2. $X^T X = \begin{bmatrix} X_1^T \\ X_2^T \end{bmatrix} \begin{bmatrix} X_1 & X_2 \end{bmatrix} = \begin{bmatrix} X_1^T X_1 & X_1^T X_2 \\ X_2^T X_1 & X_2^T X_2 \end{bmatrix}$. The partitions of X^T and X are automatically conformable for block multiplication because the columns of X^T are the rows of X. This partition of $X^T X$ is used in several computer algorithms for matrix computations.

2.5 MATRIX FACTORIZATIONS

A *factorization* of a matrix A is an equation that expresses A as a product of two or more matrices. Whereas matrix multiplication involves a *synthesis* of data (combining the effect of two or more linear transformations into a single matrix), matrix factorization is an *analysis* of data. In the language of computer science, the expression of A as a product amounts to a *preprocessing* of the data in A, organizing that data into two or more parts whose structures are more useful in some way, perhaps more accessible for computation.

Matrix factorizations and, later, factorizations of linear transformations will appear at a number of key points throughout the text. This section focuses on a factorization that lies at the heart of several important computer programs widely used in applications, such as the airflow problem described in the chapter introduction. Several other factorizations, to be studied later, are introduced in the exercises.

The LU Factorization

The LU factorization, described below, is motivated by the fairly common industrial and business problem of solving a sequence of equations, all with the same coefficient matrix:

$$A\mathbf{x} = \mathbf{b}_1, \quad A\mathbf{x} = \mathbf{b}_2, \quad \ldots, \quad A\mathbf{x} = \mathbf{b}_p \tag{1}$$

See Exercise 32, for example. Also see Section 5.8, where the inverse power method is used to estimate eigenvalues of a matrix by solving equations like those in (1), one at a time.

When A is invertible, one could compute A^{-1} and then compute $A^{-1}\mathbf{b}_1$, $A^{-1}\mathbf{b}_2$, and so on. However, it is more efficient to solve the first equation in (1) by row reduction and obtain an LU factorization of A at the same time. Thereafter, the remaining equations in (1) are solved with the LU factorization.

At first, assume that A is an $m \times n$ matrix that can be row reduced to echelon form, *without row interchanges*. (Later, we will treat the general case.) Then A can be written in the form $A = LU$, where L is an $m \times m$ lower triangular matrix with 1's on the diagonal and U is an $m \times n$ echelon form of A. For instance, see Fig. 1. Such a factorization is called an **LU factorization** of A. The matrix L is invertible and is called a *unit* lower triangular matrix.

$$A = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ * & 1 & 0 & 0 \\ * & * & 1 & 0 \\ * & * & * & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} \blacksquare & * & * & * & * \\ 0 & \blacksquare & * & * & * \\ 0 & 0 & 0 & \blacksquare & * \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{U}$$

FIGURE 1 An LU factorization.

Before studying how to construct L and U, we should look at why they are so useful. When $A = LU$, the equation $A\mathbf{x} = \mathbf{b}$ can be written as $L(U\mathbf{x}) = \mathbf{b}$. Writing $\mathbf{y}$ for $U\mathbf{x}$, we can find $\mathbf{x}$ by solving the *pair* of equations

$$\boxed{\begin{aligned} L\mathbf{y} &= \mathbf{b} \\ U\mathbf{x} &= \mathbf{y} \end{aligned}} \tag{2}$$

First solve $L\mathbf{y} = \mathbf{b}$ for $\mathbf{y}$, and then solve $U\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$. See Fig. 2. Each equation is easy to solve because L and U are triangular.

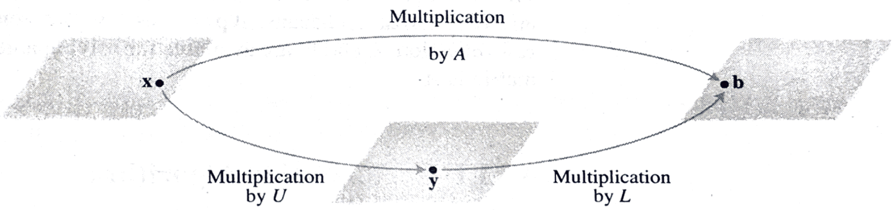

FIGURE 2 Factorization of the mapping $\mathbf{x} \mapsto A\mathbf{x}$.

EXAMPLE 1 It can be verified that

$$A = \begin{bmatrix} 3 & -7 & -2 & 2 \\ -3 & 5 & 1 & 0 \\ 6 & -4 & 0 & -5 \\ -9 & 5 & -5 & 12 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 2 & -5 & 1 & 0 \\ -3 & 8 & 3 & 1 \end{bmatrix} \begin{bmatrix} 3 & -7 & -2 & 2 \\ 0 & -2 & -1 & 2 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 \end{bmatrix} = LU$$

Use this LU factorization of A to solve $A\mathbf{x} = \mathbf{b}$, where $\mathbf{b} = \begin{bmatrix} -9 \\ 5 \\ 7 \\ 11 \end{bmatrix}$.

Solution The solution of $L\mathbf{y} = \mathbf{b}$ needs only 6 multiplications and 6 additions, because the arithmetic takes place only in column 5. (The zeros below each pivot in L are created automatically by the choice of row operations.)

$$[\,L \quad \mathbf{b}\,] = \begin{bmatrix} 1 & 0 & 0 & 0 & -9 \\ -1 & 1 & 0 & 0 & 5 \\ 2 & -5 & 1 & 0 & 7 \\ -3 & 8 & 3 & 1 & 11 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & 0 & -9 \\ 0 & 1 & 0 & 0 & -4 \\ 0 & 0 & 1 & 0 & 5 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = [\,I \quad \mathbf{y}\,]$$

Then, for $U\mathbf{x} = \mathbf{y}$, the "backward" phase of row reduction requires 4 divisions, 6 multiplications, and 6 additions. (For instance, creating the zeros in column 4 of $[\,U \quad \mathbf{y}\,]$ requires 1 division in row 4 and 3 multiplication–addition pairs to add multiples of row 4 to the rows above.)

$$[\,U \quad \mathbf{y}\,] = \begin{bmatrix} 3 & -7 & -2 & 2 & -9 \\ 0 & -2 & -1 & 2 & -4 \\ 0 & 0 & -1 & 1 & 5 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & 0 & 3 \\ 0 & 1 & 0 & 0 & 4 \\ 0 & 0 & 1 & 0 & -6 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} 3 \\ 4 \\ -6 \\ -1 \end{bmatrix}$$

To find $\mathbf{x}$ requires 28 arithmetic operations, or "flops" (floating point operations), excluding the cost of finding L and U. In contrast, row reduction of $[\,A \quad \mathbf{b}\,]$ to $[\,I \quad \mathbf{x}\,]$ takes 62 operations. ∎

The computational efficiency of the LU factorization depends on knowing L and U. The next algorithm shows that the row reduction of A to an echelon form U amounts to an LU factorization because it produces L with essentially no extra work. After the first row reduction, L and U are available for solving additional equations whose coefficient matrix is A.

An LU Factorization Algorithm

Suppose A can be reduced to an echelon form U using only row replacements that add a multiple of one row to another row *below it*. In this case, there exist unit lower triangular elementary matrices $E_1, \ldots, E_p$ such that

$$E_p \cdots E_1 A = U \tag{3}$$

Then

$$A = (E_p \cdots E_1)^{-1} U = LU$$

where

$$L = (E_p \cdots E_1)^{-1} \tag{4}$$

It can be shown that products and inverses of unit lower triangular matrices are also unit lower triangular. (For instance, see Exercise 19.) Thus L is unit lower triangular.

Note that the row operations in (3), which reduce A to U, also reduce the L in (4) to I, because $E_p \cdots E_1 L = (E_p \cdots E_1)(E_p \cdots E_1)^{-1} = I$. This observation is the key to *constructing* L.

ALGORITHM FOR AN LU FACTORIZATION

1. Reduce A to an echelon form U by a sequence of row replacement operations, if possible.
2. Place entries in L such that the *same sequence of row operations* reduces L to I.

Step 1 is not always possible, but when it is, the argument above shows that an LU factorization exists. Example 2 will show how to implement step 2. By construction, L will satisfy

$$(E_p \cdots E_1)L = I$$

using the same $E_1, \dots, E_p$ as in (3). Thus L will be invertible, by the Invertible Matrix Theorem, with $(E_p \cdots E_1) = L^{-1}$. From (3), $L^{-1}A = U$, and $A = LU$. So step 2 will produce an acceptable L.

EXAMPLE 2 Find an LU factorization of

$$A = \begin{bmatrix} 2 & 4 & -1 & 5 & -2 \\ -4 & -5 & 3 & -8 & 1 \\ 2 & -5 & -4 & 1 & 8 \\ -6 & 0 & 7 & -3 & 1 \end{bmatrix}$$

Solution Since A has four rows, L should be 4×4. The first column of L is the first column of A divided by the top pivot entry:

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 1 & & 1 & 0 \\ -3 & & & 1 \end{bmatrix}$$

Compare the first columns of A and L. *The row operations that create zeros in the first column of A will also create zeros in the first column of L.* We want this same correspondence of row operations to hold for the rest of L, so we watch a row reduction of A to an echelon form U:

$$A = \begin{bmatrix} 2 & 4 & -1 & 5 & -2 \\ -4 & -5 & 3 & -8 & 1 \\ 2 & -5 & -4 & 1 & 8 \\ -6 & 0 & 7 & -3 & 1 \end{bmatrix} \sim \begin{bmatrix} 2 & 4 & -1 & 5 & -2 \\ 0 & 3 & 1 & 2 & -3 \\ 0 & -9 & -3 & -4 & 10 \\ 0 & 12 & 4 & 12 & -5 \end{bmatrix} = A_1 \qquad (5)$$

$$\sim A_2 = \begin{bmatrix} 2 & 4 & -1 & 5 & -2 \\ 0 & 3 & 1 & 2 & -3 \\ 0 & 0 & 0 & 2 & 1 \\ 0 & 0 & 0 & 4 & 7 \end{bmatrix} \sim \begin{bmatrix} 2 & 4 & -1 & 5 & -2 \\ 0 & 3 & 1 & 2 & -3 \\ 0 & 0 & 0 & 2 & 1 \\ 0 & 0 & 0 & 0 & 5 \end{bmatrix} = U$$

The highlighted entries above determine the row reduction of A to U. At each pivot column, divide the highlighted entries by the pivot and place the result into L:

$$\begin{bmatrix} 2 \\ -4 \\ 2 \\ -6 \end{bmatrix} \begin{bmatrix} 3 \\ -9 \\ 12 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \end{bmatrix} \begin{bmatrix} 5 \end{bmatrix}$$

$$\div 2 \qquad \div 3 \qquad \div 2 \qquad \div 5$$

$$\begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ 1 & -3 & 1 & \\ -3 & 4 & 2 & 1 \end{bmatrix}, \quad \text{and} \quad L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 1 & -3 & 1 & 0 \\ -3 & 4 & 2 & 1 \end{bmatrix}$$

An easy calculation verifies that this L and U satisfy $LU = A$. ■

In practical work, row interchanges are nearly always needed, because partial pivoting is used for high accuracy. (Recall that this procedure selects, among the possible choices for a pivot, an entry in the column having the largest absolute value.) To handle row interchanges, the LU factorization above can be modified easily to produce an L that is *permuted lower triangular*, in the sense that a rearrangement (called a permutation) of the rows of L can make L (unit) lower triangular. The resulting *permuted LU factorization* solves $A\mathbf{x} = \mathbf{b}$ in the same way as before, except that the reduction of $[\,L \quad \mathbf{b}\,]$ to $[\,I \quad \mathbf{y}\,]$ follows the order of the pivots in L from left to right, starting with the pivot in the first column. A reference to an "LU factorization" usually includes the possibility that L might be permuted lower triangular. For details, see the *Study Guide*.

NUMERICAL NOTES

The following operation counts apply to an $n \times n$ dense matrix A (with most entries nonzero) for n moderately large, say, $n \geq 30$.[1]

1. Computing an LU factorization of A takes about $2n^3/3$ flops (about the same as row reducing $[\,A \quad \mathbf{b}\,]$), whereas finding A^{-1} requires about $2n^3$ flops.
2. Solving $L\mathbf{y} = \mathbf{b}$ and $U\mathbf{x} = \mathbf{y}$ requires about $2n^2$ flops, because any $n \times n$ triangular system can be solved in about n^2 flops.
3. Multiplication of $\mathbf{b}$ by A^{-1} also requires about $2n^2$ flops, but the result may not be as accurate as that obtained from L and U (because of roundoff error when computing both A^{-1} and $A^{-1}\mathbf{b}$).
4. If A is sparse (with mostly zero entries), then L and U may be sparse, too, whereas A^{-1} is likely to be dense. In this case, a solution of $A\mathbf{x} = \mathbf{b}$ with an LU factorization is *much* faster than using A^{-1}. See Exercise 31.

[1] See Section 3.8 in *Applied Linear Algebra*, 3rd ed., by Ben Noble and James W. Daniel (Englewood Cliffs, NJ: Prentice-Hall, 1988). Recall that for our purposes, a *flop* is $+$, $-$, $\times$, or $\div$.