1 Solving Sets of Equations

- Solving sets of linear equations is the most frequently used numerical procedure when real-world situations are modeled.
- The methods for solving ordinary and partial-differential equations depend on them.
  - **Matrices and Vectors**. Reviews concepts of matrices and vectors in preparation for their use in this chapter.
  - **Elimination Methods.** Describes two classical methods that change a system of equations to forms that allow getting the solution by back-substitution and shows how the errors of the solution can be minimized.
  - **The Inverse of a Matrix and Matrix Pathology.** Shows how an important derivative of a matrix, its inverse, can be computed. It shows when a matrix cannot be inverted and tells of situations where no unique solution exists to a system of equations.
  - **Ill-Conditioned Systems.** Explores systems for which getting the solution with accuracy is very difficult. A number, the condition number, is a measure of such difficulty; a property of a matrix, called its norm, is used to compute its condition number. A way to improve an inaccurate solution is described.
  - **Iterative Methods.**This section describes how a linear system can be solved in an entirely different way, by beginning with an initial estimate of the solution and performing computations that eventually arrive at the correct solution. An iterative method is particularly important in solving systems that have few nonzero coefficients.
  - **Parallel Processing.** Tells how parallel computing can be applied to the solution of linear systems. An algorithm is developed that allows a significant reduction in processing time.

1.1 Matrices and Vectors

- When a system of equations has more than two or three equations, it is difficult to discuss them without using *matrices* and *vectors*.
- A *matrix* is a rectangular array of numbers in which not only the value

of the number is important but also its position in the array.

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{nm} \end{bmatrix} = [a_{ij}]\,,\; i = 1, 2, \dots, n,\; j = 1, 2, \dots, m$$

- Two matrices of the same size may be added or subtracted. The sum of
$$A = [a_{ij}]\,, B = [b_{ij}]$$
is the matrix whose elements are the sum of the corresponding elements of A and B.
$$C = A + B = [a_{ij} + b_{ij}] = [c_{ij}]$$

- Similarly, we get the difference of two equal-sized matrices by subtracting corresponding elements. If two matrices are not equal in size, they cannot be added or subtracted.

- Multiplication of two matrices is defined as follows, when A is $n \times m$ and B is $m \times r$.
$$[a_{ij}] * [b_{ij}] = [c_{ij}] =$$
$$\begin{bmatrix} (a_{11}b_{11} + a_{12}b_{21} + \ldots + a_{1m}b_{m1}) & \dots & (a_{11}b_{1r} + \ldots + a_{1m}b_{mr}) \\ (a_{21}b_{11} + a_{22}b_{21} + \ldots + a_{2m}b_{m1}) & \dots & (a_{21}b_{1r} + \ldots + a_{2m}b_{mr}) \\ \vdots & & \\ (a_{n1}b_{11} + a_{n2}b_{21} + \ldots + a_{nm}b_{m1}) & \dots & (a_{n1}b_{1r} + \ldots + a_{nm}b_{mr}) \end{bmatrix}$$
$$c_{ij} = \sum_{k=1}^{m} a_{ik}b_{kj},\; i = 1, 2, \dots, n,\; j = 1, 2, \dots, r$$

- Unless the number of columns of A equals the number of rows of B, the matrices cannot be multiplied.

- If A is $n \times m$, B must have is m rows or else they are said to be *nonconformable* for multiplication and their product is undefined.

- In general, $AB \neq BA$, so the order of factors must be preserved in matrix multiplication.

- A matrix with only one column, $n \times 1$ in size, is termed a **column vector**, and one of only one row, $1 \times m$ in size, is called a **row vector**. When the term **vector** is used, it nearly always means a **column** vector.

- An $m \times n$ matrix times as $n \times 1$ vector gives an $m \times 1$ product. The general relation for $Ax = b$ is

$$b_i = \sum_{k=1}^{No.of.cols.} a_{ik}x_k, \; i = 1, 2, \ldots, No.of.rows$$

  This definition of matrix multiplication permits us to write the set of linear equations

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

  much more simply in matrix notation, as $Ax = b$ where

$$A = \begin{bmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{bmatrix}, x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

  For example,

$$\begin{bmatrix} 3 & 2 & 4 \\ 1 & -2 & 0 \\ -1 & 3 & 2 \end{bmatrix} * \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 14 \\ -7 \\ 2 \end{bmatrix}$$

  is the same as the set of equations

$$\begin{aligned} &3x_1 + 2x_2 + 4x_3 = 14 \\ &x_1 - 2x_2 = -7 \\ &-x_1 + 3x_2 + 2x_3 = 2 \end{aligned}$$

- A vector whose length is one is called a **unit vector** (The length of a vector is the square root of the sum of the squares of its components, an extension of the idea of the length of a two-component vector drawn from the origin).

- A vector that has all of its elements equal to zero is the **zero vector**. If all elements are zero except one, it is a *unit basis vector*. There are three distinct unit basis vectors of order-3:

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

1.1.1 Some Special Matrices and Their Properties

- Square matrices are particularly important when a system of equations is to be solved. Square matrices have some special properties.
- The elements on the *main diagonal* are those from the upper-left corner to the lower-right corner. (diagonal elements, diagonal)
- If the nonzero elements of a diagonal matrix all are equal to one, the matrix is called the *identity matrix of order n* where n equals the number of row and columns. The order-4 identity matrix is

$$I_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- An important property of an identity matrix, I, is that for any $n \times n$ matrix, A,

$$I * A = A * I = I$$

- If two rows of an identity, matrix are interchanged, it is called a transposition matrix. (We also get a transposition matrix by interchanging two columns.
- If transposition matrix P_1, is multiplied with a square matrix of the same size, A, the product $P_1 * A$ will be the A matrix but with the same two rows interchanged. i.e.:

$$P_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, A = \begin{bmatrix} 9 & 6 & 2 & 13 \\ 4 & 2 & 8 & 11 \\ 0 & 7 & 1 & 9 \\ 3 & 2 & 6 & 8 \end{bmatrix}, P_1 * A = \begin{bmatrix} 9 & 6 & 2 & 13 \\ 3 & 2 & 6 & 8 \\ 0 & 7 & 1 & 9 \\ 4 & 2 & 8 & 11 \end{bmatrix},$$

- However, if the two matrices are multiplied in reverse order, $A * P_1$, the result will be matrix A but with the columns of A interchanged.
- A permutation matrix is obtained by multiplying several transposition matrices.
- A square matrix is called a **symmetric matrix** when the pairs of elements in similar positions across the diagonal are equal.

$$\begin{bmatrix} 1 & x & y \\ x & 2 & z \\ y & z & 3 \end{bmatrix}$$

- The transpose of a matrix is the matrix obtained by writing the rows as columns or by writing the columns as rows. (A matrix does not have to be square to have a transpose.) The symbol for the transpose of matrix A is A^T.

$$A = \begin{bmatrix} 3 & -1 & 4 \\ 0 & 2 & 3 \\ 1 & 1 & 2 \end{bmatrix}, A^T = \begin{bmatrix} 3 & 0 & 1 \\ -1 & 2 & 1 \\ 4 & -3 & 2 \end{bmatrix},$$

- It should be clear that $A = A^T$ if A is symmetric, and that for any matrix, the transpose of the transpose, $(A^T)^T$, is just A itself. It is also true that $(A * B)^T = B^T * A^T$.

- When a matrix is square, a quantity called its **trace** is defined. The trace of a square matrix is the sum of the elements on its main diagonal. The trace remains the same if a square matrix is transposed. $tr(A) = tr(A^T)$

- If all the elements above the diagonal are zero, a matrix is called *lower-triangular*; it is called *upper-triangular* when all the elements below the diagonal are zero.

$$L = \begin{bmatrix} x & 0 & 0 \\ x & x & 0 \\ x & x & x \end{bmatrix}, U = \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \end{bmatrix}$$

- Tridiagonal matrices are those that have nonzero elements only on the diagonal and in the positions adjacent to the diagonal;

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

  For a tridiagonal matrix, only the nonzero values need to be recorded, and that means that the $n \times n$ matrix can be compressed into a matrix of 3 columns and n rows.

- In some important applied problems, only a few of the elements are nonzero. Such a matrix is termed a **sparse matrix** and procedures that take advantage of this sparseness are of value.

- Division of matrices is not defined, but we will discuss the inverse of a matrix later in

- The determinant of a square matrix is a number. For a 2×2 matrix, the determinant is computed by subtracting the product of the elements on the minor diagonal (from upper right to lower left) from the product of terms on the major diagonal.

$$\begin{bmatrix} -5 & 3 \\ 7 & 2 \end{bmatrix}, \; det(A) = (-5)(2) - (7)(3) = -31$$

- We expand each of the determinants of the minor until we reach 2×2 matrices.

$$A = \begin{bmatrix} 3 & 0 & -1 & 2 \\ 4 & 1 & 3 & -2 \\ 0 & 2 & -1 & 3 \\ 1 & 0 & 1 & 4 \end{bmatrix} \Rightarrow det(A) = 3 \begin{vmatrix} 1 & 3 & -2 \\ 2 & -1 & 3 \\ 0 & 1 & 4 \end{vmatrix} - 0 \begin{vmatrix} 4 & 3 & -2 \\ 0 & -1 & 3 \\ 1 & 1 & 4 \end{vmatrix}$$

$$+(-1) \begin{vmatrix} 4 & 1 & -2 \\ 0 & 2 & 3 \\ 1 & 0 & 4 \end{vmatrix} - 2 \begin{vmatrix} 4 & 1 & 3 \\ 0 & 2 & -1 \\ 1 & 0 & 1 \end{vmatrix} = -146$$

- In computing the determinant, the expansion can be about the elements of any row or column. To get the signs, give the first term a plus sign if the sum of its column number and row number is even; give it a minus if the sum is odd, with alternating signs thereafter.

- This method of calculating determinants is a lot of work if the matrix is of large size. Methods that triangularize a matrix, as described in Section 1.2, are much better ways to get the determinant.

- If a matrix, B, is triangular (either upper or lower), its determinant is just the product of the diagonal elements:

$$det(B) = \Pi B_{ii}, \; i = 1, \ldots, n$$

  It is easy to show this if the determinant of the triangular matrix is expanded by minors.

$$det \begin{bmatrix} 4 & 0 & 0 \\ 6 & -2 & 0 \\ 1 & -3 & 5 \end{bmatrix} = -40$$

- Determinants can be used to obtain the **characteristic polynomial** and the **eigenvalues** of a matrix, which are the roots of that polynomial. (Eigenvalue is a German word, the corresponding English term is characteristic value, but it is less frequently used.)

- The two terms, eigenvalue and characteristic polynomial are interrelated; For matrix A, $P_A(\lambda) = det(A - \lambda I)$.

$$A = \begin{bmatrix} 1 & 3 \\ 4 & 5 \end{bmatrix}$$

$$P_A(\lambda) = |A - \lambda I| = det \begin{bmatrix} 1-\lambda & 3 \\ 4 & 5-\lambda \end{bmatrix} = \lambda^2 - 6\lambda - 7$$

- The characteristic polynomial is always of degree n if A is $n \times n$. If we set the characteristic polynomial to zero and solve for the roots, we get the eigenvalues of A. For this example, these are $\lambda_1 = 7,\ \lambda_2 = -1$, or, in more symbolic mathematical notation:

$$\Lambda(A) = \{7, -1\}$$

- We also mention the notion of an **eigenvector** corresponding to an eigenvalue.

$$Aw = \lambda w \Longrightarrow (A - \lambda I)w = 0$$

  In the current example, the eigenvectors are

$$w_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, w_2 = \begin{bmatrix} -3 \\ 2 \end{bmatrix}$$

- Observe that the trace of A is equal to the sum of the eigenvalues: $tr(A) = 1 + 5 = \lambda_1 + \lambda_2 = 7 + (-1) = 6$ This is true for any matrix: The sum of its eigenvalues equals its trace.

- If a matrix is triangular, its eigenvalues are equal to the diagonal elements. This follows from the fact that its determinant is just the product of the diagonal elements and its characteristic polynomial is the product of the terms $(a_{ii} - \lambda)$ with i going from 1 to n, the number of rows of the matrix.

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

$$det(A - \lambda I) = det \begin{bmatrix} 1-\lambda & 2 & 3 \\ 0 & 4-\lambda & 5 \\ 0 & 0 & 6-\lambda \end{bmatrix} = (1-\lambda)(4-\lambda)(6-\lambda)$$

whose roots are clearly 1, 4, and 6. It does not matter if the matrix is upper- or lower-triangular.

1.1.2 Using Computer Algebra Systems

MATLAB can do matrix operations . We first define two matrices and a vector,*A, B,* and ν:

```
>> A = [ 4 1 -2 ; 5 1 3 ; 4 0 -1]
>> B = [ 3 3 1 ; -2 1 5 ; 2 2 0]
>> v = [ -2 3 1]
>> vt = v'
>> det(A)
>> trace (A)
We can get the characteristic polynomial;
>> poly(A)
ans =
1.000   -4.0000   2.0000   -21.0000
where the coefficients are given. This represents
x^4 - 4x^3 + 2x -21
```

1.2 Elimination Methods

- To solve a set of linear equations. The term linear equation means an equation in several variables where all of the variables occur to the first power.

- Suppose we have a system of equations that is of a special form, an *upper-triangular* system, such as

$$\begin{aligned} 5x_1 + 3x_2 - 2x_3 &= -3 \\ 6x_2 + x_3 &= -1 \\ 2x_3 &= 10 \end{aligned}$$

  we have the solution $x_1 = 2, x_2 = -1, x_3 = 5$

- The first objective of the elimination method is to change the matrix of coefficients so that it is upper triangular. Consider this example of three equations:

$$\begin{aligned} 4x_1 - 2x_2 + x_3 &= 15 \\ -3x_1 - x_2 + 4x_3 &= 8 \\ x_1 - x_2 + 3x_3 &= 13 \end{aligned}$$

$$\begin{aligned} 4x_1 - 2x_2 + x_3 &= 15 \\ -10x_2 + 19x_3 &= 77 \\ -2x_2 + 11x_3 &= 37 \end{aligned}$$

$$\begin{aligned} 4x_1 - 2x_2 + x_3 &= 15 \\ -10x_2 + 19x_3 &= 77 \\ -72x_3 &= -216 \end{aligned}$$

Now we have a triangular system and the solution is readily obtained; obviously $x_3 = 3$ from the third equation, and **back-substitution** into the second equation gives $x_2 = -2$. We continue with back-substitution by substituting both x_2, and x_3 into the first equation to get $x_1 = 2$.

- The essence of any elimination method is to reduce the coefficient matrix to a triangular matrix and then use back-substitution to get the solution.

- We now present the same problem, solved in exactly the same way, in matrix notation;

$$\begin{bmatrix} 4 & -2 & 1 \\ -3 & -1 & 4 \\ 1 & -1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 8 \\ 13 \end{bmatrix}$$

- The arithmetic operations that we have performed affect only the coefficients and the right-hand-side terms, so we work with the matrix of coefficients *augmented* with the right-hand-side vector.

- We perform elementary row transformations to convert A to upper-triangular form:

$$\begin{bmatrix} 4 & -2 & 1 & 15 \\ -3 & -1 & 4 & 8 \\ 1 & -1 & 3 & 13 \end{bmatrix}, \quad \begin{matrix} \\ 3R_1 + 4R_2 \rightarrow \\ (-1)R_1 + 4R_3 \rightarrow \end{matrix} \begin{bmatrix} 4 & -2 & 1 & 15 \\ 0 & -10 & 19 & 77 \\ 0 & -2 & 11 & 37 \end{bmatrix},$$

$$\begin{matrix} \\ \\ 2R_2 - 10R_3 \rightarrow \end{matrix} \begin{bmatrix} 4 & -2 & 1 & 15 \\ 0 & -10 & 19 & 77 \\ 0 & 0 & 72 & -216 \end{bmatrix}$$

- This array represents the equations

$$\begin{aligned} 4x_1 - 2x_2 + x_3 &= 15 \\ -10x_2 + 19x_3 &= 77 \\ -72x_3 &= -216 \end{aligned}$$

  The back-substitution step can be performed quite mechanically by solving the equations in reverse order. That is, $x_3 = 3, x_2 = -2, x_1 = 2$.

- Both the lower-and upper-triangular systems play an important part in the development of algorithms in the following sections, because these systems require fewer multiplications/divisions than the general system.

- Note that there exists the possibility that the set of equations has no solution, or that the prior procedure will fail to find it.

- During the triangularization step, if a zero is encountered on the diagonal, we cannot use that row to eliminate coefficients below that zero element. However, in that case, we can continue by interchanging rows and eventually achieve an upper-triangular matrix of coefficients.

- The real trouble is finding a zero on the diagonal after we have triangularized. If that occurs, the back-substitution fails, for we cannot divide by zero. It a1so means that the determinant is zero. There is no solution.

1.2.1 Gaussian Elimination

- The procedure just described has a major problem. While it may be satisfactory for hand computations with small systems, it is inadequate for a large system. Observe that the transformed coefficients can become very large as we convert to a triangular system.

- The method that is called *Gaussian elimination* avoids this by subtracting a_{i1}/a_{11} times the first equation from the i^{th} equation to make the transformed numbers in the first column equal to zero. We do similarly for the rest of the columns.

- We must always guard against dividing by zero. Observe that zeros may be created in the diagonal positions even if they are not present in the original matrix of coefficients. A useful strategy to avoid (if possible) such zero divisors is to rearrange the equations so as to put the coefficient of largest magnitude on the diagonal at each step. This is called **pivoting**.

- Repeat the example of the previous section,

$$\begin{bmatrix} 4 & -2 & 1 & 15 \\ -3 & -1 & 4 & 8 \\ 1 & -1 & 3 & 13 \end{bmatrix}, \begin{matrix} R_2 - (-3/4)R_1 \rightarrow \\ R_3 - (-1/4)R_1 \rightarrow \end{matrix} \begin{bmatrix} 4 & -2 & 1 & 15 \\ 0 & -2.5 & 4.75 & 19.25 \\ 0 & -0.5 & 2.75 & 9.25 \end{bmatrix},$$

$$R_3 - (-0.5/-2.5)R_2 \rightarrow \begin{bmatrix} 4 & -2 & 1 & 15 \\ 0 & -2.5 & 4.75 & 19.25 \\ 0 & 0 & 1.8 & 5.40 \end{bmatrix}$$

- The method we have just illustrated is called Gaussian elimination. (In this example, no pivoting was required to make the largest coefficients be on the diagonal.) Back-substitution, gives us $x_3 = 3, x_2 = -2, x_1 = 2$

- We shall obtain answers that are just close approximations to the exact answer because of round-off error. When there are many equations, the effects of round-off (the term is applied to the error due to chopping as well as when rounding is used) may cause large effects. In certain cases, the coefficients are such that the results are particularly sensitive to round off; such systems are called **ill-conditioned**.

- if we had stored the ratio of coefficients in place of zero (we show these in parentheses), our final form would have been

$$\begin{bmatrix} 4 & -2 & 1 & 15 \\ (-0.75) & -2.5 & 4.75 & 19.25 \\ (0.25) & (0.20) & 1.8 & 5.40 \end{bmatrix}$$

- The original matrix can be written as the product:

$$A = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ -0.75 & 1 & 0 \\ 0.25 & 0.20 & 1 \end{bmatrix}}_{L} * \underbrace{\begin{bmatrix} 4 & -2 & 1 \\ 0 & -2.5 & 4.75 \\ 0 & 0 & 1.8 \end{bmatrix}}_{U}$$

This procedure is called a *LU decomposition of A*. In this case,

$$A = L * U$$

where L is lower-triangular and U is upper-triangular.

- Because the determinant of two matrices, $B \times C$, is the product of each of the determinants, for this example we have

$$det(L * U) = det(L) * det(U) = det(U)$$

because L is triangular and has only ones on its diagonal so that $det(L) = 1$. Thus, for our example, we have

$$det(A) = det(U) = (4) * (-2.5) * (1.8) = -18$$

because U is upper-triangular and its determinant i is just the product of the diagonal elements.

- When there are row interchanges

$$det(A) = (-1)^m * u_{11} * \ldots * u_{nn}$$

where the exponent m represents the number of row interchanges.

- Solve the following system of equations using Gaussian elimination. In addition, compute the determinant of the coefficient matrix and the LU decomposition of this matrix.

$$\begin{array}{rrrrl} & 2x_2 & & +x_4 & = 0 \\ 2x_1 & +2x_2 & +3x_3 & +2x_4 & = -2 \\ 4x_1 & +2x_2 & +3x_3 & +2x_4 & = -2 \\ 2x_1 & +2x_2 & +3x_3 & +2x_4 & = -2 \end{array}$$

The augmented coefficient matrix is

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

We cannot permit a zero in the a_{11} position because that element is the pivot in reducing the first column. We could interchange the first row with any of the other rows to avoid a zero divisor, but interchanging the first and fourth rows is our best choice. This gives

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

$$\begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ 0 & 1.6667 & 5 & 3.6667 & -4 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

We again interchange before reducing the second column, not because we have a zero divisor, but because we want to preserve accuracy. Interchanging the second and third rows puts the element of largest magnitude on the diagonal.

$$\begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 1.6667 & 5 & 3.6667 & -4 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

Now we reduce in the second column

$$\begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 0 & 6.8182 & 5.6364 & -9.0001 \\ 0 & 0 & 2.1818 & 3.3636 & -5.9999 \end{bmatrix}$$

No interchange is indicated in the third column. Reducing, we get

$$\begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ 0 & -3.6667 & 4 & 4.3333 & -11 \\ 0 & 0 & 6.8182 & 5.6364 & -9.0001 \\ 0 & 0 & 0 & 1.5600 & -3.1199 \end{bmatrix}$$

Back-substitution gives $x_1 = -0.50000, x_2 = 1.0000, x_3 = 0.33325, x_4 = -1.9999$. The correct answers are $x_1 = -1/2, x_2 = 1, x_3 = 1/3, x_4 = -2$. In this calculation we have carried five significant figures and rounded each calculation. Even so, we do not have five-digit accuracy in the answers. The discrepancy is due to round off.

- In this example, if we had replaced the zeros below the main diagonal with the ratio of coefficients at each step, the resulting augmented matrix would be

$$\begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ (0.66667) & -3.6667 & 4 & 4.3333 & -11 \\ (0.33333) & (-0.45454) & 6.8182 & 5.6364 & -9.0001 \\ (0.0) & (-0.54545) & (0.32) & 1.5600 & -3.1199 \end{bmatrix}$$

This gives a LU decomposition as

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.66667 & 1 & 0 & 0 \\ 0.33333 & -0.45454 & 1 & 0 \\ 0.0 & -0.54545 & 0.32 & 1 \end{bmatrix} * \begin{bmatrix} 6 & 1 & -6 & -5 \\ 0 & -3.6667 & 4 & 4.3333 \\ 0 & 0 & 6.8182 & 5.6364 \\ 0 & 0 & 0 & 1.5600 \end{bmatrix}$$

It should be noted that the product or the matrices produces a permutation of the original matrix, call it A', where

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

The determinant of the original matrix of coefficients can be easily computed according to the formula

$$det(A) = (-1)^2 * (6) * (-3.6667) * (6.8182) * (l.5600) = -234.0028$$

which is close to the exact solution: -234. The exponent 2 is required, because there were two row interchanges in solving this system. To summarize

1. The solution to the four equations
2. The determinant of the coefficient matrix
3. A *LU* decomposition of the matrix, A', which is just the original matrix, A, after we have interchanged its rows in the process.

```
>> A = [0 2 0 1 0 ;  2 2 3 2  -2 ;  4 -3 0 1 -7 ;  6 1 -6 -5 6]
>> [L, U, P]=lu(A)
>> b = [ 0 -2 -7 6]
>> A\b
ans =
-0.5000
 1.0000
 0.3333
-2.0000
```

1.2.2 The Gauss-Jordan Method

- There are many variants to the Gaussian elimination scheme. The back-substitution step can be performed by eliminating the elements above the diagonal after the triangularization has been finished.

- The diagonal elements may all be made ones as a first step before creating zeros in their column; this performs the divisions of the back-substitution phase at an earlier time.

- One variant that is sometimes used is the *Gauss-Jordan* scheme. In it, the elements above the diagonal are made zero at the *same time* that zeros are created below the diagonal.

- Usually, the diagonal elements are made ones at the same time that the reduction is performed; this transforms the coefficient matrix into the identity matrix.

- When this has been accomplished, the column of right-hand sides has been transformed into the solution vector. Pivoting is normally employed to preserve arithmetic accuracy.

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

Interchanging rows 1 and 4, dividing the new first row by 6, and reducing the first column gives

$$\begin{bmatrix} 1 & 0.1667 & -1 & -0.8333 & 1 \\ 0 & 1.6667 & 5 & 3.3667 & -4 \\ 0 & -3.6667 & 4 & 4.3334 & -11 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

Interchanging rows 2 and 3, dividing the new second row by -3.6667, and reducing the second column (operating above the diagonal as well as below) gives

$$\begin{bmatrix} 1 & 0 & -0.8182 & -0.6364 & 0.5 \\ 0 & 1 & -1.0909 & -1.1818 & 3 \\ 0 & 0 & 6.8182 & 5.6364 & -9 \\ 0 & 0 & 2.1818 & 3.3636 & -6 \end{bmatrix}$$

No interchanges now are required. We divide the third row by 6.8182 and create zeros below and above.

$$\begin{bmatrix} 1 & 0 & 0 & 0.04 & -0.58 \\ 0 & 1 & 0 & -0.2308 & 1.56 \\ 0 & 0 & 1 & 0 & -1.32 \\ 0 & 0 & 0 & 1.5599 & -3.12 \end{bmatrix}$$

We complete by dividing the fourth row by 1.5599 and create zeros above:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & -0.5 \\ 0 & 1 & 0 & 0 & 1.0001 \\ 0 & 0 & 1 & 0 & 0.3333 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

- the fourth column is now the solution.
- While the Gauss-Jordan method might seem to require the same effort as Gaussian elimination, it really requires almost 50% more operations.

1.2.3 Using the LU Matrix for Multiple Right-Hand Sides

- Many physical situations are modelled with a large set of linear equations.
- The equations will depend on the geometry and certain external factors that will determine the right-hand sides.
- If we want the solution for many different values of these right-hand sides, it is inefficient to solve the system from the start with each one of the right-hand-side values using the LU equivalent of the coefficient matrix is preferred.
- Suppose we have solved the system $Ax = b$ by Gaussian elimination. We now know the LU equivalent of A: $A = L * U$.
- Consider now that we want to solve $Ax = b$ with some new b-vector. We can write

$$Ax = b = L * U * x = b$$

- The product of U and x is a vector, call it y. Now, we can solve for y from $Ly = b$ and this is readily done because L is lower-triangular and we get y by forward-substitution. Call the solution $y = b'$.

- Going back to the original $LUx = b$, we see that, from $Ux = y = b'$, we can get x from $Ux = b'$, which is again readily done by back-substitution (U is upper-triangular).

- i.e., Solve $Ax = b$, where we already have its L and U matrices:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.66667 & 1 & 0 & 0 \\ 0.33333 & -0.45454 & 1 & 0 \\ 0.0 & -0.54545 & 0.32 & 1 \end{bmatrix} * \begin{bmatrix} 6 & 1 & -6 & -5 \\ 0 & -3.6667 & 4 & 4.3333 \\ 0 & 0 & 6.8182 & 5.6364 \\ 0 & 0 & 0 & 1.5600 \end{bmatrix}$$

  Suppose that the b-vector is $[6, -7, -2, 0]^T$. We first get $y = Ux$ from $Ly = b$ by forward substitution:

$$y = [6, -11, -9, -3.12]^T$$

  and use it to compute x from $Ux = y$:

$$x = [-0.5, 1, 0.3333, -2]^T.$$

- Now, if we want the solution with a different b-vector;

$$bb = [14 - 31]^T$$

  we just do $Ly = bb$ to get

$$y = [1, 3.3333, -1.8182, 3.4]^T$$

  and then use this y in $Ux = y$ to find the new x:

$$x = [0.0l28, -0.5897, -2.0684, 2.1795]^T$$