28 Matrix Operations

Because operations on matrices lie at the heart of scientific computing, efficient algorithms for working with matrices have many practical applications. This chapter focuses on how to multiply matrices and solve sets of simultaneous linear equations. Appendix D reviews the basics of matrices.

Section 28.1 shows how to solve a set of linear equations using LUP decompositions. Then, Section 28.2 explores the close relationship between multiplying and inverting matrices. Finally, Section 28.3 discusses the important class of symmetric positive-definite matrices and shows how we can use them to find a least-squares solution to an overdetermined set of linear equations.

One important issue that arises in practice is ***numerical stability***. Due to the limited precision of floating-point representations in actual computers, round-off errors in numerical computations may become amplified over the course of a computation, leading to incorrect results; we call such computations ***numerically unstable***. Although we shall briefly consider numerical stability on occasion, we do not focus on it in this chapter. We refer you to the excellent book by Golub and Van Loan [144] for a thorough discussion of stability issues.

28.1 Solving systems of linear equations

Numerous applications need to solve sets of simultaneous linear equations. We can formulate a linear system as a matrix equation in which each matrix or vector element belongs to a field, typically the real numbers $\mathbb{R}$. This section discusses how to solve a system of linear equations using a method called LUP decomposition.

We start with a set of linear equations in n unknowns $x_1, x_2, \ldots, x_n$:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 , \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 , \\ &\vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n . \end{aligned} \tag{28.1}$$

A ***solution*** to the equations (28.1) is a set of values for $x_1, x_2, \ldots, x_n$ that satisfy all of the equations simultaneously. In this section, we treat only the case in which there are exactly n equations in n unknowns.

We can conveniently rewrite equations (28.1) as the matrix-vector equation

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

or, equivalently, letting $A = (a_{ij})$, $x = (x_i)$, and $b = (b_i)$, as

$$Ax = b . \tag{28.2}$$

If A is nonsingular, it possesses an inverse A^{-1}, and

$$x = A^{-1}b \tag{28.3}$$

is the solution vector. We can prove that x is the unique solution to equation (28.2) as follows. If there are two solutions, x and x', then $Ax = Ax' = b$ and, letting I denote an identity matrix,

$$\begin{aligned} x &= Ix \\ &= (A^{-1}A)x \\ &= A^{-1}(Ax) \\ &= A^{-1}(Ax') \\ &= (A^{-1}A)x' \\ &= x' . \end{aligned}$$

In this section, we shall be concerned predominantly with the case in which A is nonsingular or, equivalently (by Theorem D.1), the rank of A is equal to the number n of unknowns. There are other possibilities, however, which merit a brief discussion. If the number of equations is less than the number n of unknowns—or, more generally, if the rank of A is less than n—then the system is ***underdetermined***. An underdetermined system typically has infinitely many solutions, although it may have no solutions at all if the equations are inconsistent. If the number of equations exceeds the number n of unknowns, the system is ***overdetermined***, and there may not exist any solutions. Section 28.3 addresses the important

problem of finding good approximate solutions to overdetermined systems of linear equations.

Let us return to our problem of solving the system $Ax = b$ of n equations in n unknowns. We could compute A^{-1} and then, using equation (28.3), multiply b by A^{-1}, yielding $x = A^{-1}b$. This approach suffers in practice from numerical instability. Fortunately, another approach—LUP decomposition—is numerically stable and has the further advantage of being faster in practice.

Overview of LUP decomposition

The idea behind LUP decomposition is to find three $n \times n$ matrices L, U, and P such that

$$PA = LU \ , \tag{28.4}$$

where

- L is a unit lower-triangular matrix,
- U is an upper-triangular matrix, and
- P is a permutation matrix.

We call matrices L, U, and P satisfying equation (28.4) an ***LUP decomposition*** of the matrix A. We shall show that every nonsingular matrix A possesses such a decomposition.

Computing an LUP decomposition for the matrix A has the advantage that we can more easily solve linear systems when they are triangular, as is the case for both matrices L and U. Once we have found an LUP decomposition for A, we can solve equation (28.2), $Ax = b$, by solving only triangular linear systems, as follows. Multiplying both sides of $Ax = b$ by P yields the equivalent equation $PAx = Pb$, which, by Exercise D.1-4, amounts to permuting the equations (28.1). Using our decomposition (28.4), we obtain

$$LUx = Pb \ .$$

We can now solve this equation by solving two triangular linear systems. Let us define $y = Ux$, where x is the desired solution vector. First, we solve the lower-triangular system

$$Ly = Pb \tag{28.5}$$

for the unknown vector y by a method called "forward substitution." Having solved for y, we then solve the upper-triangular system

$$Ux = y \tag{28.6}$$

for the unknown x by a method called "back substitution." Because the permutation matrix P is invertible (Exercise D.2-3), multiplying both sides of equation (28.4) by P^{-1} gives $P^{-1}PA = P^{-1}LU$, so that

$$A = P^{-1}LU \; . \tag{28.7}$$

Hence, the vector x is our solution to $Ax = b$:

$$\begin{aligned} Ax &= P^{-1}LUx && \text{(by equation (28.7))} \\ &= P^{-1}Ly && \text{(by equation (28.6))} \\ &= P^{-1}Pb && \text{(by equation (28.5))} \\ &= b \; . \end{aligned}$$

Our next step is to show how forward and back substitution work and then attack the problem of computing the LUP decomposition itself.

Forward and back substitution

Forward substitution can solve the lower-triangular system (28.5) in $\Theta(n^2)$ time, given L, P, and b. For convenience, we represent the permutation P compactly by an array $\pi[1..n]$. For $i = 1, 2, \ldots, n$, the entry $\pi[i]$ indicates that $P_{i,\pi[i]} = 1$ and $P_{ij} = 0$ for $j \neq \pi[i]$. Thus, PA has $a_{\pi[i],j}$ in row i and column j, and Pb has $b_{\pi[i]}$ as its ith element. Since L is unit lower-triangular, we can rewrite equation (28.5) as

$$\begin{aligned} y_1 &= b_{\pi[1]} \; , \\ l_{21}y_1 + y_2 &= b_{\pi[2]} \; , \\ l_{31}y_1 + l_{32}y_2 + y_3 &= b_{\pi[3]} \; , \\ &\vdots \\ l_{n1}y_1 + l_{n2}y_2 + l_{n3}y_3 + \cdots + y_n &= b_{\pi[n]} \; . \end{aligned}$$

The first equation tells us that $y_1 = b_{\pi[1]}$. Knowing the value of y_1, we can substitute it into the second equation, yielding

$$y_2 = b_{\pi[2]} - l_{21}y_1 \; .$$

Now, we can substitute both y_1 and y_2 into the third equation, obtaining

$$y_3 = b_{\pi[3]} - (l_{31}y_1 + l_{32}y_2) \; .$$

In general, we substitute $y_1, y_2, \ldots, y_{i-1}$ "forward" into the ith equation to solve for y_i:

$$y_i = b_{\pi[i]} - \sum_{j=1}^{i-1} l_{ij} y_j \ .$$

Having solved for y, we solve for x in equation (28.6) using ***back substitution***, which is similar to forward substitution. Here, we solve the nth equation first and work backward to the first equation. Like forward substitution, this process runs in $\Theta(n^2)$ time. Since U is upper-triangular, we can rewrite the system (28.6) as

$$\begin{aligned}
u_{11}x_1 + u_{12}x_2 + \cdots + u_{1,n-2}x_{n-2} + u_{1,n-1}x_{n-1} + u_{1n}x_n &= y_1 \ , \\
u_{22}x_2 + \cdots + u_{2,n-2}x_{n-2} + u_{2,n-1}x_{n-1} + u_{2n}x_n &= y_2 \ , \\
&\vdots \\
u_{n-2,n-2}x_{n-2} + u_{n-2,n-1}x_{n-1} + u_{n-2,n}x_n &= y_{n-2} \ , \\
u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n &= y_{n-1} \ , \\
u_{n,n}x_n &= y_n \ .
\end{aligned}$$

Thus, we can solve for $x_n, x_{n-1}, \ldots, x_1$ successively as follows:

$$\begin{aligned}
x_n &= y_n/u_{n,n} \ , \\
x_{n-1} &= (y_{n-1} - u_{n-1,n}x_n)/u_{n-1,n-1} \ , \\
x_{n-2} &= (y_{n-2} - (u_{n-2,n-1}x_{n-1} + u_{n-2,n}x_n))/u_{n-2,n-2} \ , \\
&\vdots
\end{aligned}$$

or, in general,

$$x_i = \left(y_i - \sum_{j=i+1}^{n} u_{ij} x_j \right) / u_{ii} \ .$$

Given P, L, U, and b, the procedure LUP-SOLVE solves for x by combining forward and back substitution. The pseudocode assumes that the dimension n appears in the attribute $L.rows$ and that the permutation matrix P is represented by the array π.

```
LUP-SOLVE(L, U, π, b)
1  n = L.rows
2  let x and y be new vectors of length n
3  for i = 1 to n
4       y_i = b_{π[i]} − Σ_{j=1}^{i−1} l_ij y_j
5  for i = n downto 1
6       x_i = (y_i − Σ_{j=i+1}^{n} u_ij x_j) / u_ii
7  return x
```

Procedure LUP-SOLVE solves for y using forward substitution in lines 3–4, and then it solves for x using backward substitution in lines 5–6. Since the summation within each of the **for** loops includes an implicit loop, the running time is $\Theta(n^2)$.

As an example of these methods, consider the system of linear equations defined by

$$\begin{pmatrix} 1 & 2 & 0 \\ 3 & 4 & 4 \\ 5 & 6 & 3 \end{pmatrix} x = \begin{pmatrix} 3 \\ 7 \\ 8 \end{pmatrix},$$

where

$$A = \begin{pmatrix} 1 & 2 & 0 \\ 3 & 4 & 4 \\ 5 & 6 & 3 \end{pmatrix},$$

$$b = \begin{pmatrix} 3 \\ 7 \\ 8 \end{pmatrix},$$

and we wish to solve for the unknown x. The LUP decomposition is

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0.2 & 1 & 0 \\ 0.6 & 0.5 & 1 \end{pmatrix},$$

$$U = \begin{pmatrix} 5 & 6 & 3 \\ 0 & 0.8 & -0.6 \\ 0 & 0 & 2.5 \end{pmatrix},$$

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

(You might want to verify that $PA = LU$.) Using forward substitution, we solve $Ly = Pb$ for y:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0.2 & 1 & 0 \\ 0.6 & 0.5 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 8 \\ 3 \\ 7 \end{pmatrix},$$

obtaining

$$y = \begin{pmatrix} 8 \\ 1.4 \\ 1.5 \end{pmatrix}$$

by computing first y_1, then y_2, and finally y_3. Using back substitution, we solve $Ux = y$ for x:

$$\begin{pmatrix} 5 & 6 & 3 \\ 0 & 0.8 & -0.6 \\ 0 & 0 & 2.5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 8 \\ 1.4 \\ 1.5 \end{pmatrix},$$

thereby obtaining the desired answer

$$x = \begin{pmatrix} -1.4 \\ 2.2 \\ 0.6 \end{pmatrix}$$

by computing first x_3, then x_2, and finally x_1.

Computing an LU decomposition

We have now shown that if we can create an LUP decomposition for a nonsingular matrix A, then forward and back substitution can solve the system $Ax = b$ of linear equations. Now we show how to efficiently compute an LUP decomposition for A. We start with the case in which A is an $n \times n$ nonsingular matrix and P is absent (or, equivalently, $P = I_n$). In this case, we factor $A = LU$. We call the two matrices L and U an ***LU decomposition*** of A.

We use a process known as ***Gaussian elimination*** to create an LU decomposition. We start by subtracting multiples of the first equation from the other equations in order to remove the first variable from those equations. Then, we subtract multiples of the second equation from the third and subsequent equations so that now the first and second variables are removed from them. We continue this process until the system that remains has an upper-triangular form—in fact, it is the matrix U. The matrix L is made up of the row multipliers that cause variables to be eliminated.

Our algorithm to implement this strategy is recursive. We wish to construct an LU decomposition for an $n \times n$ nonsingular matrix A. If $n = 1$, then we are done, since we can choose $L = I_1$ and $U = A$. For $n > 1$, we break A into four parts:

$$\begin{aligned} A &= \left(\begin{array}{c|ccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{array}\right) \\ &= \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ v & A' \end{pmatrix}, \end{aligned}$$

where $v = (v_2, v_3, \ldots, v_n) = (a_{21}, a_{22}, \ldots, a_{n1})$ is a column $(n-1)$-vector, $w^{\mathrm{T}} = (w_2, w_3, \ldots, w_n)^{\mathrm{T}} = (a_{12}, a_{13}, \ldots, a_{1n})^{\mathrm{T}}$ is a row $(n-1)$-vector, and A' is an $(n-1) \times (n-1)$ matrix. Then, using matrix algebra (verify the equations by

simply multiplying through), we can factor A as

$$\begin{aligned} A &= \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ v & A' \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ v/a_{11} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{11} \end{pmatrix} . \end{aligned} \tag{28.8}$$

The 0s in the first and second matrices of equation (28.8) are row and column $(n-1)$-vectors, respectively. The term vw^{T}/a_{11}, formed by taking the outer product of v and w and dividing each element of the result by a_{11}, is an $(n-1) \times (n-1)$ matrix, which conforms in size to the matrix A' from which it is subtracted. The resulting $(n-1) \times (n-1)$ matrix

$$A' - vw^{\mathrm{T}}/a_{11} \tag{28.9}$$

is called the ***Schur complement*** of A with respect to a_{11}.

We claim that if A is nonsingular, then the Schur complement is nonsingular, too. Why? Suppose that the Schur complement, which is $(n-1) \times (n-1)$, is singular. Then by Theorem D.1, it has row rank strictly less than $n-1$. Because the bottom $n-1$ entries in the first column of the matrix

$$\begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{11} \end{pmatrix}$$

are all 0, the bottom $n-1$ rows of this matrix must have row rank strictly less than $n-1$. The row rank of the entire matrix, therefore, is strictly less than n. Applying Exercise D.2-8 to equation (28.8), A has rank strictly less than n, and from Theorem D.1 we derive the contradiction that A is singular.

Because the Schur complement is nonsingular, we can now recursively find an LU decomposition for it. Let us say that

$$A' - vw^{\mathrm{T}}/a_{11} = L'U' ,$$

where L' is unit lower-triangular and U' is upper-triangular. Then, using matrix algebra, we have

$$\begin{aligned} A &= \begin{pmatrix} 1 & 0 \\ v/a_{11} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{11} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ v/a_{11} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & L'U' \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ v/a_{11} & L' \end{pmatrix} \begin{pmatrix} a_{11} & w^{\mathrm{T}} \\ 0 & U' \end{pmatrix} \\ &= LU , \end{aligned}$$

thereby providing our LU decomposition. (Note that because L' is unit lower-triangular, so is L, and because U' is upper-triangular, so is U.)

Of course, if $a_{11} = 0$, this method doesn't work, because it divides by 0. It also doesn't work if the upper leftmost entry of the Schur complement $A' - vw^{\mathrm{T}}/a_{11}$ is 0, since we divide by it in the next step of the recursion. The elements by which we divide during LU decomposition are called ***pivots***, and they occupy the diagonal elements of the matrix U. The reason we include a permutation matrix P during LUP decomposition is that it allows us to avoid dividing by 0. When we use permutations to avoid division by 0 (or by small numbers, which would contribute to numerical instability), we are ***pivoting***.

An important class of matrices for which LU decomposition always works correctly is the class of symmetric positive-definite matrices. Such matrices require no pivoting, and thus we can employ the recursive strategy outlined above without fear of dividing by 0. We shall prove this result, as well as several others, in Section 28.3.

Our code for LU decomposition of a matrix A follows the recursive strategy, except that an iteration loop replaces the recursion. (This transformation is a standard optimization for a "tail-recursive" procedure—one whose last operation is a recursive call to itself. See Problem 7-4.) It assumes that the attribute $A.rows$ gives the dimension of A. We initialize the matrix U with 0s below the diagonal and matrix L with 1s on its diagonal and 0s above the diagonal. Each iteration works on a square submatrix, using its upper leftmost element as the pivot to compute the v and w vectors and the Schur complement, which becomes the square submatrix worked on by the next iteration.

```
LU-DECOMPOSITION(A)
 1  n = A.rows
 2  let L and U be new n × n matrices
 3  initialize U with 0s below the diagonal
 4  initialize L with 1s on the diagonal and 0s above the diagonal
 5  for k = 1 to n
 6      u_kk = a_kk
 7      for i = k + 1 to n
 8          l_ik = a_ik/a_kk          // a_ik holds v_i
 9          u_ki = a_ki               // a_ki holds w_i
10      for i = k + 1 to n
11          for j = k + 1 to n
12              a_ij = a_ij − l_ik u_kj
13  return L and U
```

The outer **for** loop beginning in line 5 iterates once for each recursive step. Within this loop, line 6 determines the pivot to be $u_{kk} = a_{kk}$. The **for** loop in lines 7–9 (which does not execute when $k = n$) uses the v and w vectors to update L and U.

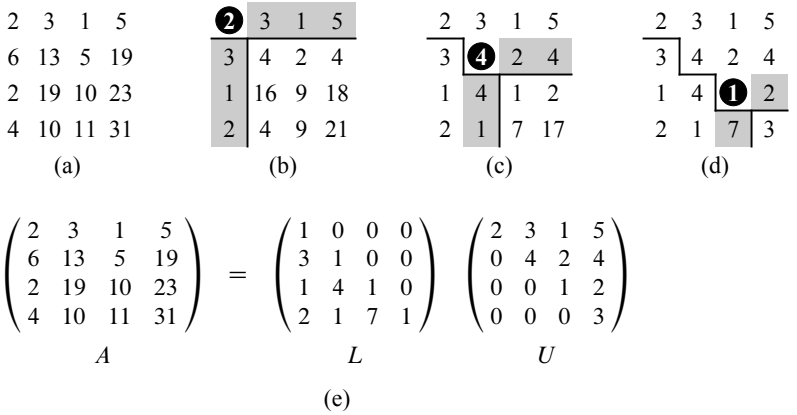

Figure 28.1 The operation of LU-DECOMPOSITION. **(a)** The matrix A. **(b)** The element $a_{11} = 2$ in the black circle is the pivot, the shaded column is v/a_{11}, and the shaded row is w^{T}. The elements of U computed thus far are above the horizontal line, and the elements of L are to the left of the vertical line. The Schur complement matrix $A' - vw^{\mathrm{T}}/a_{11}$ occupies the lower right. **(c)** We now operate on the Schur complement matrix produced from part (b). The element $a_{22} = 4$ in the black circle is the pivot, and the shaded column and row are v/a_{22} and w^{T} (in the partitioning of the Schur complement), respectively. Lines divide the matrix into the elements of U computed so far (above), the elements of L computed so far (left), and the new Schur complement (lower right). **(d)** After the next step, the matrix A is factored. (The element 3 in the new Schur complement becomes part of U when the recursion terminates.) **(e)** The factorization $A = LU$.

Line 8 determines the below-diagonal elements of L, storing v_i/a_{kk} in l_{ik}, and line 9 computes the above-diagonal elements of U, storing w_i in u_{ki}. Finally, lines 10–12 compute the elements of the Schur complement and store them back into the matrix A. (We don't need to divide by a_{kk} in line 12 because we already did so when we computed l_{ik} in line 8.) Because line 12 is triply nested, LU-DECOMPOSITION runs in time $\Theta(n^3)$.

Figure 28.1 illustrates the operation of LU-DECOMPOSITION. It shows a standard optimization of the procedure in which we store the significant elements of L and U in place in the matrix A. That is, we can set up a correspondence between each element a_{ij} and either l_{ij} (if $i > j$) or u_{ij} (if $i \leq j$) and update the matrix A so that it holds both L and U when the procedure terminates. To obtain the pseudocode for this optimization from the above pseudocode, just replace each reference to l or u by a; you can easily verify that this transformation preserves correctness.

Computing an LUP decomposition

Generally, in solving a system of linear equations $Ax = b$, we must pivot on off-diagonal elements of A to avoid dividing by 0. Dividing by 0 would, of course, be disastrous. But we also want to avoid dividing by a small value—even if A is nonsingular—because numerical instabilities can result. We therefore try to pivot on a large value.

The mathematics behind LUP decomposition is similar to that of LU decomposition. Recall that we are given an $n \times n$ nonsingular matrix A, and we wish to find a permutation matrix P, a unit lower-triangular matrix L, and an upper-triangular matrix U such that $PA = LU$. Before we partition the matrix A, as we did for LU decomposition, we move a nonzero element, say a_{k1}, from somewhere in the first column to the $(1,1)$ position of the matrix. For numerical stability, we choose a_{k1} as the element in the first column with the greatest absolute value. (The first column cannot contain only 0s, for then A would be singular, because its determinant would be 0, by Theorems D.4 and D.5.) In order to preserve the set of equations, we exchange row 1 with row k, which is equivalent to multiplying A by a permutation matrix Q on the left (Exercise D.1-4). Thus, we can write QA as

$$QA = \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ v & A' \end{pmatrix},$$

where $v = (a_{21}, a_{31}, \ldots, a_{n1})$, except that a_{11} replaces a_{k1}; $w^{\mathrm{T}} = (a_{k2}, a_{k3}, \ldots, a_{kn})^{\mathrm{T}}$; and A' is an $(n-1) \times (n-1)$ matrix. Since $a_{k1} \neq 0$, we can now perform much the same linear algebra as for LU decomposition, but now guaranteeing that we do not divide by 0:

$$\begin{aligned} QA &= \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ v & A' \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ v/a_{k1} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{k1} \end{pmatrix}. \end{aligned}$$

As we saw for LU decomposition, if A is nonsingular, then the Schur complement $A' - vw^{\mathrm{T}}/a_{k1}$ is nonsingular, too. Therefore, we can recursively find an LUP decomposition for it, with unit lower-triangular matrix L', upper-triangular matrix U', and permutation matrix P', such that

$$P'(A' - vw^{\mathrm{T}}/a_{k1}) = L'U' .$$

Define

$$P = \begin{pmatrix} 1 & 0 \\ 0 & P' \end{pmatrix} Q ,$$

which is a permutation matrix, since it is the product of two permutation matrices (Exercise D.1-4). We now have

$$
\begin{aligned}
PA &= \begin{pmatrix} 1 & 0 \\ 0 & P' \end{pmatrix} QA \\
&= \begin{pmatrix} 1 & 0 \\ 0 & P' \end{pmatrix} \begin{pmatrix} 1 & 0 \\ v/a_{k1} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{k1} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ P'v/a_{k1} & P' \end{pmatrix} \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ 0 & A' - vw^{\mathrm{T}}/a_{k1} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ P'v/a_{k1} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ 0 & P'(A' - vw^{\mathrm{T}}/a_{k1}) \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ P'v/a_{k1} & I_{n-1} \end{pmatrix} \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ 0 & L'U' \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ P'v/a_{k1} & L' \end{pmatrix} \begin{pmatrix} a_{k1} & w^{\mathrm{T}} \\ 0 & U' \end{pmatrix} \\
&= LU \,,
\end{aligned}
$$

yielding the LUP decomposition. Because L' is unit lower-triangular, so is L, and because U' is upper-triangular, so is U.

Notice that in this derivation, unlike the one for LU decomposition, we must multiply both the column vector v/a_{k1} and the Schur complement $A' - vw^{\mathrm{T}}/a_{k1}$ by the permutation matrix P'. Here is the pseudocode for LUP decomposition:

LUP-DECOMPOSITION(A)

```
 1  n = A.rows
 2  let π[1..n] be a new array
 3  for i = 1 to n
 4      π[i] = i
 5  for k = 1 to n
 6      p = 0
 7      for i = k to n
 8          if |a_ik| > p
 9              p = |a_ik|
10              k' = i
11      if p == 0
12          error "singular matrix"
13      exchange π[k] with π[k']
14      for i = 1 to n
15          exchange a_ki with a_k'i
16      for i = k + 1 to n
17          a_ik = a_ik/a_kk
18          for j = k + 1 to n
19              a_ij = a_ij − a_ik a_kj
```

Like LU-DECOMPOSITION, our LUP-DECOMPOSITION procedure replaces the recursion with an iteration loop. As an improvement over a direct implementation of the recursion, we dynamically maintain the permutation matrix P as an array π, where $\pi[i] = j$ means that the ith row of P contains a 1 in column j. We also implement the code to compute L and U "in place" in the matrix A. Thus, when the procedure terminates,

$$a_{ij} = \begin{cases} l_{ij} & \text{if } i > j \ , \\ u_{ij} & \text{if } i \le j \ . \end{cases}$$

Figure 28.2 illustrates how LUP-DECOMPOSITION factors a matrix. Lines 3–4 initialize the array π to represent the identity permutation. The outer **for** loop beginning in line 5 implements the recursion. Each time through the outer loop, lines 6–10 determine the element $a_{k'k}$ with largest absolute value of those in the current first column (column k) of the $(n - k + 1) \times (n - k + 1)$ matrix whose LUP decomposition we are finding. If all elements in the current first column are zero, lines 11–12 report that the matrix is singular. To pivot, we exchange $\pi[k']$ with $\pi[k]$ in line 13 and exchange the kth and k'th rows of A in lines 14–15, thereby making the pivot element a_{kk}. (The entire rows are swapped because in the derivation of the method above, not only is $A' - vw^{\mathrm{T}}/a_{k1}$ multiplied by P', but so is v/a_{k1}.) Finally, the Schur complement is computed by lines 16–19 in much the same way as it is computed by lines 7–12 of LU-DECOMPOSITION, except that here the operation is written to work in place.

Because of its triply nested loop structure, LUP-DECOMPOSITION has a running time of $\Theta(n^3)$, which is the same as that of LU-DECOMPOSITION. Thus, pivoting costs us at most a constant factor in time.

Exercises

28.1-1

Solve the equation

$$\begin{pmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ -6 & 5 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 14 \\ -7 \end{pmatrix}$$

by using forward substitution.

28.1-2

Find an LU decomposition of the matrix

$$\begin{pmatrix} 4 & -5 & 6 \\ 8 & -6 & 7 \\ 12 & -7 & 12 \end{pmatrix} .$$

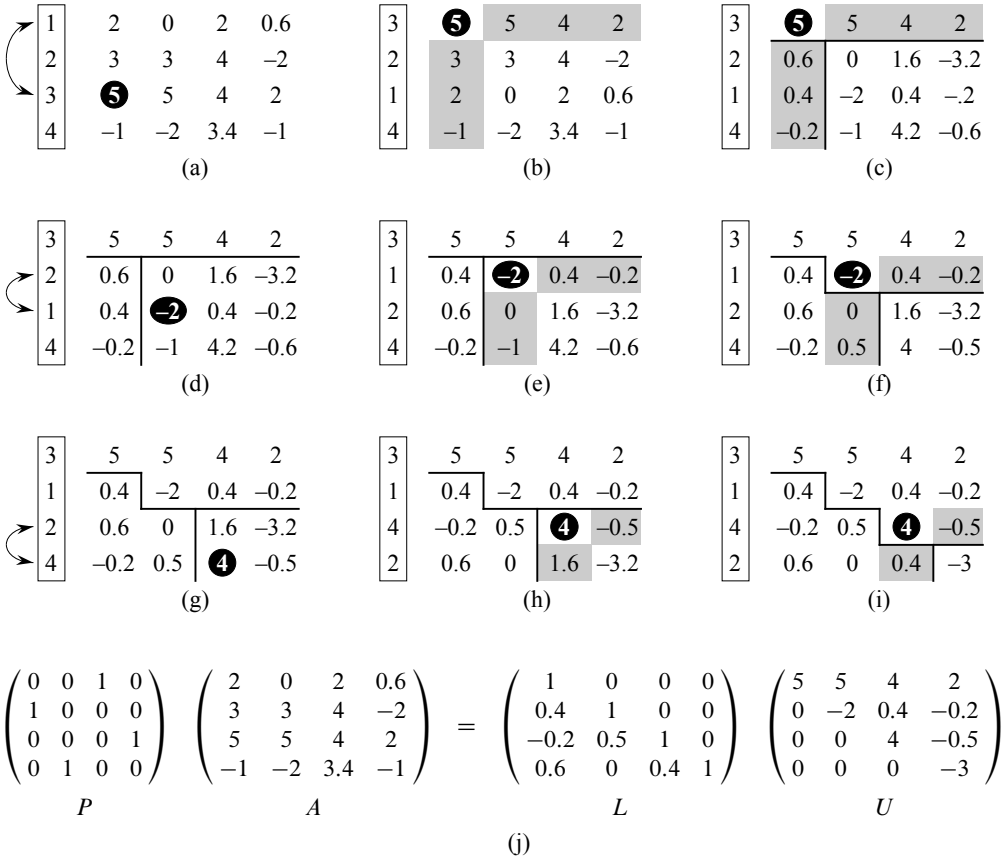

Figure 28.2 The operation of LUP-DECOMPOSITION. **(a)** The input matrix A with the identity permutation of the rows on the left. The first step of the algorithm determines that the element 5 in the black circle in the third row is the pivot for the first column. **(b)** Rows 1 and 3 are swapped and the permutation is updated. The shaded column and row represent v and w^T. **(c)** The vector v is replaced by $v/5$, and the lower right of the matrix is updated with the Schur complement. Lines divide the matrix into three regions: elements of U (above), elements of L (left), and elements of the Schur complement (lower right). **(d)–(f)** The second step. **(g)–(i)** The third step. No further changes occur on the fourth (final) step. **(j)** The LUP decomposition $PA = LU$.

28.1-3
Solve the equation

$$\begin{pmatrix} 1 & 5 & 4 \\ 2 & 0 & 3 \\ 5 & 8 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 12 \\ 9 \\ 5 \end{pmatrix}$$

by using an LUP decomposition.

28.1-4
Describe the LUP decomposition of a diagonal matrix.

28.1-5
Describe the LUP decomposition of a permutation matrix A, and prove that it is unique.

28.1-6
Show that for all $n \geq 1$, there exists a singular $n \times n$ matrix that has an LU decomposition.

28.1-7
In LU-DECOMPOSITION, is it necessary to perform the outermost **for** loop iteration when $k = n$? How about in LUP-DECOMPOSITION?

28.2 Inverting matrices

Although in practice we do not generally use matrix inverses to solve systems of linear equations, preferring instead to use more numerically stable techniques such as LUP decomposition, sometimes we need to compute a matrix inverse. In this section, we show how to use LUP decomposition to compute a matrix inverse. We also prove that matrix multiplication and computing the inverse of a matrix are equivalently hard problems, in that (subject to technical conditions) we can use an algorithm for one to solve the other in the same asymptotic running time. Thus, we can use Strassen's algorithm (see Section 4.2) for matrix multiplication to invert a matrix. Indeed, Strassen's original paper was motivated by the problem of showing that a set of a linear equations could be solved more quickly than by the usual method.

Computing a matrix inverse from an LUP decomposition

Suppose that we have an LUP decomposition of a matrix A in the form of three matrices L, U, and P such that $PA = LU$. Using LUP-SOLVE, we can solve an equation of the form $Ax = b$ in time $\Theta(n^2)$. Since the LUP decomposition depends on A but not b, we can run LUP-SOLVE on a second set of equations of the form $Ax = b'$ in additional time $\Theta(n^2)$. In general, once we have the LUP decomposition of A, we can solve, in time $\Theta(kn^2)$, k versions of the equation $Ax = b$ that differ only in b.

We can think of the equation

$$AX = I_n \,, \tag{28.10}$$

which defines the matrix X, the inverse of A, as a set of n distinct equations of the form $Ax = b$. To be precise, let X_i denote the ith column of X, and recall that the unit vector e_i is the ith column of I_n. We can then solve equation (28.10) for X by using the LUP decomposition for A to solve each equation

$$AX_i = e_i$$

separately for X_i. Once we have the LUP decomposition, we can compute each of the n columns X_i in time $\Theta(n^2)$, and so we can compute X from the LUP decomposition of A in time $\Theta(n^3)$. Since we can determine the LUP decomposition of A in time $\Theta(n^3)$, we can compute the inverse A^{-1} of a matrix A in time $\Theta(n^3)$.

Matrix multiplication and matrix inversion

We now show that the theoretical speedups obtained for matrix multiplication translate to speedups for matrix inversion. In fact, we prove something stronger: matrix inversion is equivalent to matrix multiplication, in the following sense. If $M(n)$ denotes the time to multiply two $n \times n$ matrices, then we can invert a nonsingular $n \times n$ matrix in time $O(M(n))$. Moreover, if $I(n)$ denotes the time to invert a nonsingular $n \times n$ matrix, then we can multiply two $n \times n$ matrices in time $O(I(n))$. We prove these results as two separate theorems.

Theorem 28.1 (Multiplication is no harder than inversion)
If we can invert an $n \times n$ matrix in time $I(n)$, where $I(n) = \Omega(n^2)$ and $I(n)$ satisfies the regularity condition $I(3n) = O(I(n))$, then we can multiply two $n \times n$ matrices in time $O(I(n))$.

Proof Let A and B be $n \times n$ matrices whose matrix product C we wish to compute. We define the $3n \times 3n$ matrix D by

$$D = \begin{pmatrix} I_n & A & 0 \\ 0 & I_n & B \\ 0 & 0 & I_n \end{pmatrix}.$$

The inverse of D is

$$D^{-1} = \begin{pmatrix} I_n & -A & AB \\ 0 & I_n & -B \\ 0 & 0 & I_n \end{pmatrix},$$

and thus we can compute the product AB by taking the upper right $n \times n$ submatrix of D^{-1}.

We can construct matrix D in $\Theta(n^2)$ time, which is $O(I(n))$ because we assume that $I(n) = \Omega(n^2)$, and we can invert D in $O(I(3n)) = O(I(n))$ time, by the regularity condition on $I(n)$. We thus have $M(n) = O(I(n))$. ■

Note that $I(n)$ satisfies the regularity condition whenever $I(n) = \Theta(n^c \lg^d n)$ for any constants $c > 0$ and $d \geq 0$.

The proof that matrix inversion is no harder than matrix multiplication relies on some properties of symmetric positive-definite matrices that we will prove in Section 28.3.

Theorem 28.2 (Inversion is no harder than multiplication)
Suppose we can multiply two $n \times n$ real matrices in time $M(n)$, where $M(n) = \Omega(n^2)$ and $M(n)$ satisfies the two regularity conditions $M(n+k) = O(M(n))$ for any k in the range $0 \leq k \leq n$ and $M(n/2) \leq cM(n)$ for some constant $c < 1/2$. Then we can compute the inverse of any real nonsingular $n \times n$ matrix in time $O(M(n))$.

Proof We prove the theorem here for real matrices. Exercise 28.2-6 asks you to generalize the proof for matrices whose entries are complex numbers.

We can assume that n is an exact power of 2, since we have

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

for any $k > 0$. Thus, by choosing k such that $n + k$ is a power of 2, we enlarge the matrix to a size that is the next power of 2 and obtain the desired answer A^{-1} from the answer to the enlarged problem. The first regularity condition on $M(n)$ ensures that this enlargement does not cause the running time to increase by more than a constant factor.

For the moment, let us assume that the $n \times n$ matrix A is symmetric and positive-definite. We partition each of A and its inverse A^{-1} into four $n/2 \times n/2$ submatrices:

$$A = \begin{pmatrix} B & C^{\mathrm{T}} \\ C & D \end{pmatrix} \quad \text{and} \quad A^{-1} = \begin{pmatrix} R & T \\ U & V \end{pmatrix}. \tag{28.11}$$

Then, if we let

$$S = D - CB^{-1}C^{\mathrm{T}} \tag{28.12}$$

be the Schur complement of A with respect to B (we shall see more about this form of Schur complement in Section 28.3), we have

$$A^{-1} = \begin{pmatrix} R & T \\ U & V \end{pmatrix} = \begin{pmatrix} B^{-1} + B^{-1}C^{\mathrm{T}}S^{-1}CB^{-1} & -B^{-1}C^{\mathrm{T}}S^{-1} \\ -S^{-1}CB^{-1} & S^{-1} \end{pmatrix}, \tag{28.13}$$

since $AA^{-1} = I_n$, as you can verify by performing the matrix multiplication. Because A is symmetric and positive-definite, Lemmas 28.4 and 28.5 in Section 28.3 imply that B and S are both symmetric and positive-definite. By Lemma 28.3 in Section 28.3, therefore, the inverses B^{-1} and S^{-1} exist, and by Exercise D.2-6, B^{-1} and S^{-1} are symmetric, so that $(B^{-1})^{\mathrm{T}} = B^{-1}$ and $(S^{-1})^{\mathrm{T}} = S^{-1}$. Therefore, we can compute the submatrices R, T, U, and V of A^{-1} as follows, where all matrices mentioned are $n/2 \times n/2$:

1. Form the submatrices B, C, C^{T}, and D of A.
2. Recursively compute the inverse B^{-1} of B.
3. Compute the matrix product $W = CB^{-1}$, and then compute its transpose W^{T}, which equals $B^{-1}C^{\mathrm{T}}$ (by Exercise D.1-2 and $(B^{-1})^{\mathrm{T}} = B^{-1}$).
4. Compute the matrix product $X = WC^{\mathrm{T}}$, which equals $CB^{-1}C^{\mathrm{T}}$, and then compute the matrix $S = D - X = D - CB^{-1}C^{\mathrm{T}}$.
5. Recursively compute the inverse S^{-1} of S, and set V to S^{-1}.
6. Compute the matrix product $Y = S^{-1}W$, which equals $S^{-1}CB^{-1}$, and then compute its transpose Y^{T}, which equals $B^{-1}C^{\mathrm{T}}S^{-1}$ (by Exercise D.1-2, $(B^{-1})^{\mathrm{T}} = B^{-1}$, and $(S^{-1})^{\mathrm{T}} = S^{-1}$). Set T to $-Y^{\mathrm{T}}$ and U to $-Y$.
7. Compute the matrix product $Z = W^{\mathrm{T}}Y$, which equals $B^{-1}C^{\mathrm{T}}S^{-1}CB^{-1}$, and set R to $B^{-1} + Z$.

Thus, we can invert an $n \times n$ symmetric positive-definite matrix by inverting two $n/2 \times n/2$ matrices in steps 2 and 5; performing four multiplications of $n/2 \times n/2$ matrices in steps 3, 4, 6, and 7; plus an additional cost of $O(n^2)$ for extracting submatrices from A, inserting submatrices into A^{-1}, and performing a constant number of additions, subtractions, and transposes on $n/2 \times n/2$ matrices. We get the recurrence

$$\begin{aligned} I(n) &\le 2I(n/2) + 4M(n/2) + O(n^2) \\ &= 2I(n/2) + \Theta(M(n)) \\ &= O(M(n)) \,. \end{aligned}$$

The second line holds because the second regularity condition in the statement of the theorem implies that $4M(n/2) < 2M(n)$ and because we assume that $M(n) = \Omega(n^2)$. The third line follows because the second regularity condition allows us to apply case 3 of the master theorem (Theorem 4.1).

It remains to prove that we can obtain the same asymptotic running time for matrix multiplication as for matrix inversion when A is invertible but not symmetric and positive-definite. The basic idea is that for any nonsingular matrix A, the matrix $A^{\mathrm{T}}A$ is symmetric (by Exercise D.1-2) and positive-definite (by Theorem D.6). The trick, then, is to reduce the problem of inverting A to the problem of inverting $A^{\mathrm{T}}A$.

The reduction is based on the observation that when A is an $n \times n$ nonsingular matrix, we have

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

since $((A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}})A = (A^{\mathrm{T}}A)^{-1}(A^{\mathrm{T}}A) = I_n$ and a matrix inverse is unique. Therefore, we can compute A^{-1} by first multiplying A^{T} by A to obtain $A^{\mathrm{T}}A$, then inverting the symmetric positive-definite matrix $A^{\mathrm{T}}A$ using the above divide-and-conquer algorithm, and finally multiplying the result by A^{T}. Each of these three steps takes $O(M(n))$ time, and thus we can invert any nonsingular matrix with real entries in $O(M(n))$ time. ■

The proof of Theorem 28.2 suggests a means of solving the equation $Ax = b$ by using LU decomposition without pivoting, so long as A is nonsingular. We multiply both sides of the equation by A^{T}, yielding $(A^{\mathrm{T}}A)x = A^{\mathrm{T}}b$. This transformation doesn't affect the solution x, since A^{T} is invertible, and so we can factor the symmetric positive-definite matrix $A^{\mathrm{T}}A$ by computing an LU decomposition. We then use forward and back substitution to solve for x with the right-hand side $A^{\mathrm{T}}b$. Although this method is theoretically correct, in practice the procedure LUP-DECOMPOSITION works much better. LUP decomposition requires fewer arithmetic operations by a constant factor, and it has somewhat better numerical properties.

Exercises

28.2-1

Let $M(n)$ be the time to multiply two $n \times n$ matrices, and let $S(n)$ denote the time required to square an $n \times n$ matrix. Show that multiplying and squaring matrices have essentially the same difficulty: an $M(n)$-time matrix-multiplication algorithm implies an $O(M(n))$-time squaring algorithm, and an $S(n)$-time squaring algorithm implies an $O(S(n))$-time matrix-multiplication algorithm.

28.2-2
Let $M(n)$ be the time to multiply two $n \times n$ matrices. Show that an $M(n)$-time matrix-multiplication algorithm implies an $O(M(n))$-time LUP-decomposition algorithm.

28.2-3
Let $M(n)$ be the time to multiply two $n \times n$ matrices, and let $D(n)$ denote the time required to find the determinant of an $n \times n$ matrix. Show that multiplying matrices and computing the determinant have essentially the same difficulty: an $M(n)$-time matrix-multiplication algorithm implies an $O(M(n))$-time determinant algorithm, and a $D(n)$-time determinant algorithm implies an $O(D(n))$-time matrix-multiplication algorithm.

28.2-4
Let $M(n)$ be the time to multiply two $n \times n$ boolean matrices, and let $T(n)$ be the time to find the transitive closure of an $n \times n$ boolean matrix. (See Section 25.2.) Show that an $M(n)$-time boolean matrix-multiplication algorithm implies an $O(M(n) \lg n)$-time transitive-closure algorithm, and a $T(n)$-time transitive-closure algorithm implies an $O(T(n))$-time boolean matrix-multiplication algorithm.

28.2-5
Does the matrix-inversion algorithm based on Theorem 28.2 work when matrix elements are drawn from the field of integers modulo 2? Explain.

28.2-6 ⋆
Generalize the matrix-inversion algorithm of Theorem 28.2 to handle matrices of complex numbers, and prove that your generalization works correctly. (*Hint:* Instead of the transpose of A, use the ***conjugate transpose*** A^*, which you obtain from the transpose of A by replacing every entry with its complex conjugate. Instead of symmetric matrices, consider ***Hermitian*** matrices, which are matrices A such that $A = A^*$.)

28.3 Symmetric positive-definite matrices and least-squares approximation

Symmetric positive-definite matrices have many interesting and desirable properties. For example, they are nonsingular, and we can perform LU decomposition on them without having to worry about dividing by 0. In this section, we shall

prove several other important properties of symmetric positive-definite matrices and show an interesting application to curve fitting by a least-squares approximation.

The first property we prove is perhaps the most basic.

Lemma 28.3
Any positive-definite matrix is nonsingular.

Proof Suppose that a matrix A is singular. Then by Corollary D.3, there exists a nonzero vector x such that $Ax = 0$. Hence, $x^{\mathrm{T}}Ax = 0$, and A cannot be positive-definite. ■

The proof that we can perform LU decomposition on a symmetric positive-definite matrix A without dividing by 0 is more involved. We begin by proving properties about certain submatrices of A. Define the kth ***leading submatrix*** of A to be the matrix A_k consisting of the intersection of the first k rows and first k columns of A.

Lemma 28.4
If A is a symmetric positive-definite matrix, then every leading submatrix of A is symmetric and positive-definite.

Proof That each leading submatrix A_k is symmetric is obvious. To prove that A_k is positive-definite, we assume that it is not and derive a contradiction. If A_k is not positive-definite, then there exists a k-vector $x_k \neq 0$ such that $x_k^{\mathrm{T}} A_k x_k \leq 0$. Let A be $n \times n$, and

$$A = \begin{pmatrix} A_k & B^{\mathrm{T}} \\ B & C \end{pmatrix} \tag{28.14}$$

for submatrices B (which is $(n-k)\times k$) and C (which is $(n-k)\times(n-k)$). Define the n-vector $x = (\, x_k^{\mathrm{T}} \quad 0\,)^{\mathrm{T}}$, where $n-k$ 0s follow x_k. Then we have

$$\begin{aligned} x^{\mathrm{T}}Ax &= (\, x_k^{\mathrm{T}} \quad 0\,)\begin{pmatrix} A_k & B^{\mathrm{T}} \\ B & C \end{pmatrix}\begin{pmatrix} x_k \\ 0 \end{pmatrix} \\ &= (\, x_k^{\mathrm{T}} \quad 0\,)\begin{pmatrix} A_k x_k \\ B x_k \end{pmatrix} \\ &= x_k^{\mathrm{T}} A_k x_k \\ &\leq 0\,, \end{aligned}$$

which contradicts A being positive-definite. ■

We now turn to some essential properties of the Schur complement. Let A be a symmetric positive-definite matrix, and let A_k be a leading $k \times k$ submatrix of A. Partition A once again according to equation (28.14). We generalize equation (28.9) to define the ***Schur complement*** S of A with respect to A_k as

$$S = C - BA_k^{-1}B^{\mathrm{T}} . \tag{28.15}$$

(By Lemma 28.4, A_k is symmetric and positive-definite; therefore, A_k^{-1} exists by Lemma 28.3, and S is well defined.) Note that our earlier definition (28.9) of the Schur complement is consistent with equation (28.15), by letting $k = 1$.

The next lemma shows that the Schur-complement matrices of symmetric positive-definite matrices are themselves symmetric and positive-definite. We used this result in Theorem 28.2, and we need its corollary to prove the correctness of LU decomposition for symmetric positive-definite matrices.

Lemma 28.5 (Schur complement lemma)
If A is a symmetric positive-definite matrix and A_k is a leading $k \times k$ submatrix of A, then the Schur complement S of A with respect to A_k is symmetric and positive-definite.

Proof Because A is symmetric, so is the submatrix C. By Exercise D.2-6, the product $BA_k^{-1}B^{\mathrm{T}}$ is symmetric, and by Exercise D.1-1, S is symmetric.

It remains to show that S is positive-definite. Consider the partition of A given in equation (28.14). For any nonzero vector x, we have $x^{\mathrm{T}}Ax > 0$ by the assumption that A is positive-definite. Let us break x into two subvectors y and z compatible with A_k and C, respectively. Because A_k^{-1} exists, we have

$$\begin{aligned}
x^{\mathrm{T}}Ax &= \begin{pmatrix} y^{\mathrm{T}} & z^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} A_k & B^{\mathrm{T}} \\ B & C \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} \\
&= \begin{pmatrix} y^{\mathrm{T}} & z^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} A_k y + B^{\mathrm{T}} z \\ By + Cz \end{pmatrix} \\
&= y^{\mathrm{T}} A_k y + y^{\mathrm{T}} B^{\mathrm{T}} z + z^{\mathrm{T}} By + z^{\mathrm{T}} Cz \\
&= (y + A_k^{-1}B^{\mathrm{T}}z)^{\mathrm{T}} A_k (y + A_k^{-1}B^{\mathrm{T}}z) + z^{\mathrm{T}}(C - BA_k^{-1}B^{\mathrm{T}})z , \qquad (28.16)
\end{aligned}$$

by matrix magic. (Verify by multiplying through.) This last equation amounts to "completing the square" of the quadratic form. (See Exercise 28.3-2.)

Since $x^{\mathrm{T}}Ax > 0$ holds for any nonzero x, let us pick any nonzero z and then choose $y = -A_k^{-1}B^{\mathrm{T}}z$, which causes the first term in equation (28.16) to vanish, leaving

$$z^{\mathrm{T}}(C - BA_k^{-1}B^{\mathrm{T}})z = z^{\mathrm{T}}Sz$$

as the value of the expression. For any $z \neq 0$, we therefore have $z^{\mathrm{T}}Sz = x^{\mathrm{T}}Ax > 0$, and thus S is positive-definite. ∎

Corollary 28.6
LU decomposition of a symmetric positive-definite matrix never causes a division by 0.

Proof Let A be a symmetric positive-definite matrix. We shall prove something stronger than the statement of the corollary: every pivot is strictly positive. The first pivot is a_{11}. Let e_1 be the first unit vector, from which we obtain $a_{11} = e_1^{\mathrm{T}} A e_1 > 0$. Since the first step of LU decomposition produces the Schur complement of A with respect to $A_1 = (a_{11})$, Lemma 28.5 implies by induction that all pivots are positive. ■

Least-squares approximation

One important application of symmetric positive-definite matrices arises in fitting curves to given sets of data points. Suppose that we are given a set of m data points

$$(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m) ,$$

where we know that the y_i are subject to measurement errors. We would like to determine a function $F(x)$ such that the approximation errors

$$\eta_i = F(x_i) - y_i \tag{28.17}$$

are small for $i = 1, 2, \ldots, m$. The form of the function F depends on the problem at hand. Here, we assume that it has the form of a linearly weighted sum,

$$F(x) = \sum_{j=1}^{n} c_j f_j(x) ,$$

where the number of summands n and the specific ***basis functions*** f_j are chosen based on knowledge of the problem at hand. A common choice is $f_j(x) = x^{j-1}$, which means that

$$F(x) = c_1 + c_2 x + c_3 x^2 + \cdots + c_n x^{n-1}$$

is a polynomial of degree $n - 1$ in x. Thus, given m data points $(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$, we wish to calculate n coefficients $c_1, c_2, \ldots, c_n$ that minimize the approximation errors $\eta_1, \eta_2, \ldots, \eta_m$.

By choosing $n = m$, we can calculate each y_i *exactly* in equation (28.17). Such a high-degree F "fits the noise" as well as the data, however, and generally gives poor results when used to predict y for previously unseen values of x. It is usually better to choose n significantly smaller than m and hope that by choosing the coefficients c_j well, we can obtain a function F that finds the significant patterns in the data points without paying undue attention to the noise. Some theoretical

principles exist for choosing n, but they are beyond the scope of this text. In any case, once we choose a value of n that is less than m, we end up with an overdetermined set of equations whose solution we wish to approximate. We now show how to do so.

Let

$$A = \begin{pmatrix} f_1(x_1) & f_2(x_1) & \dots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \dots & f_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_m) & f_2(x_m) & \dots & f_n(x_m) \end{pmatrix}$$

denote the matrix of values of the basis functions at the given points; that is, $a_{ij} = f_j(x_i)$. Let $c = (c_k)$ denote the desired n-vector of coefficients. Then,

$$\begin{aligned} Ac &= \begin{pmatrix} f_1(x_1) & f_2(x_1) & \dots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \dots & f_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_m) & f_2(x_m) & \dots & f_n(x_m) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \\ &= \begin{pmatrix} F(x_1) \\ F(x_2) \\ \vdots \\ F(x_m) \end{pmatrix} \end{aligned}$$

is the m-vector of "predicted values" for y. Thus,

$$\eta = Ac - y$$

is the m-vector of ***approximation errors***.

To minimize approximation errors, we choose to minimize the norm of the error vector η, which gives us a ***least-squares solution***, since

$$\|\eta\| = \left(\sum_{i=1}^{m} \eta_i^2 \right)^{1/2} .$$

Because

$$\|\eta\|^2 = \|Ac - y\|^2 = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} a_{ij} c_j - y_i \right)^2 ,$$

we can minimize $\|\eta\|$ by differentiating $\|\eta\|^2$ with respect to each c_k and then setting the result to 0:

$$\frac{d\,\|\eta\|^2}{dc_k} = \sum_{i=1}^{m} 2\left(\sum_{j=1}^{n} a_{ij}c_j - y_i\right) a_{ik} = 0\,. \tag{28.18}$$

The n equations (28.18) for $k = 1, 2, \ldots, n$ are equivalent to the single matrix equation

$$(Ac - y)^{\mathrm{T}} A = 0$$

or, equivalently (using Exercise D.1-2), to

$$A^{\mathrm{T}}(Ac - y) = 0\,,$$

which implies

$$A^{\mathrm{T}}Ac = A^{\mathrm{T}}y\,. \tag{28.19}$$

In statistics, this is called the ***normal equation***. The matrix $A^{\mathrm{T}}A$ is symmetric by Exercise D.1-2, and if A has full column rank, then by Theorem D.6, $A^{\mathrm{T}}A$ is positive-definite as well. Hence, $(A^{\mathrm{T}}A)^{-1}$ exists, and the solution to equation (28.19) is

$$\begin{aligned} c &= \left((A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}\right) y \\ &= A^{+}y\,, \end{aligned} \tag{28.20}$$

where the matrix $A^{+} = ((A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}})$ is the ***pseudoinverse*** of the matrix A. The pseudoinverse naturally generalizes the notion of a matrix inverse to the case in which A is not square. (Compare equation (28.20) as the approximate solution to $Ac = y$ with the solution $A^{-1}b$ as the exact solution to $Ax = b$.)

As an example of producing a least-squares fit, suppose that we have five data points

$$\begin{aligned} (x_1, y_1) &= (-1, 2)\,, \\ (x_2, y_2) &= (1, 1)\,, \\ (x_3, y_3) &= (2, 1)\,, \\ (x_4, y_4) &= (3, 0)\,, \\ (x_5, y_5) &= (5, 3)\,, \end{aligned}$$

shown as black dots in Figure 28.3. We wish to fit these points with a quadratic polynomial

$$F(x) = c_1 + c_2 x + c_3 x^2\,.$$

We start with the matrix of basis-function values

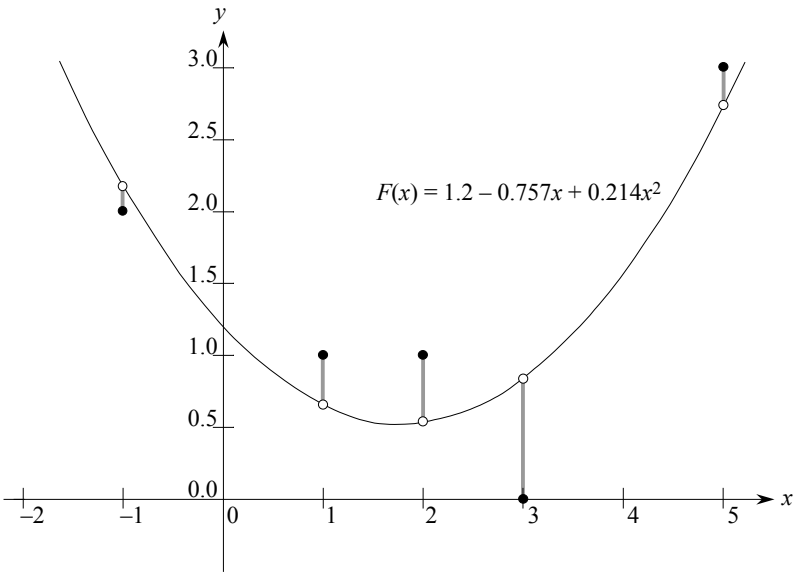

Figure 28.3 The least-squares fit of a quadratic polynomial to the set of five data points $\{(-1, 2), (1, 1), (2, 1), (3, 0), (5, 3)\}$. The black dots are the data points, and the white dots are their estimated values predicted by the polynomial $F(x) = 1.2 - 0.757x + 0.214x^2$, the quadratic polynomial that minimizes the sum of the squared errors. Each shaded line shows the error for one data point.

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \\ 1 & x_5 & x_5^2 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 5 & 25 \end{pmatrix},$$

whose pseudoinverse is

$$A^+ = \begin{pmatrix} 0.500 & 0.300 & 0.200 & 0.100 & -0.100 \\ -0.388 & 0.093 & 0.190 & 0.193 & -0.088 \\ 0.060 & -0.036 & -0.048 & -0.036 & 0.060 \end{pmatrix}.$$

Multiplying y by A^+, we obtain the coefficient vector

$$c = \begin{pmatrix} 1.200 \\ -0.757 \\ 0.214 \end{pmatrix},$$

which corresponds to the quadratic polynomial

$$F(x) = 1.200 - 0.757x + 0.214x^2$$

as the closest-fitting quadratic to the given data, in a least-squares sense.

As a practical matter, we solve the normal equation (28.19) by multiplying y by A^{T} and then finding an LU decomposition of $A^{\mathrm{T}}A$. If A has full rank, the matrix $A^{\mathrm{T}}A$ is guaranteed to be nonsingular, because it is symmetric and positive-definite. (See Exercise D.1-2 and Theorem D.6.)

Exercises

28.3-1

Prove that every diagonal element of a symmetric positive-definite matrix is positive.

28.3-2

Let $A = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$ be a 2×2 symmetric positive-definite matrix. Prove that its determinant $ac - b^2$ is positive by "completing the square" in a manner similar to that used in the proof of Lemma 28.5.

28.3-3

Prove that the maximum element in a symmetric positive-definite matrix lies on the diagonal.

28.3-4

Prove that the determinant of each leading submatrix of a symmetric positive-definite matrix is positive.

28.3-5

Let A_k denote the kth leading submatrix of a symmetric positive-definite matrix A. Prove that $\det(A_k)/\det(A_{k-1})$ is the kth pivot during LU decomposition, where, by convention, $\det(A_0) = 1$.

28.3-6

Find the function of the form

$$F(x) = c_1 + c_2 x \lg x + c_3 e^x$$

that is the best least-squares fit to the data points

$$(1, 1), (2, 1), (3, 3), (4, 8) .$$

28.3-7

Show that the pseudoinverse A^+ satisfies the following four equations:

$$\begin{aligned} AA^+A &= A\,, \\ A^+AA^+ &= A^+\,, \\ (AA^+)^{\mathrm{T}} &= AA^+\,, \\ (A^+A)^{\mathrm{T}} &= A^+A\,. \end{aligned}$$

Problems

28-1 Tridiagonal systems of linear equations

Consider the tridiagonal matrix

$$A = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix}.$$

a. Find an LU decomposition of A.

b. Solve the equation $Ax = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \end{pmatrix}^{\mathrm{T}}$ by using forward and back substitution.

c. Find the inverse of A.

d. Show how, for any $n \times n$ symmetric positive-definite, tridiagonal matrix A and any n-vector b, to solve the equation $Ax = b$ in $O(n)$ time by performing an LU decomposition. Argue that any method based on forming A^{-1} is asymptotically more expensive in the worst case.

e. Show how, for any $n \times n$ nonsingular, tridiagonal matrix A and any n-vector b, to solve the equation $Ax = b$ in $O(n)$ time by performing an LUP decomposition.

28-2 Splines

A practical method for interpolating a set of points with a curve is to use ***cubic splines***. We are given a set $\{(x_i, y_i) : i = 0, 1, \ldots, n\}$ of $n + 1$ point-value pairs, where $x_0 < x_1 < \cdots < x_n$. We wish to fit a piecewise-cubic curve (spline) $f(x)$ to the points. That is, the curve $f(x)$ is made up of n cubic polynomials $f_i(x) = a_i + b_i x + c_i x^2 + d_i x^3$ for $i = 0, 1, \ldots, n-1$, where if x falls in

the range $x_i \le x \le x_{i+1}$, then the value of the curve is given by $f(x) = f_i(x - x_i)$. The points x_i at which the cubic polynomials are "pasted" together are called ***knots***. For simplicity, we shall assume that $x_i = i$ for $i = 0, 1, \ldots, n$.

To ensure continuity of $f(x)$, we require that

$$\begin{aligned} f(x_i) &= f_i(0) = y_i \,, \\ f(x_{i+1}) &= f_i(1) = y_{i+1} \end{aligned}$$

for $i = 0, 1, \ldots, n-1$. To ensure that $f(x)$ is sufficiently smooth, we also insist that the first derivative be continuous at each knot:

$$f'(x_{i+1}) = f_i'(1) = f_{i+1}'(0)$$

for $i = 0, 1, \ldots, n-2$.

a. Suppose that for $i = 0, 1, \ldots, n$, we are given not only the point-value pairs $\{(x_i, y_i)\}$ but also the first derivatives $D_i = f'(x_i)$ at each knot. Express each coefficient a_i, b_i, c_i, and d_i in terms of the values y_i, y_{i+1}, D_i, and D_{i+1}. (Remember that $x_i = i$.) How quickly can we compute the $4n$ coefficients from the point-value pairs and first derivatives?

The question remains of how to choose the first derivatives of $f(x)$ at the knots. One method is to require the second derivatives to be continuous at the knots:

$$f''(x_{i+1}) = f_i''(1) = f_{i+1}''(0)$$

for $i = 0, 1, \ldots, n-2$. At the first and last knots, we assume that $f''(x_0) = f_0''(0) = 0$ and $f''(x_n) = f_{n-1}''(1) = 0$; these assumptions make $f(x)$ a ***natural*** cubic spline.

b. Use the continuity constraints on the second derivative to show that for $i = 1, 2, \ldots, n-1$,

$$D_{i-1} + 4D_i + D_{i+1} = 3(y_{i+1} - y_{i-1}) \,. \tag{28.21}$$

c. Show that

$$2D_0 + D_1 = 3(y_1 - y_0) \,, \tag{28.22}$$

$$D_{n-1} + 2D_n = 3(y_n - y_{n-1}) \,. \tag{28.23}$$

d. Rewrite equations (28.21)–(28.23) as a matrix equation involving the vector $D = \langle D_0, D_1, \ldots, D_n \rangle$ of unknowns. What attributes does the matrix in your equation have?

e. Argue that a natural cubic spline can interpolate a set of $n+1$ point-value pairs in $O(n)$ time (see Problem 28-1).

f. Show how to determine a natural cubic spline that interpolates a set of $n + 1$ points (x_i, y_i) satisfying $x_0 < x_1 < \cdots < x_n$, even when x_i is not necessarily equal to i. What matrix equation must your method solve, and how quickly does your algorithm run?

Chapter notes

Many excellent texts describe numerical and scientific computation in much greater detail than we have room for here. The following are especially readable: George and Liu [132], Golub and Van Loan [144], Press, Teukolsky, Vetterling, and Flannery [283, 284], and Strang [323, 324].

Golub and Van Loan [144] discuss numerical stability. They show why $\det(A)$ is not necessarily a good indicator of the stability of a matrix A, proposing instead to use $\|A\|_\infty \|A^{-1}\|_\infty$, where $\|A\|_\infty = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$. They also address the question of how to compute this value without actually computing A^{-1}.

Gaussian elimination, upon which the LU and LUP decompositions are based, was the first systematic method for solving linear systems of equations. It was also one of the earliest numerical algorithms. Although it was known earlier, its discovery is commonly attributed to C. F. Gauss (1777–1855). In his famous paper [325], Strassen showed that an $n \times n$ matrix can be inverted in $O(n^{\lg 7})$ time. Winograd [358] originally proved that matrix multiplication is no harder than matrix inversion, and the converse is due to Aho, Hopcroft, and Ullman [5].

Another important matrix decomposition is the ***singular value decomposition***, or ***SVD***. The SVD factors an $m \times n$ matrix A into $A = Q_1 \Sigma Q_2^{\mathrm{T}}$, where Σ is an $m \times n$ matrix with nonzero values only on the diagonal, Q_1 is $m \times m$ with mutually orthonormal columns, and Q_2 is $n \times n$, also with mutually orthonormal columns. Two vectors are ***orthonormal*** if their inner product is 0 and each vector has a norm of 1. The books by Strang [323, 324] and Golub and Van Loan [144] contain good treatments of the SVD.

Strang [324] has an excellent presentation of symmetric positive-definite matrices and of linear algebra in general.