D Matrices

Matrices arise in numerous applications, including, but by no means limited to, scientific computing. If you have seen matrices before, much of the material in this appendix will be familiar to you, but some of it might be new. Section D.1 covers basic matrix definitions and operations, and Section D.2 presents some basic matrix properties.

D.1 Matrices and matrix operations

In this section, we review some basic concepts of matrix theory and some fundamental properties of matrices.

Matrices and vectors

A *matrix* is a rectangular array of numbers. For example,

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$
(D.1)

is a 2×3 matrix $A = (a_{ij})$, where for i = 1, 2 and j = 1, 2, 3, we denote the element of the matrix in row i and column j by a_{ij} . We use uppercase letters to denote matrices and corresponding subscripted lowercase letters to denote their elements. We denote the set of all $m \times n$ matrices with real-valued entries by $\mathbb{R}^{m \times n}$ and, in general, the set of $m \times n$ matrices with entries drawn from a set S by $S^{m \times n}$.

The *transpose* of a matrix A is the matrix A^{T} obtained by exchanging the rows and columns of A. For the matrix A of equation (D.1),

$$A^{\mathsf{T}} = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}.$$

A *vector* is a one-dimensional array of numbers. For example,

$$x = \begin{pmatrix} 2 \\ 3 \\ 5 \end{pmatrix}$$

is a vector of size 3. We sometimes call a vector of length n an **n-vector**. We use lowercase letters to denote vectors, and we denote the ith element of a size-n vector x by x_i , for i = 1, 2, ..., n. We take the standard form of a vector to be as a **column vector** equivalent to an $n \times 1$ matrix; the corresponding **row vector** is obtained by taking the transpose:

$$x^{T} = (2 \ 3 \ 5)$$
.

The *unit vector* e_i is the vector whose *i*th element is 1 and all of whose other elements are 0. Usually, the size of a unit vector is clear from the context.

A *zero matrix* is a matrix all of whose entries are 0. Such a matrix is often denoted 0, since the ambiguity between the number 0 and a matrix of 0s is usually easily resolved from context. If a matrix of 0s is intended, then the size of the matrix also needs to be derived from the context.

Square matrices

Square $n \times n$ matrices arise frequently. Several special cases of square matrices are of particular interest:

1. A *diagonal matrix* has $a_{ij} = 0$ whenever $i \neq j$. Because all of the off-diagonal elements are zero, we can specify the matrix by listing the elements along the diagonal:

$$\operatorname{diag}(a_{11}, a_{22}, \dots, a_{nn}) = \begin{pmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn} \end{pmatrix}.$$

2. The $n \times n$ identity matrix I_n is a diagonal matrix with 1s along the diagonal:

$$I_n = \operatorname{diag}(1, 1, \dots, 1)$$

$$= \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix}.$$

When I appears without a subscript, we derive its size from the context. The ith column of an identity matrix is the unit vector e_i .

3. A *tridiagonal matrix* T is one for which $t_{ij} = 0$ if |i - j| > 1. Nonzero entries appear only on the main diagonal, immediately above the main diagonal $(t_{i,i+1}$ for i = 1, 2, ..., n - 1), or immediately below the main diagonal $(t_{i+1,i}]$ for i = 1, 2, ..., n - 1:

$$T = \begin{pmatrix} t_{11} & t_{12} & 0 & 0 & \dots & 0 & 0 & 0 \\ t_{21} & t_{22} & t_{23} & 0 & \dots & 0 & 0 & 0 \\ 0 & t_{32} & t_{33} & t_{34} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & t_{n-2,n-2} & t_{n-2,n-1} & 0 \\ 0 & 0 & 0 & 0 & \dots & t_{n-1,n-2} & t_{n-1,n-1} & t_{n-1,n} \\ 0 & 0 & 0 & 0 & \dots & 0 & t_{n,n-1} & t_{nn} \end{pmatrix}.$$

4. An *upper-triangular matrix* U is one for which $u_{ij} = 0$ if i > j. All entries below the diagonal are zero:

$$U = \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & u_{nn} \end{pmatrix}.$$

An upper-triangular matrix is *unit upper-triangular* if it has all 1s along the diagonal.

5. A *lower-triangular matrix* L is one for which $l_{ij} = 0$ if i < j. All entries above the diagonal are zero:

$$L = \begin{pmatrix} l_{11} & 0 & \dots & 0 \\ l_{21} & l_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \dots & l_{nn} \end{pmatrix}.$$

A lower-triangular matrix is *unit lower-triangular* if it has all 1s along the diagonal.

6. A *permutation matrix* P has exactly one 1 in each row or column, and 0s elsewhere. An example of a permutation matrix is

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Such a matrix is called a permutation matrix because multiplying a vector x by a permutation matrix has the effect of permuting (rearranging) the elements of x. Exercise D.1-4 explores additional properties of permutation matrices.

7. A symmetric matrix A satisfies the condition $A = A^{T}$. For example,

$$\begin{pmatrix}
1 & 2 & 3 \\
2 & 6 & 4 \\
3 & 4 & 5
\end{pmatrix}$$

is a symmetric matrix.

Basic matrix operations

The elements of a matrix or vector are numbers from a number system, such as the real numbers, the complex numbers, or integers modulo a prime. The number system defines how to add and multiply numbers. We can extend these definitions to encompass addition and multiplication of matrices.

We define *matrix addition* as follows. If $A = (a_{ij})$ and $B = (b_{ij})$ are $m \times n$ matrices, then their matrix sum $C = (c_{ij}) = A + B$ is the $m \times n$ matrix defined by

$$c_{ij} = a_{ij} + b_{ij}$$

for i = 1, 2, ..., m and j = 1, 2, ..., n. That is, matrix addition is performed componentwise. A zero matrix is the identity for matrix addition:

$$A + 0 = A = 0 + A$$
.

If λ is a number and $A = (a_{ij})$ is a matrix, then $\lambda A = (\lambda a_{ij})$ is the **scalar multiple** of A obtained by multiplying each of its elements by λ . As a special case, we define the **negative** of a matrix $A = (a_{ij})$ to be $-1 \cdot A = -A$, so that the ij th entry of -A is $-a_{ij}$. Thus,

$$A + (-A) = 0 = (-A) + A$$
.

We use the negative of a matrix to define *matrix subtraction*: A - B = A + (-B).

We define *matrix multiplication* as follows. We start with two matrices A and B that are *compatible* in the sense that the number of columns of A equals the number of rows of B. (In general, an expression containing a matrix product AB is always assumed to imply that matrices A and B are compatible.) If $A = (a_{ik})$ is an $m \times n$ matrix and $B = (b_{kj})$ is an $n \times p$ matrix, then their matrix product C = AB is the $m \times p$ matrix $C = (c_{ij})$, where

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \tag{D.2}$$

for $i=1,2,\ldots,m$ and $j=1,2,\ldots,p$. The procedure SQUARE-MATRIX-MULTIPLY in Section 4.2 implements matrix multiplication in the straightforward manner based on equation (D.2), assuming that the matrices are square: m=n=p. To multiply $n\times n$ matrices, SQUARE-MATRIX-MULTIPLY performs n^3 multiplications and $n^2(n-1)$ additions, and so its running time is $\Theta(n^3)$.

Matrices have many (but not all) of the algebraic properties typical of numbers. Identity matrices are identities for matrix multiplication:

$$I_m A = A I_n = A$$

for any $m \times n$ matrix A. Multiplying by a zero matrix gives a zero matrix:

$$A 0 = 0$$
.

Matrix multiplication is associative:

$$A(BC) = (AB)C$$

for compatible matrices A, B, and C. Matrix multiplication distributes over addition:

$$A(B+C) = AB + AC,$$

$$(B+C)D = BD + CD.$$

For n > 1, multiplication of $n \times n$ matrices is not commutative. For example, if $A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, then

$$AB = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$BA = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

We define matrix-vector products or vector-vector products as if the vector were the equivalent $n \times 1$ matrix (or a $1 \times n$ matrix, in the case of a row vector). Thus, if A is an $m \times n$ matrix and x is an n-vector, then Ax is an m-vector. If x and y are n-vectors, then

$$x^{\mathrm{T}}y = \sum_{i=1}^{n} x_i y_i$$

is a number (actually a 1×1 matrix) called the *inner product* of x and y. The matrix xy^{T} is an $n \times n$ matrix Z called the *outer product* of x and y, with $z_{ij} = x_i y_j$. The *(euclidean) norm* ||x|| of an n-vector x is defined by

$$||x|| = (x_1^2 + x_2^2 + \dots + x_n^2)^{1/2}$$

= $(x^T x)^{1/2}$.

Thus, the norm of x is its length in n-dimensional euclidean space.

Exercises

D.1-1

Show that if A and B are symmetric $n \times n$ matrices, then so are A + B and A - B.

D.1-2

Prove that $(AB)^{T} = B^{T}A^{T}$ and that $A^{T}A$ is always a symmetric matrix.

D.1-3

Prove that the product of two lower-triangular matrices is lower-triangular.

D.1-4

Prove that if P is an $n \times n$ permutation matrix and A is an $n \times n$ matrix, then the matrix product PA is A with its rows permuted, and the matrix product AP is A with its columns permuted. Prove that the product of two permutation matrices is a permutation matrix.

D.2 Basic matrix properties

In this section, we define some basic properties pertaining to matrices: inverses, linear dependence and independence, rank, and determinants. We also define the class of positive-definite matrices.

Matrix inverses, ranks, and determinants

We define the *inverse* of an $n \times n$ matrix A to be the $n \times n$ matrix, denoted A^{-1} (if it exists), such that $AA^{-1} = I_n = A^{-1}A$. For example,

$$\left(\begin{array}{cc} 1 & 1 \\ 1 & 0 \end{array}\right)^{-1} = \left(\begin{array}{cc} 0 & 1 \\ 1 & -1 \end{array}\right).$$

Many nonzero $n \times n$ matrices do not have inverses. A matrix without an inverse is called *noninvertible*, or *singular*. An example of a nonzero singular matrix is

$$\left(\begin{array}{cc} 1 & 0 \\ 1 & 0 \end{array}\right).$$

If a matrix has an inverse, it is called *invertible*, or *nonsingular*. Matrix inverses, when they exist, are unique. (See Exercise D.2-1.) If A and B are nonsingular $n \times n$ matrices, then

$$(BA)^{-1} = A^{-1}B^{-1}$$
.

The inverse operation commutes with the transpose operation:

$$(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$$
.

The vectors x_1, x_2, \ldots, x_n are *linearly dependent* if there exist coefficients c_1, c_2, \ldots, c_n , not all of which are zero, such that $c_1x_1 + c_2x_2 + \cdots + c_nx_n = 0$. The row vectors $x_1 = (1 \ 2 \ 3), x_2 = (2 \ 6 \ 4),$ and $x_3 = (4 \ 11 \ 9)$ are linearly dependent, for example, since $2x_1 + 3x_2 - 2x_3 = 0$. If vectors are not linearly dependent, they are *linearly independent*. For example, the columns of an identity matrix are linearly independent.

The **column rank** of a nonzero $m \times n$ matrix A is the size of the largest set of linearly independent columns of A. Similarly, the **row rank** of A is the size of the largest set of linearly independent rows of A. A fundamental property of any matrix A is that its row rank always equals its column rank, so that we can simply refer to the **rank** of A. The rank of an $m \times n$ matrix is an integer between 0 and $\min(m, n)$, inclusive. (The rank of a zero matrix is 0, and the rank of an $n \times n$ identity matrix is n.) An alternate, but equivalent and often more useful, definition is that the rank of a nonzero $m \times n$ matrix A is the smallest number r such that there exist matrices B and C of respective sizes $m \times r$ and $r \times n$ such that

$$A = BC$$
.

A square $n \times n$ matrix has **full rank** if its rank is n. An $m \times n$ matrix has **full column rank** if its rank is n. The following theorem gives a fundamental property of ranks.

Theorem D.1

A square matrix has full rank if and only if it is nonsingular.

A *null vector* for a matrix A is a nonzero vector x such that Ax = 0. The following theorem (whose proof is left as Exercise D.2-7) and its corollary relate the notions of column rank and singularity to null vectors.

Theorem D.2

A matrix A has full column rank if and only if it does not have a null vector.

Corollary D.3

A square matrix A is singular if and only if it has a null vector.

The ij th **minor** of an $n \times n$ matrix A, for n > 1, is the $(n-1) \times (n-1)$ matrix $A_{[ij]}$ obtained by deleting the ith row and jth column of A. We define the **determinant** of an $n \times n$ matrix A recursively in terms of its minors by

$$\det(A) = \begin{cases} a_{11} & \text{if } n = 1, \\ \sum_{j=1}^{n} (-1)^{1+j} a_{1j} \det(A_{[1j]}) & \text{if } n > 1. \end{cases}$$

The term $(-1)^{i+j} \det(A_{[ij]})$ is known as the *cofactor* of the element a_{ij} .

The following theorems, whose proofs are omitted here, express fundamental properties of the determinant.

Theorem D.4 (Determinant properties)

The determinant of a square matrix A has the following properties:

- If any row or any column of A is zero, then det(A) = 0.
- The determinant of A is multiplied by λ if the entries of any one row (or any one column) of A are all multiplied by λ .
- The determinant of A is unchanged if the entries in one row (respectively, column) are added to those in another row (respectively, column).
- The determinant of A equals the determinant of A^{T} .
- The determinant of A is multiplied by -1 if any two rows (or any two columns) are exchanged.

Also, for any square matrices A and B, we have det(AB) = det(A) det(B).

Theorem D.5

An $n \times n$ matrix A is singular if and only if det(A) = 0.

Positive-definite matrices

Positive-definite matrices play an important role in many applications. An $n \times n$ matrix A is **positive-definite** if $x^{T}Ax > 0$ for all n-vectors $x \neq 0$. For example, the identity matrix is positive-definite, since for any nonzero vector $x = (x_1 \ x_2 \ \cdots \ x_n)^{T}$,

$$x^{\mathrm{T}} I_n x = x^{\mathrm{T}} x$$
$$= \sum_{i=1}^n x_i^2$$
$$> 0.$$

Matrices that arise in applications are often positive-definite due to the following theorem.

Theorem D.6

For any matrix A with full column rank, the matrix $A^{T}A$ is positive-definite.

Proof We must show that $x^{T}(A^{T}A)x > 0$ for any nonzero vector x. For any vector x,

$$x^{\mathrm{T}}(A^{\mathrm{T}}A)x = (Ax)^{\mathrm{T}}(Ax)$$
 (by Exercise D.1-2)
= $||Ax||^2$.

Note that $||Ax||^2$ is just the sum of the squares of the elements of the vector Ax. Therefore, $||Ax||^2 \ge 0$. If $||Ax||^2 = 0$, every element of Ax is 0, which is to say Ax = 0. Since A has full column rank, Ax = 0 implies x = 0, by Theorem D.2. Hence, A^TA is positive-definite.

Section 28.3 explores other properties of positive-definite matrices.

Exercises

D.2-1

Prove that matrix inverses are unique, that is, if B and C are inverses of A, then B = C.

D.2-2

Prove that the determinant of a lower-triangular or upper-triangular matrix is equal to the product of its diagonal elements. Prove that the inverse of a lower-triangular matrix, if it exists, is lower-triangular.

D.2-3

Prove that if P is a permutation matrix, then P is invertible, its inverse is P^{T} , and P^{T} is a permutation matrix.

D.2-4

Let A and B be $n \times n$ matrices such that AB = I. Prove that if A' is obtained from A by adding row j into row i, then subtracting column i from column j of B yields the inverse B' of A'.

D.2-5

Let A be a nonsingular $n \times n$ matrix with complex entries. Show that every entry of A^{-1} is real if and only if every entry of A is real.

D.2-6

Show that if A is a nonsingular, symmetric, $n \times n$ matrix, then A^{-1} is symmetric. Show that if B is an arbitrary $m \times n$ matrix, then the $m \times m$ matrix given by the product BAB^{T} is symmetric.

D.2-7

Prove Theorem D.2. That is, show that a matrix A has full column rank if and only if Ax = 0 implies x = 0. (*Hint:* Express the linear dependence of one column on the others as a matrix-vector equation.)

D.2-8

Prove that for any two compatible matrices A and B,

$$rank(AB) \leq min(rank(A), rank(B))$$
,

where equality holds if either A or B is a nonsingular square matrix. (*Hint:* Use the alternate definition of the rank of a matrix.)

Problems

D-1 Vandermonde matrix

Given numbers $x_0, x_1, \ldots, x_{n-1}$, prove that the determinant of the *Vandermonde* matrix

$$V(x_0, x_1, \dots, x_{n-1}) = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^{n-1} \\ 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n-1} & x_{n-1}^2 & \cdots & x_{n-1}^{n-1} \end{pmatrix}$$

is

$$\det(V(x_0, x_1, \dots, x_{n-1})) = \prod_{0 \le j < k \le n-1} (x_k - x_j).$$

(*Hint*: Multiply column i by $-x_0$ and add it to column i+1 for i=n-1, $n-2,\ldots,1$, and then use induction.)

D-2 Permutations defined by matrix-vector multiplication over GF(2)

One class of permutations of the integers in the set $S_n = \{0, 1, 2, ..., 2^n - 1\}$ is defined by matrix multiplication over GF(2). For each integer x in S_n , we view its binary representation as an n-bit vector

$$\begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{n-1} \end{pmatrix},$$

where $x = \sum_{i=0}^{n-1} x_i 2^i$. If A is an $n \times n$ matrix in which each entry is either 0 or 1, then we can define a permutation mapping each value x in S_n to the number whose binary representation is the matrix-vector product Ax. Here, we perform all arithmetic over GF(2): all values are either 0 or 1, and with one exception the usual rules of addition and multiplication apply. The exception is that 1 + 1 = 0. You can think of arithmetic over GF(2) as being just like regular integer arithmetic, except that you use only the least significant bit.

As an example, for $S_2 = \{0, 1, 2, 3\}$, the matrix

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

defines the following permutation π_A : $\pi_A(0) = 0$, $\pi_A(1) = 3$, $\pi_A(2) = 2$, $\pi_A(3) = 1$. To see why $\pi_A(3) = 1$, observe that, working in GF(2),

$$\pi_A(3) = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 \cdot 1 + 0 \cdot 1 \\ 1 \cdot 1 + 1 \cdot 1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

which is the binary representation of 1.

For the remainder of this problem, we work over GF(2), and all matrix and vector entries are 0 or 1. We define the rank of a 0-1 matrix (a matrix for which each entry is either 0 or 1) over GF(2) the same as for a regular matrix, but with all arithmetic that determines linear independence performed over GF(2). We define the **range** of an $n \times n$ 0-1 matrix A by

$$R(A) = \{y : y = Ax \text{ for some } x \in S_n\}$$
,

so that R(A) is the set of numbers in S_n that we can produce by multiplying each value x in S_n by A.

a. If r is the rank of matrix A, prove that $|R(A)| = 2^r$. Conclude that A defines a permutation on S_n only if A has full rank.

For a given $n \times n$ matrix A and a given value $y \in R(A)$, we define the **preimage** of y by

$$P(A, y) = \{x : Ax = y\}$$
,

so that P(A, y) is the set of values in S_n that map to y when multiplied by A.

b. If r is the rank of $n \times n$ matrix A and $y \in R(A)$, prove that $|P(A, y)| = 2^{n-r}$.

Let $0 \le m \le n$, and suppose we partition the set S_n into blocks of consecutive numbers, where the *i*th block consists of the 2^m numbers $i2^m, i2^m + 1$, $i2^m + 2, ..., (i + 1)2^m - 1$. For any subset $S \subseteq S_n$, define B(S, m) to be the set of size- 2^m blocks of S_n containing some element of S. As an example, when n = 3, m = 1, and $S = \{1, 4, 5\}$, then B(S, m) consists of blocks 0 (since 1 is in the 0th block) and 2 (since both 4 and 5 are in block 2).

c. Let r be the rank of the lower left $(n-m) \times m$ submatrix of A, that is, the matrix formed by taking the intersection of the bottom n-m rows and the leftmost m columns of A. Let S be any size- 2^m block of S_n , and let $S' = \{y : y = Ax \text{ for some } x \in S\}$. Prove that $|B(S', m)| = 2^r$ and that for each block in B(S', m), exactly 2^{m-r} numbers in S map to that block.

Because multiplying the zero vector by any matrix yields a zero vector, the set of permutations of S_n defined by multiplying by $n \times n$ 0-1 matrices with full rank over GF(2) cannot include all permutations of S_n . Let us extend the class of permutations defined by matrix-vector multiplication to include an additive term, so that $x \in S_n$ maps to Ax + c, where c is an n-bit vector and addition is performed over GF(2). For example, when

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

and

$$c = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

we get the following permutation $\pi_{A,c}$: $\pi_{A,c}(0) = 2$, $\pi_{A,c}(1) = 1$, $\pi_{A,c}(2) = 0$, $\pi_{A,c}(3) = 3$. We call any permutation that maps $x \in S_n$ to Ax + c, for some $n \times n$ 0-1 matrix A with full rank and some n-bit vector c, a *linear permutation*.

- **d.** Use a counting argument to show that the number of linear permutations of S_n is much less than the number of permutations of S_n .
- e. Give an example of a value of n and a permutation of S_n that cannot be achieved by any linear permutation. (*Hint*: For a given permutation, think about how multiplying a matrix by a unit vector relates to the columns of the matrix.)

Appendix notes

Linear-algebra textbooks provide plenty of background information on matrices. The books by Strang [323, 324] are particularly good.