned}$$

We conclude that every eigenvalue lies in some similar disk; that is, the spectrum lies in the union of such disks.

Since $\sigma(A^{\mathrm{T}}) = \sigma(A)$, using the same argument as above, we can define another collection of n Gershgorin disks based on column sums:

$$|z - a_{jj}| \leq s_j \quad \text{where } s_j = \sum_{1 \leq i \leq n;\ i \neq j} |a_{ij}|. \tag{3.240}$$

All eigenvalues of A lie within the union of these disks.

Combining the two restrictions, we see that all eigenvalues of A lie within the intersection of these two unions of Gershgorin disks.

3.8.6 Similarity Transformations

Two $n \times n$ matrices, A and B, are said to be *similar* if there exists a nonsingular matrix P such that

$$B = P^{-1}AP. \tag{3.241}$$

The transformation in equation (3.241) is called a *similarity transformation*. (Compare similar matrices with *equivalent matrices* on page 110. The matrices A and B in equation (3.241) are also equivalent, as we see using equations (3.153) and (3.154).)

It is clear from the definition that the similarity relationship is both commutative and transitive.

If A and B are similar, as in equation (3.241), then for any scalar c

$$\begin{aligned} \det(A - cI) &= \det(P^{-1})\det(A - cI)\det(P) \\ &= \det(P^{-1}AP - cP^{-1}IP) \\ &= \det(B - cI), \end{aligned}$$

and, hence, A and B have the same eigenvalues. (This simple fact was stated as property 9 on page 137.)

3.8.6.1 Orthogonally and Unitarily Similar Transformations

An important type of similarity transformation is based on an orthogonal matrix in equation (3.241). If Q is orthogonal and

$$B = Q^{\mathrm{T}}AQ, \tag{3.242}$$

A and B are said to be *orthogonally similar*.

If B in equation (3.242) $B = Q^{\mathrm{T}}AQ$ 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.

The concepts of orthogonally similar and orthogonal diagonalization are very important, but for matrices with complex entries or for real matrices with complex eigenvalues, generalizations of the concepts based on unitary matrices are more useful. If U is unitary and

$$B = U^{\mathrm{H}}AU, \tag{3.243}$$

A and B are said to be *unitarily similar*. Since an orthogonal matrix is unitary, two matrices that are orthogonally similar are also unitarily similar.

If B in equation (3.243) $B = U^{\mathrm{H}}AU$ is a diagonal matrix, A is said to be *unitarily diagonalizable*, and QBQ^{T} is called the *unitarily diagonal factorization* or *unitarily similar factorization* of A. A matrix that is orthogonally diagonalizable is also unitarily diagonalizable.

We will discuss characteristics of orthogonally diagonalizable matrices in Sects. 3.8.8 through 3.8.10 below. The significant fact that we will see there is that a matrix is orthogonally diagonalizable if and only if it is symmetric.

We will discuss characteristics of unitarily diagonalizable matrices in Sect. 8.2.3 on page 345. The significant fact that we will see there is that a matrix is unitarily diagonalizable if and only if it is normal (which includes symmetric matrices).

3.8.6.2 Uses of Similarity Transformations

Similarity transformations are very useful in establishing properties of matrices, such as convergence properties of sequences (see, for example, Sect. 3.9.6). Similarity transformations are also used in algorithms for computing eigenvalues (see, for example, Sect. 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 3.29b).

3.8.7 Schur Factorization

If B in equation (3.242) is an upper triangular matrix, QBQ^{T} is called the *Schur factorization* of A:

$$A = QBQ^{\mathrm{T}}. \tag{3.244}$$

This is also called the "Schur form" of A.

For any square matrix, the Schur factorization exists. Although the matrices in the factorization are not unique, the diagonal elements of the upper triangular matrix B are the eigenvalues of A.

There are various forms of the Schur factorization. Because in general the eigenvalues and eigenvectors may contain imaginary components, the orthogonal matrices in equation (3.244) may contain imaginary components, and furthermore, the Schur factorization is particularly useful in studying factorizations involving unitary matrices, we will describe the Schur factorization that use unitary matrices.

The general form of the Schur factorization for a square matrix A is

$$A = UTU^{\mathrm{H}}, \tag{3.245}$$

where U is a unitary matrix and T is an upper triangular matrix whose diagonal entries are the eigenvalues of A.

The Schur factorization exists for any square matrix, which we can see by induction. It clearly exists in the degenerate case of a 1×1 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 a unitary matrix U_1 with v as its first column. Let U_2 be the matrix consisting of the remaining columns; that is, U_1 is partitioned as $[v \,|\, U_2]$.

$$\begin{aligned} U_1^{\mathrm{H}} A U_1 &= \begin{bmatrix} v^{\mathrm{H}} A v & v^{\mathrm{H}} A U_2 \\ U_2^{\mathrm{H}} A v & U_2^{\mathrm{H}} A U_2 \end{bmatrix} \\ &= \begin{bmatrix} c & v^{\mathrm{H}} A U_2 \\ 0 & U_2^{\mathrm{H}} A U_2 \end{bmatrix} \\ &= T, \end{aligned}$$

where $U_2^{\mathrm{H}} A U_2$ is an $(n-1) \times (n-1)$ matrix. Now the eigenvalues of $U^{\mathrm{H}} A U$ are the same as those of A; hence, if $n = 2$, then $U_2^{\mathrm{H}} A U_2$ is a scalar and must equal the other eigenvalue, and so the statement is proven for a 2×2 matrix.

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

$$U_1^{\mathrm{H}} A U_1 = \begin{bmatrix} c & v^{\mathrm{H}} A U_2 \\ 0 & U_2^{\mathrm{H}} A U_2 \end{bmatrix}.$$

Now, since $U_2^{\mathrm{H}} A U_2$ is an $(n-1) \times (n-1)$ matrix, by the induction hypothesis there exists an $(n-1) \times (n-1)$ Hermitian matrix V such that $V^{\mathrm{H}} (U_2^{\mathrm{H}} A U_2) V = T_1$, where T_1 is upper triangular. Now let

$$U = U_1 \begin{bmatrix} 1 & 0 \\ 0 & V \end{bmatrix}.$$

By multiplication, we see that $U^{\mathrm{H}} U = I$ (that is, Q is Hermitian). Now form

$$U^{\mathrm{H}} A U = \begin{bmatrix} c & v^{\mathrm{H}} A U_2 V \\ 0 & V^{\mathrm{H}} U_2^{\mathrm{H}} A U_2 V \end{bmatrix} = \begin{bmatrix} c & v^{\mathrm{H}} A U_2 V \\ 0 & T_1 \end{bmatrix} = T.$$

We see that T is upper triangular because T_1 is, and so by induction the Schur factorization exists for any $n \times n$ matrix.

The steps in the induction did not necessarily involve unique choices except for the eigenvalues on the diagonal of T.

Note that the Schur factorization is also based on unitarily similar transformations, but the term "unitarily similar factorization" is generally used only to refer to the diagonal factorization.

3.8.8 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 (3.218)) we can write

$$AV = VC. \tag{3.246}$$

Now, if V is nonsingular, we have

$$A = VCV^{-1}. \tag{3.247}$$

Expression (3.247) 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 (3.247). It obviously depends on V being nonsingular; that is, that the eigenvectors are linearly independent. If a matrix can be factored as in (3.247), 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 (that is, distinct) is diagonalizable (because, as we saw on page 143, 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 $l = 1, \ldots, k$,

$$\text{rank}(A - \lambda_l I) = n - m_l \tag{3.248}$$

(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 (3.246)) 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 λ_l, and for each λ_l, we have $\lambda_l = c_{l_1} = c_{l_{m_l}}$ 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 143 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 $u = \sum b_k w_k$, and so $Au = A\sum b_k w_k = c_i \sum b_k w_k = c_i u$, 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 113), we have $\text{rank}(A - c_i I) = n - m_i$.

3.8.8.1 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 (3.164), we have

$$\text{rank}\left(B^2\right) = \text{rank}\left(B^{\mathrm{T}}B\right) = \text{rank}(B) = r.$$

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 (3.221) 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 $n - m = r = \text{rank}(A - cI)$.

As we will see below in Sect. 3.8.10, a symmetric matrix A is not only diagonalizable in the form (3.247), $A = VCV^{-1}$, the matrix V can be chosen as an orthogonal matrix, so we have $A = UCU^{\mathrm{T}}$. We will say that the symmetric matrix is *orthogonally diagonalizable*.

3.8.8.2 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 $A - c_2 I$:

$$A - I = \begin{bmatrix} -1 & 1 & 2 \\ 2 & 2 & 0 \\ 0 & 4 & 4 \end{bmatrix}.$$

This is clearly of rank 2; hence the rank of the null space of $A - c_2 I$ (that is, the geometric multiplicity of c_2) is $3 - 2 = 1$. The matrix A is not diagonalizable.

3.8.8.3 The Jordan Decomposition

Although not all matrices can be diagonalized in the form of equation (3.247), $V^{-1}AV = C = \text{diag}(c_i)$, any square matrix A can be expressed in the form

$$X^{-1}AX = \text{diag}(J_{j_i}), \tag{3.249}$$

where the J_{j_i} are *Jordan blocks* associated with a single eigenvalue λ_j, of the form

$$J_{j_i}(\lambda_j) = \begin{bmatrix} \lambda_j & 1 & 0 & \cdots & 0 & 0 \\ 0 & \lambda_j & 1 & \cdots & 0 & 0 \\ 0 & 0 & \lambda_j & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \lambda_j & 1 \\ 0 & 0 & \cdots & 0 & 0 & \lambda_j \end{bmatrix},$$

or, in the degenerate case, $J_{j_i}(\lambda_j) = [\lambda_j]$, where λ_j is a specific distinct eigenvalue (that is, $\lambda_j \neq \lambda_k$ if $j \neq k$). (Compare this with the Jordan form of a nilpotent matrix following equation (3.51) on page 77, in which the diagonal elements are 0s.) If each Jordan block J_{j_i} is 1×1, the Jordan decomposition is a diagonal decomposition.

There are some interesting facts about the Jordan decomposition. If there are g_j Jordan blocks associated with the eigenvalue λ_j, then λ_j has geometric multiplicity g_j. The algebraic multiplicity of λ_j is the total number of diagonal elements in all the Jordan blocks associated with λ_j; hence, if each Jordan block J_{j_i} is 1×1 then all eigenvalues are semisimple. While these two facts appear rather profound, they are of little interest for our purposes, and we will not give proofs. (Proofs can be found in Horn and Johnson (1991).) The problem of computing a Jordan decomposition is ill-conditioned because slight perturbations in the elements of A can obviously result in completely different sets of Jordan blocks.

3.8.9 Properties of Diagonalizable Matrices

If the matrix A has the similar canonical factorization VCV^{-1} of equation (3.247), 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 (3.227) and (3.228) 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

$$\mathrm{tr}(A) = \mathrm{tr}(VCV^{-1}) = \mathrm{tr}(V^{-1}VC) = \mathrm{tr}(C).$$

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, $\sum_{i=1}^{k} m_i = \mathrm{rank}(A)$, for the matrix A with k distinct eigenvalues with multiplicities m_i.

3.8.9.1 Matrix Functions

We can use the diagonal factorization (3.247) of the matrix $A = VCV^{-1}$ to define a function of the matrix that corresponds to a scalar-valued function of a scalar, $f(x)$,

$$f(A) = V\mathrm{diag}((f(c_1), \ldots, f(c_n)))V^{-1}, \tag{3.250}$$

if $f(\cdot)$ is defined for each eigenvalue c_i. (Notice the relationship of this definition to the Cayley-Hamilton theorem, page 138, and to Exercise 3.26.)

Another useful feature of the diagonal factorization of the matrix A in equation (3.247) is that it allows us to study functions of powers of A because $A^k = VC^kV^{-1}$. 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 $\mathrm{e}^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$, we can define the *matrix exponential* for the square matrix A as the matrix

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}, \tag{3.251}$$

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

$$\begin{aligned} e^A &= V \sum_{k=0}^{\infty} \frac{C^k}{k!} V^{-1} \\ &= V \operatorname{diag}\left((e^{c_1}, \ldots, e^{c_n})\right) V^{-1}. \end{aligned}$$

This is called the *matrix exponential* for the square matrix A.

The expression $\exp(A)$ is generally interpreted as $\exp(A) = (\exp(a_{ij}))$, while the expression e^A is interpreted as in equation (3.251), 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 `expm` for the matrix exponential. (In R, `expm` is in the `Matrix` package.)

3.8.10 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.

3.8.10.1 Orthogonality of Eigenvectors: Orthogonal Diagonalization

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 $v_1^{\mathrm{T}} v_2$. Multiplying this by c_2, we get

$$c_2 v_1^{\mathrm{T}} v_2 = v_1^{\mathrm{T}} A v_2 = v_2^{\mathrm{T}} A v_1 = c_1 v_2^{\mathrm{T}} v_1 = c_1 v_1^{\mathrm{T}} v_2.$$

Because $c_1 \neq c_2$, we have $v_1^{\mathrm{T}} v_2 = 0$.

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

$$\tilde{v}_j = \frac{1}{\|v_j - \langle v_i, v_j \rangle v_i\|} \left(v_j - \langle v_i, v_j \rangle v_i\right),$$

as in equation (2.56) on page 38, yielding a vector orthogonal to v_i. Now, we have

$$\begin{aligned} A\tilde{v}_j &= \frac{1}{\|v_j - \langle v_i, v_j\rangle v_i\|}\,(Av_j - \langle v_i, v_j\rangle Av_i) \\ &= \frac{1}{\|v_j - \langle v_i, v_j\rangle v_i\|}\,(c_j v_j - \langle v_i, v_j\rangle c_i v_i) \\ &= c_j \frac{1}{\|v_j - \langle v_i, v_j\rangle v_i\|}\,(v_j - \langle v_i, v_j\rangle v_i) \\ &= c_j \tilde{v}_j; \end{aligned}$$

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 (3.247) can be chosen to be orthogonal, and can be written as

$$A = VCV^{\mathrm{T}}, \tag{3.252}$$

where $VV^{\mathrm{T}} = V^{\mathrm{T}}V = I$, and so we also have

$$V^{\mathrm{T}}AV = C. \tag{3.253}$$

Such a matrix is orthogonally similar to a diagonal matrix formed from its eigenvalues.

Not only is a symmetric matrix orthogonally diagonalizable, any matrix that is orthogonally diagonalizable is symmetric. This is easy to see. Suppose $B = VCV^{\mathrm{T}}$, where V is orthogonal and C is diagonal. Then

$$B^{\mathrm{T}} = (VCV^{\mathrm{T}})^{\mathrm{T}} = VCV^{\mathrm{T}} = B; \tag{3.254}$$

hence, B is symmetric.

3.8.10.2 Spectral Decomposition

When A is symmetric and the eigenvectors v_i are chosen to be orthonormal,

$$I = \sum_i v_i v_i^{\mathrm{T}}, \tag{3.255}$$

so

$$\begin{aligned} A &= A\sum_i v_i v_i^{\mathrm{T}} \\ &= \sum_i Av_i v_i^{\mathrm{T}} \\ &= \sum_i c_i v_i v_i^{\mathrm{T}}. \end{aligned} \tag{3.256}$$

This representation is called the *spectral decomposition* of the symmetric matrix A. It is essentially the same as equation (3.252), so $A = VCV^{\mathrm{T}}$ 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

$$P_i = v_i v_i^{\mathrm{T}}. \tag{3.257}$$

Then we have

$$P_i P_i = P_i, \tag{3.258}$$

$$P_i P_j = 0 \text{ for } i \neq j, \tag{3.259}$$

$$\sum_i P_i = I, \tag{3.260}$$

and the spectral decomposition,

$$A = \sum_i c_i P_i. \tag{3.261}$$

The P_i are called *spectral projectors*.

The spectral decomposition also applies to powers of A,

$$A^k = \sum_i c_i^k v_i v_i^{\mathrm{T}}, \tag{3.262}$$

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 (3.261) with projection matrices that satisfy properties (3.258) through (3.260). 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 $x_j y_j^{\mathrm{H}} / y_j^{\mathrm{H}} x_j$. (Note that because the eigenvectors may not be real, we take the conjugate transpose.) This is Exercise 3.30.

3.8.10.3 Kronecker Products of Symmetric Matrices: Orthogonal Diagonalization

If A and B are symmetric, then $A \otimes B$ is symmetric. (We have already mentioned this fact, but it is easy to see using equation (3.100) on page 96.)

Now if A and B are symmetric, we can orthogonally diagonalize them as in equation (3.252): $A = VCV^{\mathrm{T}}$ and $B = UDU^{\mathrm{T}}$. This immediately yields an orthogonal diagonalization of the symmetric matrix $A \otimes B$:

$$\begin{aligned} A \otimes B &= VCV^{\mathrm{T}} \otimes UDU^{\mathrm{T}} \\ &= (V \otimes U)(C \otimes D)(V^{\mathrm{T}} \otimes U^{\mathrm{T}}), \end{aligned} \tag{3.263}$$

which we obtain by using equation (3.101) twice. Using equation (3.101) again, we have $(V \otimes U)(V^{\mathrm{T}} \otimes U^{\mathrm{T}}) = (VV^{\mathrm{T}} \otimes UU^{\mathrm{T}}) = I$ and since $C \otimes D$ is obviously diagonal, equation (3.263) is in the orthogonally diagonalized form of equation (3.252).

3.8.10.4 Quadratic Forms and the Rayleigh Quotient

Equation (3.256) 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 $x^{\mathrm{T}}Ax$ we have

$$\begin{aligned} x^{\mathrm{T}}Ax &= x^{\mathrm{T}} \sum_i c_i v_i v_i^{\mathrm{T}} x \\ &= \sum_i b^{\mathrm{T}} V^{\mathrm{T}} v_i v_i^{\mathrm{T}} V b c_i \\ &= \sum_i b_i^2 c_i. \end{aligned}$$

This immediately gives the inequality

$$x^{\mathrm{T}}Ax \leq \max\{c_i\} b^{\mathrm{T}} b.$$

(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 $x \neq 0$, $b^{\mathrm{T}}b = x^{\mathrm{T}}x$, and we have the important inequality

$$\frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x} \leq \max\{c_i\}. \tag{3.264}$$

Equality is achieved if x is the eigenvector corresponding to $\max\{c_i\}$, so we have

$$\max_{x \neq 0} \frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x} = \max\{c_i\}. \tag{3.265}$$

If $c_1 > 0$, this is the spectral radius, $\rho(A)$.

The expression on the left-hand side in (3.264) as a function of x is called the *Rayleigh quotient* of the symmetric matrix A and is denoted by $R_A(x)$:

$$\begin{aligned} R_A(x) &= \frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x} \\ &= \frac{\langle x,\, Ax\rangle}{\langle x,\, x\rangle}. \end{aligned} \tag{3.266}$$

Because if $x \neq 0$, $x^{\mathrm{T}}x > 0$, it is clear that the Rayleigh quotient is nonnegative for all x if and only if A is nonnegative definite, and it is positive for all x if and only if A is positive definite.

3.8.10.5 The Fourier Expansion

The $v_i v_i^{\mathrm{T}}$ matrices in equation (3.256) have the property that $\langle v_i v_i^{\mathrm{T}}, v_j v_j^{\mathrm{T}}\rangle = 0$ for $i \neq j$ and $\langle v_i v_i^{\mathrm{T}}, v_i v_i^{\mathrm{T}}\rangle = 1$, and so the spectral decomposition is a Fourier expansion as in equation (3.113) and the eigenvalues are Fourier coefficients. From equation (3.114), we see that the eigenvalues can be represented as the inner product

$$c_i = \langle A,\, v_i v_i^{\mathrm{T}}\rangle. \tag{3.267}$$

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 $\{v_1 v_1^{\mathrm{T}}, \ldots, v_n v_n^{\mathrm{T}}\}$ are partial sums of the form of equation (3.256). In Sect. 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.

3.8.10.6 Powers of a Symmetric Matrix

If (c, v) is an eigenpair of the symmetric matrix A with $v^{\mathrm{T}}v = 1$, then for any $k = 1, 2, \ldots$,

$$\left(A - cvv^{\mathrm{T}}\right)^k = A^k - c^k vv^{\mathrm{T}}. \tag{3.268}$$

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 $k - 1$

$$\left(A - cvv^{\mathrm{T}}\right)^{k-1} = A^{k-1} - c^{k-1} vv^{\mathrm{T}},$$

then by multiplying both sides by $(A - cvv^{\mathrm{T}})$, we see it is true for k:

$$\begin{aligned} \left(A - cvv^{\mathrm{T}}\right)^k &= \left(A^{k-1} - c^{k-1} vv^{\mathrm{T}}\right)\left(A - cvv^{\mathrm{T}}\right) \\ &= A^k - c^{k-1} vv^{\mathrm{T}} A - cA^{k-1} vv^{\mathrm{T}} + c^k vv^{\mathrm{T}} \\ &= A^k - c^k vv^{\mathrm{T}} - c^k vv^{\mathrm{T}} + c^k vv^{\mathrm{T}} \end{aligned}$$

$$= A^k - c^k v v^{\mathrm{T}}.$$

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 $w^{\mathrm{T}}v = 1$. (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 $A^{\mathrm{T}}w = cw$.) The only property of symmetry used above was that we could scale $v^{\mathrm{T}}v$ to be 1; hence, we just need $w^{\mathrm{T}}v \neq 0$. 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 Sects. 8.7.2 and 8.7.3, positive matrices and irreducible nonnegative matrices.

If w and v are left and right eigenvectors of A associated with the same eigenvalue c and $w^{\mathrm{T}}v = 1$, then for $k = 1, 2, \ldots$,

$$\left(A - cvw^{\mathrm{T}}\right)^k = A^k - c^k v w^{\mathrm{T}}. \tag{3.269}$$

We can prove this by induction as above.

3.8.10.7 The Trace and Sums of Eigenvalues

For a general $n \times n$ matrix A with eigenvalues $c_1, \ldots, c_n$, we have $\mathrm{tr}(A) = \sum_{i=1}^n c_i$. (This is equation (3.228).) This is particularly easy to see for symmetric matrices because of equation (3.252), rewritten as $V^{\mathrm{T}}AV = C$, 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

$$\mathrm{tr}(U^{\mathrm{T}}AU) \leq \sum_{i=1}^{k} c_i. \tag{3.270}$$

To see this, we represent U in terms of the columns of V, which span $\mathbb{R}^n$, as $U = VX$. Hence,

$$\begin{aligned} \mathrm{tr}(U^{\mathrm{T}}AU) &= \mathrm{tr}(X^{\mathrm{T}}V^{\mathrm{T}}AVX) \\ &= \mathrm{tr}(X^{\mathrm{T}}CX) \\ &= \sum_{i=1}^{n} x_i^{\mathrm{T}} x_i \, c_i, \end{aligned} \tag{3.271}$$

where x_i^{T} is the i^{th} row of X.

Now $X^{\mathrm{T}}X = X^{\mathrm{T}}V^{\mathrm{T}}VX = U^{\mathrm{T}}U = I_k$, so either $x_i^{\mathrm{T}}x_i = 0$ or $x_i^{\mathrm{T}}x_i = 1$, and $\sum_{i=1}^n x_i^{\mathrm{T}}x_i = k$. Because $c_1 \geq \cdots \geq c_n$, therefore $\sum_{i=1}^n x_i^{\mathrm{T}}x_i \, c_i \leq \sum_{i=1}^k c_i$, and so from equation (3.271) we have $\mathrm{tr}(U^{\mathrm{T}}AU) \leq \sum_{i=1}^k c_i$.

3.8.11 Positive Definite and Nonnegative Definite Matrices

The factorization of symmetric matrices in equation (3.252) yields some useful properties of positive definite and nonnegative definite matrices (introduced on page 91). We will briefly discuss these properties here and then return to the subject in Sect. 8.3 and discuss more properties of positive definite and nonnegative definite matrices.

3.8.11.1 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 (3.252) 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 $x^{\mathrm{T}}Ax = x^{\mathrm{T}}VCV^{\mathrm{T}}x = y^{\mathrm{T}}Cy$, where $y = V^{\mathrm{T}}x$, and so

$$x^{\mathrm{T}}Ax > (\geq)\, 0$$

if and only if

$$y^{\mathrm{T}}Cy > (\geq)\, 0.$$

This, together with the resulting inequality (3.161) on page 114, implies that if P is a nonsingular matrix and D is a diagonal matrix, $P^{\mathrm{T}}DP$ 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.

3.8.11.2 Inverse of Positive Definite Matrices

If A is positive definite and $A = VCV^{\mathrm{T}}$ as in equation (3.252), then $A^{-1} = VC^{-1}V^{\mathrm{T}}$, and A^{-1} is positive definite because the elements of C^{-1} are positive.

3.8.11.3 Diagonalization of Positive Definite Matrices

If A is positive definite, the elements of the diagonal matrix C in equation (3.252) are positive, and so their square roots can be absorbed into V to form a nonsingular matrix P. The diagonalization in equation (3.253), $V^{\mathrm{T}}AV = C$, can therefore be reexpressed as

$$P^{\mathrm{T}}AP = I. \tag{3.272}$$

3.8.11.4 Square Roots of Positive and Nonnegative Definite Matrices

The factorization (3.252) 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 (3.252): $A = VCV^{\mathrm{T}}$. Now, let S be a diagonal matrix whose elements are the nonnegative square roots of the corresponding elements of C. Then $(VSV^{\mathrm{T}})^2 = A$; hence, we write

$$A^{\frac{1}{2}} = VSV^{\mathrm{T}} \tag{3.273}$$

and call this matrix the *square root* of A. This definition of the square root of a matrix is an instance of equation (3.250) 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.

Notice that if $A = I_2$ (the identity) and if $J = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, then $J^2 = A$, but by the definition, J is not a square root of A.

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 Sect. 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.)

3.8.12 Generalized Eigenvalues and Eigenvectors

The characterization of an eigenvalue as a root of the determinant equation (3.220) can be extended to define a *generalized eigenvalue* of the square matrices A and B to be a root in c of the equation

$$\det(A - cB) = 0 \tag{3.274}$$

if a root exists.

Equation (3.274) is equivalent to $A - cB$ being singular; that is, for some c and some nonzero, finite v,

$$Av = cBv. \tag{3.275}$$

Such a c (if it exists) is called a *generalized eigenvalue* of A and B, and such a v (if it exists) is called a *generalized eigenvector* of A and B. In contrast to the existence of eigenvalues of any square matrix with finite elements, the generalized eigenvalues of two matrices may not exist; that is, they may be infinite. Notice that if (and only if) c is nonzero and finite, the roles of A and B can be interchanged in equation (3.275), and the generalized eigenvalue of B and A is $1/c$.

If A and B are $n \times n$ (that is, square) and B is nonsingular, then all n generalized 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 $0 = \det(AB^{-1} - c_0 I) = \det(B^{-1}A - c_0 I) = \det(A - c_0 B) = 0$. 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 also yields some useful properties, which we will discuss in Sect. 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.

3.8.12.1 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).

3.8.13 Singular Values and the Singular Value Decomposition (SVD)

An $n \times m$ matrix A can be factored as

$$A = UDV^{\mathrm{T}}, \tag{3.276}$$

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 (3.276) 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.

The SVD, which is unique, as we establish below, is one of the most important and most useful decompositions in all of matrix theory and applications.

There are $\min(n, m)$ singular values. We can rearrange the entries in D so that $d_1 \geq \cdots \geq d_{\min(n,m)}$, and by rearranging the columns of U correspondingly, nothing is changed.

We see that the SVD exists for any matrix by forming a square symmetric matrix and then using the decomposition in equation (3.252) on page 154. Let A be an $n \times m$ matrix A, and form $A^{\mathrm{T}}A = VCV^{\mathrm{T}}$. If $n \geq m$, we have

$$\begin{aligned} A^{\mathrm{T}}A &= VCV^{\mathrm{T}} \\ &= V[I\ 0] \begin{bmatrix} C \\ 0 \end{bmatrix} V^{\mathrm{T}} \\ &= \begin{bmatrix} V & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} C \\ 0 \end{bmatrix} V^{\mathrm{T}} \\ &= UDV^{\mathrm{T}}, \end{aligned}$$

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.

This same development follows for AA^{T}, and it is clear that the nonzero elements of the corresponding "C" matrix are the same (or property 14 on page 140 ensures that they are the same.)

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 (3.158) and (3.159).)

From this development, we see that the squares of the singular values of A are the eigenvalues of $A^{\mathrm{T}}A$ and of AA^{T}, which are necessarily nonnegative. To state this more clearly (and using some additional facts developed previously, including property 13 on page 140), let A be an $n \times m$ matrix with rank r, and let d be a singular value of A. We have

- $c = d^2$ is an eigenvalue of $A^{\mathrm{T}}A$;
- $c = d^2$ is an eigenvalue of AA^{T};
- if c is a nonzero eigenvalue of $A^{\mathrm{T}}A$, then there is a singular value d of A such that $d^2 = c$; and
- there are r nonzero singular values of A, and r nonzero eigenvalues of $A^{\mathrm{T}}A$ and of AA^{T}.

These relationships between singular values and eigenvalues are some of the most important properties of singular values and the singular value de-

composition. In particular, from these we can see that the singular value decomposition is unique (with the same qualifications attendant to uniqueness of eigenvalues and eigenvectors, relating to ordering of the elements and selection of vectors corresponding to nonunique values).

An additional observation is that if A is symmetric, the singular values of A are the absolute values of the eigenvalues of A.

From the factorization (3.276) defining the singular values, we see that

- the singular values of A^{T} are the same as those of A.

As pointed out above, 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.

We often partition D to separate the zero singular values. If the rank of the matrix is r, we have $d_1 \geq \cdots \geq d_r > 0$ (with the common indexing), 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 $D_r = \mathrm{diag}((d_1, \ldots, d_r))$.

3.8.13.1 The Fourier Expansion in Terms of the Singular Value Decomposition

From equation (3.276), we see that the general matrix A with rank r also has a Fourier expansion, similar to equation (3.256), in terms of the singular values and outer products of the columns of the U and V matrices:

$$A = \sum_{i=1}^{r} d_i u_i v_i^{\mathrm{T}}. \tag{3.277}$$

This is also called a spectral decomposition. The $u_i v_i^{\mathrm{T}}$ matrices in equation (3.277) have the property that $\langle u_i v_i^{\mathrm{T}}, u_j v_j^{\mathrm{T}} \rangle = 0$ for $i \neq j$ and $\langle u_i v_i^{\mathrm{T}}, u_i v_i^{\mathrm{T}} \rangle = 1$, and so the spectral decomposition is a Fourier expansion as in equation (3.113), 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 (3.114), we see that the singular values can be represented as the inner product

$$d_i = \langle A, u_i v_i^{\mathrm{T}} \rangle.$$

After we have discussed matrix norms in the next section, we will formulate Parseval's identity for this Fourier expansion.

The spectral decomposition is a *rank-one decomposition*, since each of the matrices $u_i v_i^{\mathrm{T}}$ has rank one.

3.9 Matrix Norms

Norms on matrices are scalar functions of matrices with the three properties on page 25 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 25, 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.

A matrix norm, as any norm, is necessarily convex. (See page 26.)

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, $\|A^{\mathrm{T}}\| \neq \|A\|$. 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 (3.110), 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

$$\|A^k\| \leq \|A\|^k \tag{3.278}$$

for any positive integer k.

A matrix norm $\|\cdot\|$ is *orthogonally 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 $\|\cdot\|_{\mathrm{v}}$ and a matrix norm as $\|\cdot\|_{\mathrm{M}}$. (This notation is meant to be generic; that is, $\|\cdot\|_{\mathrm{v}}$ represents any vector norm.) For the matrix $A \in \mathbb{R}^{n\times m}$, the matrix norm $\|\cdot\|_{\mathrm{M}}$ *induced* by $\|\cdot\|_{\mathrm{v}}$ is defined by

$$\|A\|_{\mathrm{M}} = \max_{x\neq 0} \frac{\|Ax\|_{\mathrm{v}}}{\|x\|_{\mathrm{v}}}. \tag{3.279}$$

(Note that there are some minor subtleties here; $Ax \in \mathbb{R}^n$ while $x \in \mathbb{R}^m$, so the two vector norms are actually different. Of course, in practice, an induced norm is defined in terms of vector norms of the same "type", for example L_p norms with the same p.)

An induced matrix norm is also sometimes called an *operator norm*.

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 (3.279) 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 (3.279) 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 (3.279) that

$$\|Ax\| \leq \|A\|\,\|x\| \tag{3.280}$$

because $\|x\| \geq 0$.

3.9.1.1 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

$$\|A\|_p = \max_{\|x\|_p=1} \|Ax\|_p. \tag{3.281}$$

(Notice that the restriction on $\|x\|_p$ makes this an induced norm as defined in equation (3.279). 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_∞ norms have interesting simplifications of equation (3.279):

$$\|A\|_1 = \max_j \sum_i |a_{ij}|, \tag{3.282}$$

so the L_1 is also called the *column-sum norm*; and

$$\|A\|_\infty = \max_i \sum_j |a_{ij}|, \tag{3.283}$$

so the L_∞ is also called the *row-sum norm*. We see these relationships by considering the L_p norm of the vector

$$v = (a_{1*}^{\mathrm{T}}x, \ldots, a_{n*}^{\mathrm{T}}x),$$

where a_{i*} 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 $\sum_i |a_{i*}^{\mathrm{T}}x|$. 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 $|\sum_i a_{ik}| \geq |\sum_i a_{ij}|$, 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 (3.282).

For the row-sum norm, the L_∞ norm of v is

$$\max_i |a_{i*}^{\mathrm{T}}x| = \max_i \sum_j |a_{ij}|\,|x_j|$$

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 ± 1. The maximum $|a_{i*}^{\mathrm{T}}x|$ 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 (3.283).

From equations (3.282) and (3.283), we see that

$$\|A^{\mathrm{T}}\|_\infty = \|A\|_1. \tag{3.284}$$

Alternative formulations of the L_2 norm of a matrix are not so obvious from equation (3.281). 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 142):

$$\|A\|_2 = \sqrt{\rho(A^{\mathrm{T}}A)}, \tag{3.285}$$

(see Exercise 3.34, page 182). 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 $A^{\mathrm{T}}A$ are the same as those of AA^{T}; hence, $\|A^{\mathrm{T}}\|_2 = \|A\|_2$.

For Q orthogonal, the L_2 vector norm has the important property

$$\|Qx\|_2 = \|x\|_2 \tag{3.286}$$

(see Exercise 3.35a, page 182). 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 (3.286) that

$$\|Q\|_2 = 1. \tag{3.287}$$

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).

3.9.1.2 L_1, L_2, and L_∞ Norms of Symmetric Matrices

For a symmetric matrix A, we have the obvious relationships

$$\|A\|_1 = \|A\|_\infty \tag{3.288}$$

and, from equation (3.285),

$$\|A\|_2 = \rho(A). \tag{3.289}$$

3.9.2 The Frobenius Norm—The "Usual" Norm

The *Frobenius norm* is defined as

$$\|A\|_{\mathrm{F}} = \sqrt{\sum_{i,j} a_{ij}^2}. \tag{3.290}$$

It is easy to see that this measure has the consistency property (Exercise 3.37), as a norm must. The Frobenius norm is sometimes called the *Euclidean matrix norm* and denoted by $\|\cdot\|_{\mathrm{E}}$, although the L_2 matrix norm is more directly based on the Euclidean vector norm, as we mentioned above. We will usually use the notation $\|\cdot\|_{\mathrm{F}}$ 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 $\|A^{\mathrm{T}}\|_{\mathrm{F}} = \|A\|_{\mathrm{F}}$. We have seen that the L_2 matrix norm also has this property.

Another important property of the Frobenius norm that is obvious from the definition is

$$\|A\|_{\mathrm{F}} = \sqrt{\mathrm{tr}(A^{\mathrm{T}}A)} \tag{3.291}$$

$$= \sqrt{\langle A, A\rangle}; \tag{3.292}$$

that is,

- the Frobenius norm is the norm that arises from the matrix inner product (see page 97).

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:

$$\|A\|_{\mathrm{F}} = \sqrt{\sum c_i \bar{c}_i}, \tag{3.293}$$

and if A is also symmetric,

$$\|A\|_{\mathrm{F}} = \sqrt{\sum c_i^2}, \tag{3.294}$$

These follow from equation (3.291) and equation (3.228) on page 141.

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

$$\mathrm{angle}(A, B) = \cos^{-1}\left(\frac{\langle A, B\rangle}{\|A\|_{\mathrm{F}}\|B\|_{\mathrm{F}}}\right). \tag{3.295}$$

If Q is an $n \times m$ orthogonal matrix, then

$$\|Q\|_{\mathrm{F}} = \sqrt{m} \tag{3.296}$$

(see equation (3.216)).

If A and B are orthogonally similar (see equation (3.242)), then

$$\|A\|_{\mathrm{F}} = \|B\|_{\mathrm{F}};$$

that is, the Frobenius norm is an orthogonally invariant norm. To see this, let $A = Q^{\mathrm{T}}BQ$, where Q is an orthogonal matrix. Then

$$\begin{aligned}\|A\|_{\mathrm{F}}^2 &= \mathrm{tr}(A^{\mathrm{T}}A)\\ &= \mathrm{tr}(Q^{\mathrm{T}}B^{\mathrm{T}}QQ^{\mathrm{T}}BQ)\end{aligned}$$

$$\begin{aligned} &= \mathrm{tr}(B^{\mathrm{T}}BQQ^{\mathrm{T}}) \\ &= \mathrm{tr}(B^{\mathrm{T}}B) \\ &= \|B\|_{\mathrm{F}}^2. \end{aligned}$$

(The norms are nonnegative, of course, and so equality of the squares is sufficient.)

3.9.2.1 The Frobenius Norm and the Singular Values

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 (3.277), we mentioned that the singular values have the general properties of Fourier coefficients; for example, they satisfy Parseval's identity, equation (2.60), on page 41. 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 it is the L_2 norm of the vector of singular values of the matrix. For the $n \times m$ matrix A, let d be the $\min(n, m)$-vector of singular values of A. Then

$$\|A\|_{\mathrm{F}}^2 = \|d\|_2. \tag{3.297}$$

Compare equations (3.293) and (3.294) for square matrices.

3.9.3 Other Matrix Norms

There are two different ways of generalizing the Frobenius norm. One is a simple generalization of the definition in equation (3.290). For $p \geq 1$, it is the *Frobenius p norm*:

$$\|A\|_{\mathrm{F}_p} = \left(\sum_{i,j} |a_{ij}|^p \right)^{1/p}. \tag{3.298}$$

Some people refer to this as the L_p norm of the matrix. As we have seen, the L_p matrix norm is different, but there is a simple relationship of the Frobenius p matrix norm to the L_p vector norm:

$$\|A\|_{\mathrm{F}_p} = \|\mathrm{vec}(A)\|_p. \tag{3.299}$$

This relationship of the matrix norm to a vector norm sometimes makes computational problems easier.

The Frobenius 2 norm is the ordinary Frobenius norm.

Another generalization of the Frobenius norm arises from its relation to the singular values given in equation (3.297). For $p \geq 1$, it is the *Schatten p norm*:

$$\|A\|_{\mathrm{S}_p} = \|d\|_p, \tag{3.300}$$

where d is the vector of singular values of A.

The Schatten 2 norm is the ordinary Frobenius norm.

The Schatten 1 norm is called the *nuclear norm* (because of its relationship to "nuclear operators", which are linear operators that preserve local convexity). It is also sometimes called the *trace norm*, because

$$\|d\|_1 = \mathrm{tr}\left((A^{\mathrm{T}}A)^{1/2}\right). \tag{3.301}$$

The Schatten ∞ norm is the spectral norm.

3.9.4 Matrix Norm Inequalities

There is an equivalence among any two matrix norms similar to that of expression (2.39) 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,

$$r\|A\|_b \leq \|A\|_a \leq s\|A\|_b. \tag{3.302}$$

We will not prove this result in general but, in Exercise 3.39, 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 (3.302):

$$\|A\|_\infty \leq \sqrt{m}\,\|A\|_{\mathrm{F}}, \tag{3.303}$$

$$\|A\|_{\mathrm{F}} \leq \sqrt{\min(n,m)}\,\|A\|_2, \tag{3.304}$$

$$\|A\|_2 \leq \sqrt{m}\,\|A\|_1, \tag{3.305}$$

$$\|A\|_1 \leq \sqrt{n}\,\|A\|_2, \tag{3.306}$$

$$\|A\|_2 \leq \|A\|_{\mathrm{F}}, \tag{3.307}$$

$$\|A\|_{\mathrm{F}} \leq \sqrt{n}\,\|A\|_\infty. \tag{3.308}$$

See Exercise 3.40 on page 182.

Compare these inequalities with those for L_p vector norms on page 28. 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 (2.34):

$$\|x\|_\infty \leq \|x\|_2 \leq \|x\|_1.$$

There is a related inequality involving matrices:

$$\|A\|_2^2 \leq \|A\|_1 \|A\|_\infty. \tag{3.309}$$

3.9.5 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 (3.289), the spectral radius is not a norm (see Exercise 3.41a).

We have for any norm $\|\cdot\|$ and any square matrix A that

$$\rho(A) \leq \|A\|. \tag{3.310}$$

To see this, we consider the associated eigenvalue and eigenvector, c_i and v_i, and form the matrix $V = [v_i|0|\cdots|0]$. This yields $c_i V = AV$, and by the consistency property of any matrix norm,

$$\begin{aligned} |c_i|\|V\| &= \|c_i V\| \\ &= \|AV\| \\ &\leq \|A\|\,\|V\|, \end{aligned}$$

or

$$|c_i| \leq \|A\|,$$

(see also Exercise 3.41b).

The inequality (3.310) and the L_1 and L_∞ 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. (These were inequalities (3.235) and (3.236) on page 142.)

The inequality (3.310) and equation (3.289) also yield a minimum property of the L_2 norm of a symmetric matrix A:

$$\|A\|_2 \leq \|A\|.$$

3.9.6 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 32). 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 (3.310), 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.

3.9.6.1 Conditions for Convergence of a Sequence of Powers to 0

For a square matrix A, we have the important fact that

$$A^k \to 0, \quad \text{if } \|A\| < 1, \tag{3.311}$$

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 (3.278) 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, $A^k x \to 0$; in particular, for the eigenvector $v_1 \neq 0$ corresponding to the dominant eigenvalue c_1, 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:

$$A^k \to 0 \quad \text{if } \rho(A) < 1. \tag{3.312}$$

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 (3.311) to establish the convergence.

Let $A = QTQ^{\mathrm{T}}$ 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 $D = \mathrm{diag}((d^1, \ldots, d^n))$. Notice that DTD^{-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 DTD^{-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

$$\|DTD^{-1}\|_1 = \max_j \left(|c_j| + \sum_{i=1}^{j-1} d^{-(j-i)}|t_{ij}| \right) < \rho(A) + \epsilon.$$

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

$$\|X\|_d = \|(QD^{-1})^{-1} X (QD^{-1})\|_1. \tag{3.313}$$

It is clear that $\|\cdot\|_d$ is a norm (Exercise 3.42). Furthermore,

$$\begin{aligned}\|A\|_d &= \|(QD^{-1})^{-1}A(QD^{-1})\|_1 \\ &= \|DTD^{-1}\|_1 \\ &< \rho(A) + \epsilon,\end{aligned}$$

and so if $\rho(A) < 1$, ϵ and d can be chosen so that $\|A\|_d < 1$, and by equation (3.311) above, we have $A^k \to 0$; hence, we conclude that

$$A^k \to 0 \quad \text{if and only if } \rho(A) < 1. \tag{3.314}$$

Informally, we see that A^k goes to 0 more rapidly the smaller is $\rho(A)$.

We will discuss convergence of a sequence of powers of an important special class of matrices with spectral radii possibly greater than or equal to 1 on page 378.

3.9.6.2 Another Perspective on the Spectral Radius: Relation to Norms

From inequality (3.310) and the fact that $\rho(A^k) = \rho(A)^k$, we have

$$\rho(A) \leq \|A^k\|^{1/k}, \tag{3.315}$$

where $\|\cdot\|$ is any matrix norm. Now, for any $\epsilon > 0$, $\rho\big(A/(\rho(A)+\epsilon)\big) < 1$ and so

$$\lim_{k\to\infty} \big(A/(\rho(A)+\epsilon)\big)^k = 0$$

from expression (3.314); hence,

$$\lim_{k\to\infty} \frac{\|A^k\|}{(\rho(A)+\epsilon)^k} = 0.$$

There is therefore a positive integer M_ϵ 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

$$\lim_{k\to\infty} \|A^k\|^{1/k} = \rho(A). \tag{3.316}$$

Compare this with the inequality (3.310).

3.9.6.3 Convergence of a Power Series: Inverse of $I - A$

Consider the power series in an $n \times n$ matrix such as in equation (3.186) on page 120,

$$I + A + A^2 + A^3 + \cdots .$$

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 (3.186). Therefore,

$$(I - A)^{-1} = I + A + A^2 + A^3 + \cdots \quad \text{if } \|A\| < 1. \tag{3.317}$$

3.9.6.4 Nilpotent Matrices

As we discussed on page 77, for some nonzero square matrices, $A^k = 0$ for a finite integral value of k. If $A^2 = 0$, such a matrix is a *nilpotent* matrix (otherwise, it is nilpotent with an index greater than 2). A matrix such as we discussed above for which $A^k \to 0$, but for any finite k, $A^k \neq 0$, is not called a nilpotent matrix.

From the definition, it is clear that the Drazin inverse of any nilpotent matrix is 0.

We have seen in equation (3.314) that $A^k \to 0$ if and only if $\rho(A) < 1$. The condition in equation (3.311) on any norm is not necessary, however; that is, if $A^k \to 0$, it may be the case that, for some norm, $\|A\| > 1$. In fact, even for an idempotent matrix (for which $A^k = 0$ for finite k), it may be the case that $\|A\| > 1$. A simple example is

$$A = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}.$$

For this matrix, $A^2 = 0$, yet $\|A\|_1 = \|A\|_2 = \|A\|_\infty = \|A\|_{\mathrm{F}} = 2$.

At this point, I list some more properties of nilpotent matrices that involve concepts we had not introduced when we first discussed nilpotent matrices. It is easy to see that if $A_{n\times n}$ is nilpotent, then

$$\mathrm{tr}(A) = 0, \tag{3.318}$$

$$\det(A) = 0, \tag{3.319}$$

$$\rho(A) = 0, \tag{3.320}$$

(that is, all eigenvalues of A are 0), and

$$\text{rank}(A) \leq n - 1. \tag{3.321}$$

You are asked to supply the proofs of these statements in Exercise 3.43b.

In applications, for example in time series or other stochastic processes, because of expression (3.314), 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 Sect. 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 428; or variable selection as in Sect. 9.5.2, 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 Sect. 9.5.6).

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.

Finally, we may wish to represent a matrix as a sum or a product of other matrices with restrictions on those matrices that do not allow an exact representation. (A nonnegative factorization as discussed in Sect. 5.10.1 is an example.)

3.10.1 Measures of the Difference Between 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 32. If $\widetilde{A}$ is an approximation to A, we could measure the quality of the approximation by $\Delta(A, \widetilde{A}) = \|A - \widetilde{A}\|$ for some norm $\|\cdot\|$. The measure $\Delta(A, \widetilde{A})$ is a metric, as defined on page 32, and is a common way of measuring the "distance" between two matrices.

Other ways of measuring the difference between two matrices may be based on how much the entropy of one divergences from that of the other. This may make sense if all elements in the matrices are positive. The Kullback-Leibler divergence between distributions is based on this idea. Because one distribution is used to normalize the other one, the Kullback-Leibler divergence is not a metric. If all elements of the matrices $\widetilde{A}$ and A are positive, the Kullback-Leibler divergence measure for how much the matrix $\widetilde{A}$ differs from A is

$$d_{\mathrm{KL}}(A - \widetilde{A}) = \sum_{ij} \left(\tilde{a}_{ij} \log \left(\frac{\tilde{a}_{ij}}{a_{ij}} \right) - \tilde{a}_{ij} + a_{ij} \right). \tag{3.322}$$

The most commonly-used measure of the goodness of an approximation uses the norm that arises from the inner product (the Frobenius norm).

3.10.2 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 $\widetilde{A}$ in $\mathbb{R}^{n \times m}$ but with smaller rank, say k; that is, we want to find $\widetilde{A}$ of rank k such that

$$\|A - \widetilde{A}\|_{\mathrm{F}} \tag{3.323}$$

is a minimum for all $\widetilde{A} \in \mathbb{R}^{n \times m}$ of rank k.

We have an orthogonal basis in terms of the singular value decomposition, equation (3.277), 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 (2.65). 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 (2.65).) 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 $\|A - \widetilde{A}\|_{\mathrm{F}}^2$. Neither the Fourier expansion nor the restriction $\mathcal{V}(\widetilde{A}) \subset \mathcal{V}(A)$ permits 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 (3.323) that occurs within $\mathcal{V}(A)$, and a minimum is at the truncated Fourier expansion in the singular values (equation (3.277)).

To state this more precisely, let A be an $n \times m$ matrix of rank r with singular value decomposition

$$A = U \begin{bmatrix} D_r & 0 \\ 0 & 0 \end{bmatrix} V^{\mathrm{T}},$$

where $D_r = \mathrm{diag}((d_1, \ldots, d_r))$, 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 $k < r$,

$$\|A - X\|_{\mathrm{F}}^2 \geq \sum_{i=k+1}^{r} d_i^2, \tag{3.324}$$

and this minimum occurs for $X = \widetilde{A}$, where

$$\widetilde{A} = U \begin{bmatrix} D_k & 0 \\ 0 & 0 \end{bmatrix} V^{\mathrm{T}}. \tag{3.325}$$

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 $k \times m$ matrix, also of rank k. The minimization problem now is

$$\min_{Y} \|A - QY\|_{\mathrm{F}}$$

with the restriction $\mathrm{rank}(Y) = k$.

Now, expanding, completing the Gramian and using its nonnegative definiteness, and permuting the factors within a trace, we have

$$\begin{aligned}
\|A - QY\|_{\mathrm{F}}^2 &= \mathrm{tr}\left((A - QY)^{\mathrm{T}}(A - QY)\right) \\
&= \mathrm{tr}\left(A^{\mathrm{T}}A\right) + \mathrm{tr}\left(Y^{\mathrm{T}}Y - A^{\mathrm{T}}QY - Y^{\mathrm{T}}Q^{\mathrm{T}}A\right) \\
&= \mathrm{tr}\left(A^{\mathrm{T}}A\right) + \mathrm{tr}\left((Y - Q^{\mathrm{T}}A)^{\mathrm{T}}(Y - Q^{\mathrm{T}}A)\right) - \mathrm{tr}\left(A^{\mathrm{T}}QQ^{\mathrm{T}}A\right) \\
&\geq \mathrm{tr}\left(A^{\mathrm{T}}A\right) - \mathrm{tr}\left(Q^{\mathrm{T}}AA^{\mathrm{T}}Q\right).
\end{aligned}$$

The squares of the singular values of A are the eigenvalues of $A^{\mathrm{T}}A$, and so $\mathrm{tr}(A^{\mathrm{T}}A) = \sum_{i=1}^{r} d_i^2$. The eigenvalues of $A^{\mathrm{T}}A$ are also the eigenvalues of AA^{T}, and so, from inequality (3.270), $\mathrm{tr}(Q^{\mathrm{T}}AA^{\mathrm{T}}Q) \leq \sum_{i=1}^{k} d_i^2$, and so

$$\|A - X\|_{\mathrm{F}}^2 \geq \sum_{i=1}^{r} d_i^2 - \sum_{i=1}^{k} d_i^2;$$

hence, we have inequality (3.324). (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 Sect. 3.3.10.)

Direct expansion of $\|A - \widetilde{A}\|_{\mathrm{F}}^2$ yields

$$\mathrm{tr}\left(A^{\mathrm{T}}A\right) - 2\mathrm{tr}\left(A^{\mathrm{T}}\widetilde{A}\right) + \mathrm{tr}\left(\widetilde{A}^{\mathrm{T}}\widetilde{A}\right) = \sum_{i=1}^{r} d_i^2 - \sum_{i=1}^{k} d_i^2,$$

and hence $\widetilde{A}$ is the best rank k approximation to A under the Frobenius norm.

Equation (3.325) can be stated another way: the best approximation of A of rank k is

$$\widetilde{A} = \sum_{i=1}^{k} d_i u_i v_i^{\mathrm{T}}. \tag{3.326}$$

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 342, 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 Sect. 9.4).

Exercises

3.1. Vector spaces of matrices.
   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 (3.92) on page 93.

3.3. Show that for any quadratic form $x^{\mathrm{T}}Ax$ there is a symmetric matrix A_s such that $x^{\mathrm{T}}A_sx = x^{\mathrm{T}}Ax$. (The proof is by construction, with $A_s = \frac{1}{2}(A+A^{\mathrm{T}})$, first showing A_s is symmetric and then that $x^{\mathrm{T}}A_sx = x^{\mathrm{T}}Ax$.)

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 (3.95) is a metric (that is, show that it satisfies the properties listed on page 32).

3.6. Verify the relationships for Kronecker products shown in equations (3.97) through (3.103) on page 95.
Hint: Make liberal use of equation (3.96) and previously verified equations.

3.7. Verify the relationship between the vec function and Kronecker multiplication given in equation (3.106), $\mathrm{vec}(ABC) = (C^{\mathrm{T}} \otimes A)\mathrm{vec}(B)$.
Hint: Just determine an expression for the i^{th} term in the vector on either side of the equation.

3.8. Cauchy-Schwarz inequalities for matrices.
   a) Prove the Cauchy-Schwarz inequality for the dot product of matrices ((3.111), page 98), which can also be written as

$$(\mathrm{tr}(A^{\mathrm{T}}B))^2 \leq \mathrm{tr}(A^{\mathrm{T}}A)\mathrm{tr}(B^{\mathrm{T}}B).$$

   b) Prove the Cauchy-Schwarz inequality for determinants of matrices A and B of the same shape:

$$\det(A^{\mathrm{T}}B)^2 \leq \det(A^{\mathrm{T}}A)\det(B^{\mathrm{T}}B).$$

   Under what conditions is equality achieved?
   c) Let A and B be matrices of the same shape, and define

$$p(A, B) = \det(A^{\mathrm{T}}B).$$

   Is $p(\cdot,\cdot)$ an inner product? Why or why not?

3.9. Prove that a square matrix that is either row or column (strictly) diagonally dominant is nonsingular.

3.10. Prove that a positive definite matrix is nonsingular.

3.11. 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?

3.12. Bounds on ranks.

a) Show that the bound in inequality (3.128) is sharp by finding two matrices A and B such that $\text{rank}(AB) = \min(\text{rank}(A), \text{rank}(B))$.

b) Show that the bound in inequality (3.170) is sharp by finding an $n \times n$ matrix A and a matrix B with n rows such that $\text{rank}(AB) = \text{rank}(A) + \text{rank}(B) - n$.

c) Show that the bound in inequality (3.129) is sharp by finding two matrices A and B such that $\text{rank}(A + B) = \text{rank}(A) + \text{rank}(B)$.

d) Show that the bound in inequality (3.130) is sharp by finding two matrices A and B such that $\text{rank}(A + B) = |\text{rank}(A) - \text{rank}(B)|$.

3.13. The affine group $\mathcal{A}L(n)$.

a) What is the identity in $\mathcal{A}L(n)$?

b) Let (A, v) be an element of $\mathcal{A}L(n)$. What is the inverse of (A, v)?

3.14. Let A be an $n \times m$ matrix of rank one. Show that A can be written as an outer product

$$A = xy^{\mathrm{T}},$$

where x is some n-vector and y is some m-vector.

3.15. 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 (3.172) on page 118 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.

3.16. Verify the relationships shown in equations (3.176) through (3.183) on page 119. Do this by multiplying the appropriate matrices. For example, equation (3.176) 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 (3.173) 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.

3.17. Verify equation (3.184).

3.18. In equations (3.176) through (3.183) on page 119, 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.

3.19. Prove that if A is nonsingular and lower triangular, then A^{-1} is lower triangular.

3.20. By writing $AA^{-1} = I$, derive the expression for the inverse of a partitioned matrix given in equation (3.190).

3.21. Show that the expression given in equation (3.209) on page 128 is a Moore-Penrose inverse of A. (Show that properties 1 through 4 hold.)

3.22. Properties of Drazin inverses (page 129).

a) Show that a Drazin inverse is a g_1 inverse; that is,

$$AA^{\mathrm{D}}A = A.$$

b) Prove equation (3.212), for any square matrix A and any positive integer k,

$$A^{\mathrm{D}} = A^k(A^{2k+1})^+A^k;$$

inter alia, show that for positive integers j and k,

$$A^j(A^{2j+1})^+A^j = A^k(A^{2k+1})^+A^k.$$

3.23. Show that the expression given for the generalized inverse in equation (3.214) on page 131 is correct.

3.24. In computational explorations involving matrices, it is often convenient to work with matrices whose elements are integers. If eigenvalues are involved, it would be nice to know that the eigenvalues are also integers. This is similar in spirit to matrices with integral elements whose inverses also have integral elements, as was the problem considered in Exercise 3.15. Matrices like this also provide convenient test problems for algorithms or sogtware.
The use of the companion matrix (equation (3.225)) gives us a convenient way of obtaining "nice" matrices for numerically exploring properties of eigenvalues. Using other properties of eigenvalues/vectors such as those listed on page 136 and with similarity transforms, we can generate "interesting" matrices that have nice eigenvalues.
For instance, a 3×3 matrix in equation (3.237) was generated by choosing a set of eigenvalues $\{a, 1 + \mathrm{i}, 1 - \mathrm{i}\}$.
Next, I used the relationship between the eigenvalues of A and $A - dI$, and finally, I squared the matrix, so that the eigenvalues are squared. The resulting spectrum is $\{(a-d)^2, (1-d+\mathrm{i})^2, (1-d-\mathrm{i}\}$. After initializing a and d, the R statements are

```
B <- matrix(c(-d,0,2*a, 1,-d,-2*a+2, 0,1,a+2-d),nrow=3)
A <- B%*%B
```

```
eigen(A)
```

and the Matlab statements are

```
B = [-d, 0, 2*a;  1, -d, -2*a+2;  0, 1, a+2-d];
A = B*B;
eigen(A)
```

Can you tell what values of a and d were used in generating the matrix in equation (3.237) following these steps?

a) Using R, Matlab, or some other system you like, construct *two different* 3×3 matrices whose elements are all integers and whose eigenvalues are $\{7, 5, 3\}$.
b) Determine the six Gershgorin disks for each of your matrices. (Are they the same?)

3.25. Write formal proofs of the properties of eigenvalues/vectors listed on page 136.

3.26. 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.)

3.27. Write formal proofs of the properties of eigenvalues/vectors listed on page 139.

3.28. Prove that for any square matrix, the algebraic multiplicity of a given eigenvalue is at least as great as the geometric multiplicity of that eigenvalue.

3.29. 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 (3.241), let A be a 2×2 diagonal matrix (so you know its eigenvalues and eigenvectors) with unequal values along the diagonal, and let P be a 2×2 upper triangular matrix, so that you can invert it. Form B and check the eigenvectors.

3.30. Let A be a diagonalizable matrix (not necessarily symmetric) with a spectral decomposition of the form of equation (3.261), $A = \sum_i c_i P_i$. 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 $y_j^{\mathrm{H}} x_j \neq 0$.
b) Show that the projection matrix P_j is $x_j y_j^{\mathrm{H}} / y_j^{\mathrm{H}} x_j$.

3.31. If A is nonsingular, show that for any (conformable) vector x

$$(x^{\mathrm{T}} Ax)(x^{\mathrm{T}} A^{-1} x) \geq (x^{\mathrm{T}} x)^2.$$

Hint: Use the square roots and the Cauchy-Schwarz inequality.

3.32. Prove that the induced norm (page 165) is a matrix norm; that is, prove that it satisfies the consistency property.

3.33. Prove the inequality (3.280) for an induced matrix norm on page 165:

$$\|Ax\| \leq \|A\| \, \|x\|.$$

3.34. Prove that, for the square matrix A,

$$\|A\|_2^2 = \rho(A^{\mathrm{T}} A).$$

Hint: Show that $\|A\|_2^2 = \max x^{\mathrm{T}} A^{\mathrm{T}} Ax$ for any normalized vector x.

3.35. Let Q be an $n \times n$ orthogonal matrix, and let x be an n-vector.
a) Prove equation (3.286):

$$\|Qx\|_2 = \|x\|_2.$$

Hint: Write $\|Qx\|_2$ as $\sqrt{(Qx)^{\mathrm{T}} Qx}$.
b) Give examples to show that this does not hold for other norms.

3.36. 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_∞ norm.
c) Prove the triangle inequality for the matrix Frobenius norm.

3.37. Prove that the Frobenius norm satisfies the consistency property.

3.38. The Frobenius p norm and the Shatten p norm.
a) Prove that the expression in equation (3.298), the "Frobenius p norm", is indeed a norm.
b) Prove that the expression in equation (3.300), the "Shatten p norm", is indeed a norm.
c) Prove equation (3.301).

3.39. If $\|\cdot\|_a$ and $\|\cdot\|_b$ are matrix norms induced respectively by the vector norms $\|\cdot\|_{v_a}$ and $\|\cdot\|_{v_b}$, prove inequality (3.302); that is, show that there are positive numbers r and s such that, for any A,

$$r\|A\|_b \leq \|A\|_a \leq s\|A\|_b.$$

3.40. Prove inequalities (3.303) through (3.309), and show that the bounds are sharp by exhibiting instances of equality.

3.41. 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, $\rho(A) \leq \|A\|$.

3.42. Show that the function $\|\cdot\|_d$ defined in equation (3.313) is a norm.
Hint: Just verify the properties on page 164 that define a norm.

3.43. Nilpotent matrices.

a) Prove that a nilpotent matrix is singular without using the properties listed on page 174.

b) Prove equations (3.318) through (3.321).

3.44. Prove equations (3.324) and (3.325) under the restriction that $\mathcal{V}(X) \subseteq \mathcal{V}(A)$; that is, where $X = BL$ for a matrix B whose columns span $\mathcal{V}(A)$.