3. LINEAR ALGEBRA

3.1 INTRODUCTION

A large number of situations in engineering reduce to the need for solving a set of algebraic equations. Therefore, it is essential to have basic definitions and techniques available with some understanding of limitations and pitfalls that can occur from a strictly numerical viewpoint. As shown later on, there is usually a strong correlation between a poor physical understanding of a problem and an improper mathematical formulation, and between an improper mathematical formulation and problems associated with numerical simulation. The intent of these sections on linear algebra is to provide a convenient compilation of definitions and results that form an essential part of computational mechanics. With this background, the reader can then appreciate the material in a more comprehensive book such as the one by Strang (1988) who provides insight that is essential for a thorough understanding of linear algebra.

3.2. VECTORS

3.2.1 Notation

A **column vector**, {v}, is taken here to be a column of ordered terms, called components, v_1, v_2, ... Alternative notations are $\mathbf{v}$, $\overline{v}$, $\vec{v}$, and some authors just define v to be a vector with no particular identifying feature. Most undergraduate engineering texts use bold face to represent physical vectors in one, two and three dimensions. In general, we will now be considering vectors in a more abstract sense so will just use the word **vector** and consistently use the notation, {v}, to indicate the column format. Also, because this is intended to be an introductory text and reference book, the bracket notation should be clearer for those not intimate with the concepts of vector and matrix theory. As the material becomes familiar, a more compact notation, such as bold type, for vectors becomes preferable.

Sometimes the components are arranged in a row, <v>, in which case the vector is called a **row vector**. As before, the variables that form a row vector are called components or elements of the vector. The number of components, n, is the size of the vector or the dimension of the vector. The elements are ordered as follows for the column and row notations:

$$\{v\} = \begin{Bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{Bmatrix}, \qquad <v> = \langle v_1 \quad v_2 \quad \cdots \quad v_n \rangle \tag{3.2-1}$$

The transpose, denoted by a superscript, T, is used to imply that a column is replaced by a row, and vice versa, so the following notation also holds:

$$\{v\}^T = <v> \qquad <v>^T = \{v\} \tag{3.2-2}$$

If two vectors, {u} and {v}, have the same size, then the **inner product** is defined to be the scalar

$$<u>\{v\} = <v>\{u\} = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n \tag{3.2-3}$$

The magnitude of a vector, {v}, is denoted by $|v|$ and is obtained by taking the inner product of the vector with itself:

$$|v| = (<v>\{v\})^{1/2} \tag{3.2-4}$$

The unit vectors associated with {u} and {v} are

$$\{\bar{u}\} = \frac{\{u\}}{|u|} \qquad \{\bar{v}\} = \frac{\{v\}}{|v|} \tag{3.2-5}$$

The angle, θ_{uv} between the vectors {u} and {v}, is defined by the equation

$$\cos\theta_{uv} = <\bar{u}>\{\bar{v}\} \tag{3.2-6}$$

3.2.2 Vector Spaces

A real vector space is a set of vectors together with rules for vector addition and multiplication by real numbers [Strang, 1988; pg. 64]. Let the vectors be labelled $\{v\}^i$. The rules are:

1. $\{v\}^1 + \{v\}^2 = \{v\}^2 + \{v\}^1$,
2. $\{v\}^1 + \{\{v\}^2 + \{v\}^3\} = \{\{v\}^1 + \{v\}^2\} + \{v\}^3$,
3. There is a unique zero vector, {0}, such that {v} + {0} = {v} for all {v},
4. For each {v}, there is a unique vector -{v} such that $\{v\} + \{-\{v\}\} = \{0\}$,
5. The product of the scalar 1 and {v} is again {v}, or, 1{v} = {v},
6. $(c_1 c_2)\{v\} = c_1\{c_2\{v\}\}$,

7. $c\{\{v\}^1 + \{v\}^2\} = c\{v\}^1 + c\{v\}^2$, and
8. $(c_1 + c_2)\{v\} = c_1\{v\} + c_2\{v\}$.

In Rule 2, large brackets have been placed around $\{v\}^2 + \{v\}^3$ to emphasize the point that the result is, itself, a vector. The same notation has been used in Rules 4, 6 and 7.

The vector space is denoted by R^n where n indicates the number of components. Note that the set of vectors must be given. The number of given vectors may be smaller than, equal to, or larger than n.

The dimension of a vector space is the number of independent vectors given in the definition of the vector space. Note that this concept is totally different from that associated with the size or dimension of a vector. The vectors $\{v\}^1,..., \{v\}^m$ are linearly independent if

$$\sum_{i=1}^{m} \alpha_i \{v\}^i = \{0\} \tag{3.2-7}$$

implies that $\alpha_i = 0$ for i = 1,..., m. It is not a trivial matter to determine the dimension of a vector space so the issue will be addressed later.

The maximum dimension of R^n is n in which case the vector space is denoted by R^n_n. If the dimension of R^n is m, then the set of given vectors define a subspace, R^n_m, which implies that n is the number of components and m is the number of independent vectors, $m \leq n$, and we have what is called an m-dimensional subspace.

3.2.3 Basis for Vector Spaces

Consider a vector space R^n_m. Any set of m linearly independent vectors form a **basis** for that **vector space**. Suppose the set of vectors $\{v\}^i$, i = 1,..., m, represents such a basis. Then any vector {x} in that same vector space can be represented as the linear combination

$$\{x\} = \sum_{i=1}^{m} x_i^v \{v\}^i \tag{3.2-8}$$

By definition, x_i^v are the components of {x} with respect to the basis $\{v\}^i$.

Suppose another set of vectors $\{u\}^1,...,\{u\}^p$ are given to define a vector space of dimension m^* and denoted by $R^n_{m^*}$ with $m^* \leq m$. If each vector in this space is also in the vector space R^n_m, then $R^n_{m^*}$ is said to be a **vector subspace** of R^n_m. The given set of vectors is said to **span** the subspace. If each of $\{w\}^1,...,\{w\}^q$ can be expressed as some combination of the $\{u\}^i$'s, then $\{w\}^1,...,\{w\}^q$ span the same subspace. A subspace is often defined by the notation

$$S = \text{span}\left(\{u\}^1,\ldots,\{u\}^p\right) \tag{3.2-9}$$

The dimension of S, denoted by dim(S), is defined to be the number of independent vectors in the subspace.

Unless specified otherwise, the basis that is normally implied for R^n is the **coordinate basis**

$$\{I\}^i = \begin{Bmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{Bmatrix} \quad \text{i.e., the i' th component is one and all other components are zero} \tag{3.2-10}$$

for i = 1,..., n. Let I^i_j denote the j'th component of the i'th base vector. Then (3.2-10) implies that $I^i_j = \delta^i_j$, the Kronecker delta. The components of any vector, {x}, are merely the components with respect to the **coordinate basis**:

$$\{x\} = \begin{Bmatrix} x_1 \\ \vdots \\ x_n \end{Bmatrix} = x_1\{I\}^1 + \cdots + x_n\{I\}^n \tag{3.2-11}$$

Consider a set of vectors, $\{u\}^i$, i = 1,...,n. The following special properties often hold:

(i) The vectors are **normal** if $<u>^i\{u\}^i = 1$ for all i.
(ii) The vectors are **orthogonal** if $<u>^i\{u\}^j = 0$ for all i and j with $i \neq j$.
(iii) The vectors are **orthonormal** if $<u>^i\{u\}^j = \delta_{ij}$ for all i and j.

If the vectors, $\{u\}^i$, of a set are linearly independent and orthonormal, then these vectors form an orthonormal basis for the particular subspace spanned by the set of vectors. The coordinate basis is one example of an orthonormal basis.

An orthonormal basis is particularly convenient if it is necessary to obtain components with respect to that basis. If {x} is an arbitrary vector, $\{u\}^i$ is the basis, and x^u_i the i'th component of {x} with respect to this basis, then

$$\{x\} = x^u_1\{u\}^1 + \cdots + x^u_j\{u\}^j + \cdots + x^u_n\{u\}^n \tag{3.2-12}$$

Take an inner product of each term with $<u>^i$ and use the orthonormal relation. It follows that the i'th component is merely

$$x^u_i = <u>^i \{x\} \tag{3.2-13}$$

Note that this relation becomes much more complicated if the base vectors are not orthonormal.

Suppose a set of independent vectors, $\{g\}^i \in R^n$ is known. An alternative set of orthonormal vectors with the same span can be constructed by the **Gram-Schmidt** procedure as follows [Strang, 1988; Pg. 172]:

1. First set $\{u\}^1 = \dfrac{\{g\}^1}{|\{g\}^1|}$.

2. Remove the part of $\{g\}^2$ in the $\{u\}^1$ direction from $\{g\}^2$:

$$\{u\}^{*2} = \{g\}^2 - (< u >^1 \{g\}^2)\{u\}^1$$

   Normalize

$$\{u\}^2 = \frac{\{u\}^{*2}}{|\{u\}^{*2}|}$$

3. Remove the parts of $\{g\}^3$ in the $\{u\}^1$ and $\{u\}^2$ directions from $\{g\}^3$:

$$\{u\}^{*3} = \{g\}^3 - (< u >^1 \{g\}^3)\{u\}^1 - (< u >^2 \{g\}^3)\{u\}^2$$

   Normalize

$$\{u\}^3 = \frac{\{u\}^{*3}}{|\{u\}^{*3}|}$$

4. Continue in a similar fashion to obtain an orthonormal set.

If the vectors, $\{g\}^i$, are not independent, then the result will be a zero vector for one or more of the $\{u\}^i$'s. In fact, this is one procedure for determining the dimension of a vector space.

Example Problem:

Suppose a vector space is defined by the following set of vectors ε R^3:

$$\{g\}^1 = \begin{Bmatrix} 1 \\ 2 \\ 1 \end{Bmatrix}, \qquad \{g\}^2 = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}, \qquad \{g\}^3 = \begin{Bmatrix} 3 \\ 4 \\ 3 \end{Bmatrix}$$

Determine the dimension of the space and construct a set of orthonormal vectors that span the space.

Solution: Since $\{g\}^1$ is not a scalar times $\{g\}^2$, the space is of dimension at least two. Because $\{g\}^3 = \{g\}^1 + 2\{g\}^2$ the space is of dimension only 2 and the vectors define a two-dimensional subspace. The Gram-Schmidt procedure yields

$$\{u\}^1 = \frac{1}{\sqrt{6}}\begin{Bmatrix}1\\2\\1\end{Bmatrix}, \qquad \{u\}^2 = \frac{1}{\sqrt{3}}\begin{Bmatrix}1\\-1\\1\end{Bmatrix}, \qquad \{u\}^3 = \begin{Bmatrix}0\\0\\0\end{Bmatrix}$$

The first two vectors span the space. The details of verification are left as an exercise for the reader.

3.3 MATRICES

3.3.1 Notation

A **matrix** [A], of size m x n, is an ordered array of n column vectors, $\{A\}^i$, or of m row vectors $<A>^i$:

$$[A]_{m\,x\,n} = \begin{bmatrix}\{A\}^1 & \{A\}^2 & \cdots & \{A\}^n\end{bmatrix} = \begin{bmatrix}<A>^1\\ <A>^2\\ \vdots\\ <A>^m\end{bmatrix} \tag{3.3-1}$$

More conventionally, a matrix $[A]_{mxn}$ is also considered an ordered array of terms or components identified as A_{ij} in which i varies from 1 to m and denotes the row, and j varies from 1 to n and denotes the column:

$$[A]_{m\,x\,n} = \begin{bmatrix}A_{11} & A_{12} & \cdots & A_{1n}\\ A_{21} & A_{22} & \cdots & A_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ A_{m1} & A_{m2} & \cdots & A_{mn}\end{bmatrix} \tag{3.3-2}$$

The complete set of components occupies m rows and n columns. One alternative notation is **A**. Sometimes authors merely use A after stating that A is a matrix. If the size of the matrix is understood, we will use the notation [A] for a matrix, in analogy with the notation {v} for a column vector. Matrices and functions can also be considered as elements of vector spaces. R^{mxn} denotes the vector space of all real m x n matrices, and the dimension of the vector space is the number of independent matrices used to define the space. Sometimes the pair (m, n) that describe the numbers of rows, m, and columns, n, is called the dimension of the matrix. In this context, the concepts of dimension of the space and of dimension of the matrix must be carefully separated.

A special matrix is that of a column matrix, introduced previously as a column vector, but now with two notations of $[x]_{mx1}$, and $\{x\}$, having components x_i, i =1,..., m.

The **transpose** of [A], denoted by $[A]^T$ is another matrix whose rows (columns) are formed from the columns (rows) of [A], which implies that $[A]^T$ has n rows and m columns. The components of the two matrices are related by the equation $A^T_{ij} = A_{ji}$.

If the sizes of [A] and [B] are identical, then [A] = [B] if and only if $A_{ij} = B_{ij}$. Also, the addition of two matrices can be defined: [C] = [A] + [B] where $C_{ij} = A_{ij} + B_{ij}$ for all i and j. The multiplication of a matrix [A] by a scalar α is defined to be a new matrix [B] with components $B_{ij} = \alpha A_{ij}$.

3.3.2 Matrix Multiplication

Matrix multiplication is defined only if a particular restriction is met on one of the dimensions of each matrix, specifically [C] = [A][B] is defined only if the number of columns of [A] equals the number of rows of [B]. If $A \in R^{mxp}$ and $B \in R^{pxn}$, then $C \in R^{mxn}$. The components of [C] are given explicitly by

$$C_{ij} = \sum_{k=1}^{p} A_{ik} B_{kj}, \qquad i = 1,...,m \quad \text{and} \quad j = 1,...,n \tag{3.3-3}$$

There are several equivalent forms for expressing matrix multiplication. One way is to write the first matrix in terms of row vectors and the second matrix in terms of column vectors. The result is

$$[C] = [A][B] = \begin{bmatrix} <A>^1 \\ <A>^2 \\ \vdots \end{bmatrix} \begin{bmatrix} \{B\}^1 & \{B\}^2 & \cdots \end{bmatrix} \tag{3.3-4}$$

or

$$C_{ij} = <A>^i \{B\}^j \tag{3.3-5}$$

which is just (3.3-3). If the alternative method for writing [A] and [B] is used, the result is

$$\begin{aligned} [A][B] &= \begin{bmatrix} \{A\}^1 & \{A\}^2 & \cdots \end{bmatrix} \begin{bmatrix} <B>^1 \\ <B>^2 \\ \vdots \end{bmatrix} \\ &= \{A\}^1 <B>^1 + \{A\}^2 <B>^2 + \cdots + \{A\}^n <B>^n \end{aligned} \tag{3.3-6}$$

Yet another form is

$$[A][B] = \left[\{[A]\{B\}^1\} \quad \{[A]\{B\}^2\} \quad \{[A]\{B\}^3\} \quad \cdots \quad \{[A]\{B\}^n\} \right] \tag{3.3-7}$$

which shows the intimate relationship between matrix and vector theory. Matrix multiplication satisfies the following relations:

$$[\,[A] + [B]\,][C] = [A][C] + [B][C] \qquad \text{Distributive Law} \tag{3.3-8}$$

$$[\,[A][B]\,][C] = [A][\,[B][C]\,] \qquad \text{Associative Law} \tag{3.3-9}$$

In general, matrices do not commute when multiplied, i.e.,

$$[A][B] \neq [B][A] \tag{3.3-10}$$

A special matrix equation is the case when [A] and {b} are known and an unknown vector {x} is to be determined from the following linear algebraic equation:

$$[A]\{x\} = \{b\} \tag{3.3-11}$$

An alternative form for (3.3-11) is

$$x_1\{A\}^1 + x_2\{A\}^2 + \cdots + x_n\{A\}^n = \{b\} \tag{3.3-12}$$

i.e., {b} is just a linear combination of the basis formed from the columns of [A]. We will return later to discuss techniques for solving (3.3-11).

3.3.3 Derivative of a Matrix

If the components of a matrix depend on a scalar, then the **derivative of the matrix** is defined to be the matrix of component derivatives:

$$\frac{d}{d\alpha}[A] = \left[\frac{dA_{ij}}{d\alpha} \right] \tag{3.3-13}$$

3.3.4 Transpose of the Product of Matrices

The transpose of the product of two matrices is the product of the transposed matrices in reverse order:

$$[[A][B]]^T = [B]^T[A]^T \tag{3.3-14}$$

To show that this relation holds, let [C] = [A][B] and [D] = $[B]^T[A]^T$. With the use of indicial notation, (3.3-14) is shown as follows:

$$\left.\begin{aligned} C_{ij} &= \sum_k A_{ik}B_{kj} \\ C^T_{ij} = C_{ji} &= \sum_k B_{ki}A_{jk} \\ D_{ij} = \sum_k B^T_{ik}A^T_{kj} &= \sum_k B_{ki}A_{jk} = C^T_{ij} \end{aligned}\right\} \tag{3.3-15}$$

3.3.5 Partitioned Matrices

Frequently, it is useful to partition vectors and matrices into vectors and matrices of reduced dimensions. An example is the situation when a set of constraints are to be applied and the variables, {x}, are separated into a subset of independent, $\{x\}_q$, and a subset of dependent variables, $\{x\}_{n-q}$. To illustrate the procedure, consider the set of algebraic equations [A]{x} ={b} or

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{Bmatrix} \tag{3.3-16}$$

in which the matrices are separated as follows:

$$\begin{bmatrix} \begin{bmatrix} A_{11} & \cdots & \cdots & A_{1q} \\ \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ A_{s1} & \cdots & \cdots & A_{sq} \end{bmatrix} & \begin{bmatrix} A_{1,q+1} & \cdots & \cdots & A_{1n} \\ \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ A_{s,q+1} & \cdots & \cdots & A_{sn} \end{bmatrix} \\ \begin{bmatrix} A_{s+1,1} & \cdots & \cdots & A_{s+1,q} \\ \vdots & \vdots & \cdots & \vdots \\ A_{m1} & \cdots & \cdots & A_{mq} \end{bmatrix} & \begin{bmatrix} A_{s+1,q+1} & \cdots & \cdots & A_{s+1,n} \\ \vdots & \vdots & \vdots & \vdots \\ A_{m,q+1} & \cdots & \cdots & A_{mn} \end{bmatrix} \end{bmatrix} \begin{Bmatrix} \begin{Bmatrix} x_1 \\ \vdots \\ \vdots \\ x_q \end{Bmatrix} \\ \begin{Bmatrix} x_{q+1} \\ \vdots \\ \vdots \\ x_n \end{Bmatrix} \end{Bmatrix} = \begin{Bmatrix} \begin{Bmatrix} b_1 \\ \vdots \\ \vdots \\ b_s \end{Bmatrix} \\ \begin{Bmatrix} b_{s+1} \\ \vdots \\ b_m \end{Bmatrix} \end{Bmatrix}$$

or

$$\begin{bmatrix} [A]_{11} & [A]_{12} \\ [A]_{21} & [A]_{22} \end{bmatrix} \begin{Bmatrix} \{x\}_1 \\ \{x\}_2 \end{Bmatrix} = \begin{Bmatrix} \{b\}_1 \\ \{b\}_2 \end{Bmatrix} \tag{3.3-17}$$

which can be expanded into two sets of algebraic equations

$$\begin{aligned} [A]_{11}\{x\}_1 + [A]_{12}\{x\}_2 &= \{b\}_1 \\ [A]_{21}\{x\}_1 + [A]_{22}\{x\}_2 &= \{b\}_2 \end{aligned} \tag{3.3-18}$$

Note that $[A]_{11}$, as an example, is a matrix, not the component A_{11}. We see that the structure of the notation yields the convenient result that rules for multiplication using submatrices are identical to those for multiplication using components in conventional matrix notation. The sizes of the submatrices, which satisfy the restrictions necessary for matrix multiplication, are:

$$\begin{array}{ll} [A]_{11} \in R^{s\,x\,q}\,, & [A]_{12} \in R^{s\,x\,(n-q)} \\ [A]_{21} \in R^{(m-s)x\,q}\,, & [A]_{12} \in R^{(m-s)\,x(n-q)} \\ \{x\}_1 \in R^{q}\,, & \{x\}_2 \in R^{n-q} \\ \{b\}_1 \in R^{s}\,, & \{b\}_2 \in R^{m-s} \end{array} \tag{3.3-19}$$

3.3.6 Outer Product of Vectors

Suppose $\{u\} \in R^m$ and $\{v\} \in R^n$. Then the **outer product** of these vectors is the matrix $[A] \in R^{m\,x\,n}$:

$$[A] = \{u\}\langle v\rangle = \begin{bmatrix} u_1v_1 & u_1v_2 & \cdots & u_1v_n \\ u_2v_1 & u_2v_2 & \cdots & u_2v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_mv_1 & u_mv_2 & \cdots & u_mv_n \end{bmatrix} \tag{3.3-20}$$

3.3.7 Special Matrices

Matrices with a special structure occur often in practice and are identified with particular adjectives. Suppose $[A] \in R^{m\,x\,n}$. Then [A] is said to be

Diagonal	if	$A_{ij} = 0$	whenever	$i \neq j$
Tridiagonal	if	$A_{ij} = 0$	whenever	$\lvert i - j \rvert > 1$
Upper Bidiagonal	if	$A_{ij} = 0$	whenever	$i > j$ or $j > i + 1$
Upper Triangular	if	$A_{ij} = 0$	whenever	$i > j$
Strictly Upper Triangular	if	$A_{ij} = 0$	whenever	$i \geq j$
Upper Hessenberg	if	$A_{ij} = 0$	whenever	$i > j + 1$

Analogous definitions hold with upper replaced by lower; just replace [A] with $[A]^T$ in the definitions given above. [A] has **lower bandwidth** w_l and **upper bandwidth** w_u if $A_{ij} = 0$ whenever $i > j + w_l$ and $j > i + w_u$. If $w_l = w_u = w$, then [A] has **bandwidth** w. A matrix is **sparse** if it has relatively few nonzero entries.

3.3.8 Applications of Vector Spaces to Matrices

There are four subspaces associated with $[A] \in R^{m \times n}$:

(i) The **range** of [A] is the vector space defined by the columns of [A] and denoted by R[A]. The range of [A] is also called the column space of [A].

(ii) The **null space** of [A], denoted by N[A], is a vector space which contains all vectors {x} such that $[A]\{x\} = \{0\}$. The null space is also called the **kernel** of [A].

(iii) The **row space** of [A] is the space defined by the row vectors of [A] and is the same as the column space of $[A]^T$.

(iv) The **left null space** of [A], which is the same as the null space of $[A]^T$, consists of all vectors {y} such that $\langle y\rangle[A] = \langle 0\rangle$ or $[A]^T\{y\} = \{0\}$.

Let the dimension of the column space (range) be r. It follows that (the proof is omitted for the sake of brevity) the dimension of the row space is also r, i.e., r equals the number of independent column vectors which is also the number of independent row vectors and is called the **rank** of the matrix. An alternative notation is to say that the **rank** of the matrix is defined by

$$r = \text{rank}\left([A]\right) = \dim R\left([A]\right) = \text{rank}\left([A]^T\right)$$

If there are n columns, then $r \le n$.

In summary, the range of [A] is the vector space formed from the columns of [A]. The rank of [A] equals the dimension of the range of [A], which, in turn, equals the number of independent columns of [A], which also equals the number of independent rows of [A].

The nullspace of [A] has dimension n - r. Similarly, the left nullspace has dimension m - r.

Example Problem:

Consider the matrix [A] given as follows:

$$[A] = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 4 & 1 \end{bmatrix}$$

For this matrix, determine the range, the null space, the row space, the left null space and the rank.

Solution: The vectors formed from the columns are the following:

$$\{A\}^1 = \begin{Bmatrix} 1 \\ 2 \\ 4 \end{Bmatrix}, \qquad \{A\}^2 = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}$$

As can be easily verified, the column vectors are linearly independent. Therefore, $n = 2$ and the rank of [A] is $r = 2$. These vectors form the range or column space of [A]. Because the columns are independent vectors, there is no vector, {x} such that [A]{x} = {0} so the null space of [A] is empty ($n - r = 0$). The vectors formed from the rows are the following:

$$\langle A\rangle^1 = \langle 1 \quad 1\rangle, \qquad \langle A\rangle^2 = \langle 2 \quad 1\rangle, \qquad \langle A\rangle^3 = \langle 4 \quad 1\rangle$$

$\langle A\rangle^1$ and $\langle A\rangle^2$ are linearly independent but $\langle A\rangle^3 = 3\langle A\rangle^2 - 2\langle A\rangle^1$. Therefore, there are two independent vectors and we determine, again, that the rank is two. The row space of [A] is the vector space formed from any two of the three vectors.

Since $\langle A\rangle^3 = 3\langle A\rangle^2 - 2\langle A\rangle^1$, let $\langle x\rangle = \langle 2, -3, 1\rangle$. By direct substitution, it is seen that $\langle x\rangle[A] = \langle 0\rangle$. No other independent vector satisfies this relation so $\langle x\rangle$ forms the left null space which is a vector space of dimension $m - r = 3 - 2 = 1$.

3.4 SQUARE MATRICES

3.4.1 Notation

The matrix [A] is **square** if $m = n$, i.e., $[A] \in R^{n\times n}$. In this special (and common) case properties identified solely with square matices can be defined. For example, [A] is **symmetric** if $[A] = [A]^T$ or $A_{ij} = A_{ji}$. [A] is **skew-symmetric** if $[A] = -[A]^T$ or $A_{ij} = -A_{ji}$. It follows that the diagonal terms of a skew-symmetric matrix are zero. Any matrix can be decomposed into its symmetric and skew-symmetric parts:

$$[A] = \tfrac{1}{2}\left[[A] + [A]^T\right] + \tfrac{1}{2}\left[[A] - [A]^T\right] \qquad (3.4\text{-}1)$$

If [A] is symmetric, then so is $[B]^T[A][B]$. This is shown by recalling the rule for taking the transpose of a product of matrices and using $[A] = [A]^T$ as follows:

$$\left[[B]^T[A][B]\right]^T = [B]^T[A]^T[B] = [B]^T[A][B] \qquad (3.4\text{-}2)$$

The **trace** of a square matrix is defined to be the sum of the diagonal components:

$$\mathrm{tr}\,[A] = \sum_{i=1}^{n} A_{ii} \qquad (3.4\text{-}3)$$

3.4.2 The Identity Matrix

The **identity matrix** [I] is defined such that

$$[I]\{x\} = \{x\} \qquad \text{for any } \{x\} \qquad (3.4\text{-}4)$$

It follows that

$$[I] = \left[\{I\}^1 \quad \{I\}^2 \quad \cdots \quad \{I\}^n\right] \qquad (3.4\text{-}5)$$

in which $\{I\}^i$ denotes the i'th coordinate basis. The components of [I] are given by $I_{ij} = \delta_{ij}$. Matrix multiplication with the identity matrix yields

$$[A][I] = [A] \qquad [I][A] = [A] \qquad (3.4\text{-}6)$$

The **left and right inverses** of [A], denoted by $[A_L]^{-1}$ and $[A_R]^{-1}$, respectively, are defined such that

$$[A_L]^{-1}\,[A] = [I] \qquad [A][A_R]^{-1} = [I] \qquad (3.4\text{-}7)$$

A matrix without an inverse is said to be **singular**.

Theorem: If $[A_L]^{-1}$ exists, then

$$[A_R]^{-1} = [A_L]^{-1} = [A]^{-1} \qquad (3.4\text{-}8)$$

The matrix, $[A]^{-1}$, is called the **inverse** to [A], i.e., $[A]^{-1}[A] = [A][A]^{-1} = [I]$.

Proof: Suppose the left and right inverses exist. Then (3.4-6) implies

$$[A_L]^{-1} = [A_L]^{-1}\,[I]$$

Now apply (3.4-7) to the right side obtain

$$[A_L]^{-1}\,[I] = [A_L]^{-1}\,\big[[A][A_R]^{-1}\big]$$

Rearrange the order of multiplication to get the equation

$$[A_L]^{-1}\,\big[[A][A_R]^{-1}\big] = \big[[A_L]^{-1}\,[A]\big][A_R]^{-1}$$

Use (3.4-7) again to finally obtain

$$[[A_L]^{-1} [A]][A_R]^{-1} = [I][A_R]^{-1} = [A_R]^{-1}$$

and (3.4-8) is derived. **QED**

Theorem: The inverse of the product of two matrices is the product in reverse order of the inverses of the matrices:

$$[[A][B]]^{-1} = [B]^{-1}[A]^{-1} \tag{3.4-9}$$

Proof: Let $[C] = [[A][B]]^{-1}$. Then from the definition of an inverse, we have

$$[C][A][B] = [I]$$

Multiply on the right by the inverse of [B] to obtain

$$[C][A] = [I][B]^{-1} = [B]^{-1}$$

Now multiply on the right by the inverse of [A] with the following result:

$$[C] = [B]^{-1}[A]^{-1}$$ **QED**

3.4.3 Orthogonal Matrices

A square matrix [Q] is **orthogonal** if

$$[Q]^T[Q] = [Q][Q]^T = [I] \tag{3.4-10}$$

Therefore, a matrix is orthogonal if its inverse equals its transpose, i.e.,

$$[Q]^{-1} = [Q]^T \tag{3.4-11}$$

Theorem: The columns of orthogonal matrices must be orthonormal.
Proof: Set the product of a matrix and its transpose equal to the identity matrix as follows:

$$[I] = [Q]^T[Q] = \begin{bmatrix} <Q>^1 \\ <Q>^2 \\ \cdots \\ <Q>^n \end{bmatrix} \begin{bmatrix} \{Q\}^1 & \{Q\}^2 & \cdots & \{Q\}^n \end{bmatrix}$$

Based on (3.3-5) for matrix multiplication, the component form of this equation is

$$\delta_{ij} = <Q>^i \{Q\}^j$$

This equation is just the relationship satisfied by orthonormal vectors. **QED**

Examples of orthogonal matrices are given as follows:

Example 1. **Identity Matrix**. The identity matrix satisfies trivially the definition of an orthogonal matrix.

Example 2. **Rotation Matrices**. A set of rotation matrices $[Q]_{ij}$ are defined to have the components

$$Q_{ii} = \cos\theta \qquad Q_{ij} = -\sin\theta$$
$$Q_{ji} = \sin\theta \qquad Q_{jj} = \cos\theta$$

The other diagonal components are unity; other off-diagonal components are zero. As one example, suppose n = 4, i = 2 and j = 4. The resulting orthogonal matrix is the following:

$$[Q]_{24} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & 0 & -\sin\theta \\ 0 & 0 & 1 & 0 \\ 0 & \sin\theta & 0 & \cos\theta \end{bmatrix}$$

It is left as an exercise to verify that this is an orthogonal matrix.

Example 3. **Reflection Matrices**. A reflection matrix is of the form

$$[Q] = [I] - \alpha\{v\}\{v\}^T, \qquad \alpha = \frac{2}{<v>\{v\}}$$

where {v} is any vector. To verify that [Q] is orthogonal, take the product of [Q] and its transpose, and show that the identity is obtained. The first step is to note that $[\{v\}\{v\}^T]^T = \{v\}\{v\}^T$. Then

$$
\begin{aligned}
[Q][Q]^T &= [[I] - \alpha\{v\}\{v\}^T][[I] - \alpha\{v\}\{v\}^T] \\
&= [I] - 2\alpha\{v\}\{v\}^T + \alpha^2\{v\}(\{v\}^T\{v\})\{v\}^T
\end{aligned}
$$

In the last term, we note that we can identify the product contained within the brackets as simply the scalar $(\{v\}^T\{v\}) = 2/\alpha$. The same kind of observation is used later in connection with the Sherman-Morrison Formula. When this result is used, we obtain $[Q][Q]^T = [I]$.

[Q] is called a reflection matrix because [Q]{w} can be interpreted as the reflection of the vector{w} with respect to the plane whose normal is {v}. To show this let

$$
\{w\} = \gamma\{v\} + \{u\} \qquad \text{where} \qquad <v>\{u\} = 0
$$

i.e., {w} is decomposed into a vector parallel to {v} and a vector {u} perpendicular to {v}. Then,

$$
\begin{aligned}
[Q]\{w\} &= \gamma[Q]\{v\} + [Q]\{u\} \\
&= \gamma[[I] - \alpha\{v\}<v>]\{v\} + [Q]\{u\} \\
&= \gamma\{v\} - \gamma\alpha\{v\}(<v>\{v\}) + \{u\} - \alpha\{v\}(<v>\{u\})
\end{aligned}
$$

However, two of the terms are the following:

$$
<v>\{v\} = \frac{2}{\alpha}\ , \qquad <v>\{u\} = 0
$$

The result is

$$
[Q]\{w\} = \{u\} - \gamma\{v\}
$$

for which a geometric interpretation is given in Fig. 3.4-1.

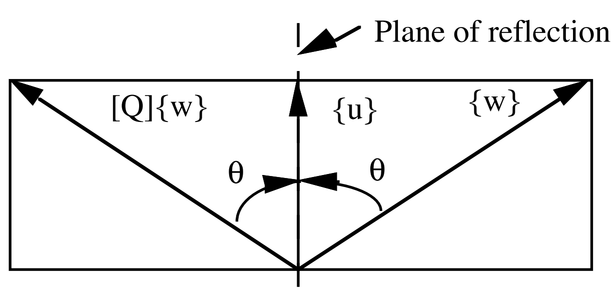

Fig. 3.4-1. A geometrical interpretation of reflection matrices.

3.4.4 Positive Definite Matrices

A matrix [A] is **positive definite** if

$$\{x\}^T[A]\{x\} > 0 \qquad \text{for all } \{x\} \neq \{0\} \tag{3.4-12}$$

Theorem: If a matrix [A] is positive definite, then $A_{ii} > 0$ for every i.
Proof: Choose $\{x\} = \{I\}^i$. Then $\{I\}^{iT}[A]\{I\}^i = A_{ii} > 0$. **QED**

Theorem: If [A] is symmetric and positive definite, then

$$\left|A_{ij}\right| \leq \frac{1}{2}(A_{ii} + A_{jj}) \qquad \text{for} \quad i \neq j \tag{3.4-13}$$

and

$$\left|A_{ij}\right| \leq \sqrt{A_{ii}A_{jj}} \tag{3.4-14}$$

Proof: See the text by Golub and Van Loan (1983), page 90.

This theorem implies that the largest component in a positive definite, symmetric matrix must appear on the diagonal.

3.4.5 Congruence and Similarity

The matrices [A] and $[A^c]$ are said to be **congruent** if they are related through a nonsingular matrix [S] such that

$$[A^c] = [S][A][S]^T \tag{3.4-15}$$

[S] is called the congruent transformation. Note that properties of symmetry, skew-symmetry and positive definiteness are preserved under congruent transformations. The matrices [A] and $[A^s]$ are said to be **similar** if they are related through a nonsingular matrix [S] such that

$$[A^s] = [S][A][S]^{-1} \tag{3.4-16}$$

The matrix [S] is called the **similarity transformation**. If [S] is orthogonal, then $[S]^T = [S]^{-1}$ and congruent and similarity transformations are identical.

3.4.6 Elementary Matrices

Elementary matrices, [E], are matrices which, when used to multiply with [A], cause rows or columns in [A] to be scaled, cause rows or columns in [A] to be interchanged, or cause linear combinations of rows or columns in [A] to be combined. In general, premultiplying by an elementary matrix [E] affects rows, postmultiplication by [E] affects columns.

<u>Scaling</u>

Suppose each component of row k in [A] is to be scaled by a factor s. To accomplish this, define an elementary matrix as follows:

$$[E] = \left[\{I\}^1 \quad \{I\}^2 \quad \cdots \quad s\{I\}^k \quad \cdots \quad \{I\}^n \right]$$

i.e., start with the identity matrix and set $E_{kk} = s$. The operation [E][A] scales the k'th row of [A] by s; the operation [A][E] scales the k'th column of [A] by s.

<u>Interchanging Rows or Columns</u>

Consider an elementary matrix formed by interchanging the k'th and l'th rows of the identity matrix, i.e., set $E_{kk} = 0$, $E_{ll} = 0$, $E_{kl} = 1$, $E_{lk} = 1$ with all other components unchanged. Then the operation [E][A] interchanges the k'th and l'th rows of [A]; conversely, [A][E] interchanges the k'th and l'th columns of [A].

<u>Linear Combinations of Rows or Columns</u>

Suppose s times the l'th row is to be added to the k'th row of [A]. Define an elementary matrix that begins as the identity matrix but with $E_{kl} = s$. Then the task is accomplished by the operation [E] [A]. The operation [A][E] causes s times the l'th column to be added to the k'th column. For example, if n = 3 and if

$$[E] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 4 & 1 \end{bmatrix}$$

then the operation [E][A] will result in a matrix where 4 times the second row of [A] is added to the third row.

Several elementary operations can be combined into one elementary matrix, e.g.,

$$[E]^1[E]^2[E]^3[A] = [E][A] \qquad \text{where} \qquad [E] = [E]^1[E]^2[E]^3$$

where it is understood that $[E]^3$ is conducted first, then $[E]^2$ and, finally, $[E]^1$.

<u>Example Problem</u>:

Suppose [A] is the following symmetric matrix:

$$[A]=\begin{bmatrix}1&2&3&4\\2&5&6&7\\3&6&8&9\\4&7&9&10\end{bmatrix}$$

Construct an operation that interchanges the first and third rows and the first and third columns of [A].

Solution: Construct [E] to interchange the first and third rows. Then [E] and [E][A] are

$$[E]=\begin{bmatrix}0&0&1&0\\0&1&0&0\\1&0&0&0\\0&0&0&1\end{bmatrix} \qquad [E][A]=\begin{bmatrix}3&6&8&9\\2&5&6&7\\1&2&3&4\\4&7&9&10\end{bmatrix}$$

Note that [E][A] is not symmetric. Now, postmultiply by [E] to interchange the first and third columns, the result is the symmetric matrix:

$$[E][A][E]=\begin{bmatrix}8&6&3&9\\6&5&2&7\\3&2&1&4\\9&7&4&10\end{bmatrix}$$

which is the desired objective.

3.4.7 Determinants

Determinants are of practically no use for computational purposes; however, their study is of significant theoretical benefit and provides a unifying insight to linear algebra. The **determinant** of [A], denoted as det [A] or $|[A]|$, is a single number associated with a square matrix. Examples for small matrices are:

$$\begin{aligned}&\det[A_{11}]=A_{11}\\&\det\begin{bmatrix}A_{11}&A_{12}\\A_{21}&A_{22}\end{bmatrix}=A_{11}A_{22}-A_{12}A_{21}\\&\det\begin{bmatrix}A_{11}&A_{12}&A_{13}\\A_{21}&A_{22}&A_{23}\\A_{31}&A_{32}&A_{33}\end{bmatrix}=\begin{matrix}A_{11}A_{22}A_{33}+A_{12}A_{23}A_{31}+A_{13}A_{21}A_{32}\\-A_{13}A_{22}A_{31}-A_{23}A_{32}A_{11}-A_{12}A_{21}A_{33}\end{matrix}\end{aligned} \tag{3.4-17}$$

The determinant of a matrix obtained by deleting the i'th row and j'th column of [A] is called a **minor** M_{ij} of [A]. The number

$$M^c_{ij} = (-1)^{i+j} M_{ij} \tag{3.4-18}$$

is called a **cofactor** of [A]. The general definition of the determinant is defined inductively. Define the determinant of a one-by-one matrix to be the component, itself: det $[A_{11}] = A_{11}$. Then the determinant of [A] can be obtained by either a row sum or a column sum as follows:

$$\det[A] = \sum_{j=1}^{n} A_{pj} M^c_{pj} = \sum_{i=1}^{n} A_{iq} M^c_{iq} \qquad \text{for any p or q} \tag{3.4-19}$$

<u>Example</u>:

$$[A] = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \qquad [M]^c = \begin{bmatrix} A_{22} & -A_{21} \\ -A_{12} & A_{11} \end{bmatrix}$$

$$\sum_{j=1}^{2} A_{1j} M^c_{1j} = A_{11}A_{22} + A_{12}(-A_{21})$$

With the formula established for a two-by-two matrix, the determinant of a three-by-three matrix can be obtained by using (3.4-19). Then determinants of matrices with n = 4, 5, ... can be obtained similarly up to the size desired.

Some properties of determinants are summarized as follows [Strang, 1988]:

(i)

$$\det[A]^T = \det[A] \tag{3.4-20}$$

The reason is that a row expansion of $[A]^T$ is identical to a column expansion of [A].

(ii)

$$\det[cA] = c^n \det[A] \tag{3.4-21}$$

(iii) If the entries of any row or column are zero, then det [A] = 0.

(iv) If any row (column) is a linear combination of the other rows (columns), i.e., if the dimension of the vector space defined by the rows (columns) is less then n, then det [A] = 0.

(v) If two rows or columns are interchanged, then the determinant changes sign.

(vi) The value of a determinant is unchanged if a multiple of one row (column) is added to another row (column).

(vii) The determinant of a product of two matrices is the product of the determinants:

$$\det\left[[A][B]\right] = \det [A] \det [B] \tag{3.4-22}$$

(viii) The determinant of a diagonal matrix is just the product of the diagonal components.
(ix) The determinant of a triangular matrix, either upper or lower, is the product of the diagonal terms.

Item (ix) is particularly important in the context of solutions to algebraic equations. To verify the property, consider an upper triangular matrix:

$$[U] = \begin{bmatrix} U_{11} & U_{12} & U_{13} & \cdots & U_{1n} \\ 0 & U_{22} & U_{23} & \cdots & U_{2n} \\ 0 & 0 & U_{33} & \cdots & U_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & U_{nn} \end{bmatrix} \tag{3.4-23}$$

Let M^c_{ij} denote the cofactors. Perform a row expansion based on the last row:

$$\det [U] = U_{nn}(-1)^{n+n} M_{nn} \tag{3.4-24}$$

where

$$M_{nn} = \det \begin{bmatrix} U_{11} & U_{12} & \cdots & U_{1,n-1} \\ 0 & U_{22} & \cdots & U_{2,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & U_{n-1,n-1} \end{bmatrix} \tag{3.4-25}$$
$$= U_{n-1,n-1}(-1)^{(n+1)+(n+1)} M_{n-2,n-1}$$

Proceed until the last term is obtained:

$$\det [U] = U_{nn}(-1)^{n+n} U_{n-1,n-1}(-1)^{(n+1)+(n+1)} \cdots U_{22}(-1)^{1+1} U_{11} \tag{3.4-26}$$

The exponents are all even. Therefore

$$\det [U] = \prod_{i=1}^{n} U_{ii} \tag{3.4-27}$$

A similar development holds for a lower triangular matrix. A diagonal matrix is just a special case of a lower or upper triangular matrix.

A Formula for the Inverse of [A]

Recall that

$$\det[A] = \sum_{j=1}^{n} A_{pj} M^{c}_{pj} = \sum_{i=1}^{n} A_{iq} M^{c}_{iq} \qquad \text{for any } p \text{ or } q \tag{3.4-28}$$

Theorem: The sums of particular products of components of the matrix [A] and cofactors are zero:

$$\left.\begin{aligned} \sum_{j=1}^{n} A_{pj} M^{c}_{qj} &= 0 \qquad p \neq q \\ \sum_{i=1}^{n} A_{iq} M^{c}_{ip} &= 0 \qquad p \neq q \end{aligned}\right\} \tag{3.4-29}$$

Proof: See Strang [1988].

The two sets of Equations (3.4-28) and (3.4-29) can be written together as

$$\sum_{j=1}^{n} A_{pj} M^{c}_{qj} = \delta_{pq} \det[A] \qquad \text{and} \qquad \sum_{i=1}^{n} A_{iq} M^{c}_{ip} = \delta_{pq} \det[A] \tag{3.4-30}$$

or

$$\sum_{j=1}^{n} A_{pj} M^{cT}_{jq} = \delta_{pq} \det[A] \qquad \text{and} \qquad \sum_{i=1}^{n} M^{cT}_{pi} A_{iq} = \delta_{pq} \det[A] \tag{3.4-31}$$

Equation (3.4-31) suggests the formation of certain matrices. Define the cofactor matrix $[M]^c$ to be the matrix with components $M^c{}_{ij}$ and the **adjoint matrix** $[M]^a$ to be the transpose of the cofactor matrix:

$$[M]^a = [M]^{cT} \tag{3.4-32}$$

In matrix notation, (3.4-31) becomes

$$[A][M]^a = [I] \det[A] \qquad \text{and} \qquad [M]^a[A] = [I] \det[A] \tag{3.4-33}$$

or

$$[A]^{-1} = \frac{1}{\det[A]} [M]^a \tag{3.4-34}$$

The inverse of [A] is proportional to the adjoint matrix and exists only if $\det[A] \neq 0$.

Derivative of the Determinant

Suppose we wish to know how sensitive det[A] is to one of the components of [A], which is labelled A_{pq}. A measure of sensitivity, s, is the derivative

$$s = \frac{\partial \det[A]}{\partial A_{pq}} \tag{3.4-35}$$

To obtain an expression for the derivative, consider a row expansion for det[A] using row p:

$$\det[A] = \sum_{j=1}^{n} A_{pj} M^c_{pj} \tag{3.4-36}$$

But M^c_{pj} contains no terms that involve A_{pq} because M^c_{pj} is obtained by deleting row p and column q from [A]. Therefore

$$\frac{\partial \det[A]}{\partial A_{pq}} = \sum_{j=1}^{n} \frac{\partial A_{pj}}{\partial A_{pq}} M^c_{pj} \tag{3.4-37}$$

But

$$\frac{\partial A_{pj}}{\partial A_{pq}} = \delta_{qj} \tag{3.4-38}$$

i.e., the derivative is zero unless the same component (independent variable) appears in both the numerator and denominator in which case the answer is one. The result is that the sensitivity factor for the determinant with respect to the component A_{pq} is just the corresponding component of the cofactor matrix:

$$\frac{\partial \det[A]}{\partial A_{pq}} = M^c_{pq} \tag{3.4-39}$$

Examples of Determinants:

For some of the more common matrices, the determinants are known. Examples are the following:

(i) det [I] = 1.

(ii) Recall that for an orthogonal matrix, $[Q]^T[Q] = [I]$. The determinant of a product of matrices is the product of the determinants, and the determinant of the transpose equals the determinant of the matrix. Therefore det $[Q] = \pm 1$.

(iii) Let [E] be the elementary matrix for interchanging the first and second rows or columns, i.e., [E] = [I] except that the first and second rows are interchanged. Then det [E] = -1.

3.5 GAUSSIAN ELIMINATION

3.5.1 The Algebraic Problem

A problem of considerable interest is one of solving for the column vector {x} that satisfies the following equation:

$$[A]\{x\} = \{b\} \tag{3.5-1}$$

One direct approach is to obtain the inverse using the adjoint matrix

$$[A]^{-1} = \frac{1}{\det[A]}[M]^a \tag{3.5-2}$$

If the terms in (3.5-1) are multiplied on the left by $[A]^{-1}$, the solution is

$$\{x\} = [A]^{-1}\{b\} \tag{3.5-3}$$

Although the result is theoretically correct, this approach is computationally inefficient and is rarely used. Of more general use is **Gaussian elimination**, which is a general term that describes a number of schemes for solving the linear algebraic problem of (3.5-1) through the successive elimination of variables. The procedures are also said to be direct. This section describes several of the most commonly used **direct procedures**.

3.5.2 Cramer's Rule

Another application of the use of determinants is **Cramer's rule** for obtaining the solution to a set of algebraic equations. The solution to (3.5-1) for the i'th component of {x} is

$$x_i = \frac{\det\left[\{A\}^1 \;\cdots\; \{A\}^{i-1} \;\; \{b\} \;\; \{A\}^{i+1} \;\cdots\; \{A\}^n\right]}{\det[A]} \tag{3.5-4}$$

in which the numerator is the determinant of a matrix obtained by replacing the i'th column of [A] with {b}. Again, it is seen that no solution exists if det [A] is zero, i.e., if [A] is singular.

3.5.3 LU Decomposition

A solution to the matrix equation (3.5-1) is desired. For the moment, suppose that [A] is the product of a lower triangular matrix [L] and an upper triangular matrix [U] in which [U] has 1's on the diagonal (Crout decomposition). An alternative approach is to assign 1's on the diagonal of [L] (Doolittle's decomposition). Suppose the Crout decomposition is available:

$$[A] = [L][U]$$

$$[L] = \begin{bmatrix} L_{11} & 0 & 0 & \cdots \\ L_{21} & L_{22} & 0 & \cdots \\ L_{31} & L_{32} & L_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \qquad [U] = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots \\ \cdots & 1 & U_{n-2,n-1} & U_{n-2,n} \\ \cdots & 0 & 1 & U_{n-1,n} \\ \cdots & 0 & 0 & 1 \end{bmatrix} \tag{3.5-5}$$

Let

$$\{y\} = [U]\{x\} \qquad \text{and} \qquad [L]\{y\} = \{b\} \tag{3.5-6}$$

With [L] known, the second equation becomes

$$\begin{aligned} L_{11}y_1 &= b_1 \\ L_{21}y_1 + L_{22}y_2 &= b_2 \\ L_{31}y_1 + L_{32}y_2 + L_{33}y_3 &= b_3 \ , \end{aligned} \tag{3.5-7}$$

etc.

The first equation is used to determine y_1, the second for y_2, and so on. Next, with {y} considered known, the first of (3.5-6), in reverse order, becomes

$$\begin{aligned} x_n &= y_n \\ x_{n-1} + U_{n-1,n}x_n &= y_{n-1} \\ x_{n-2} + U_{n-2,n-1}x_{n-1} + U_{n-2,n}x_n &= y_{n-2} \ , \end{aligned} \tag{3.5-8}$$

etc.

Therefore, if [L] and [U] are known, a vector {y} is obtained first with a **forward substitution** and then the solution {x} is obtained with a **back substitution**. These are particularly simple and efficient operations, especially if multiple solutions are to be obtained for several vectors, {b}. The decomposition of [A] into the lower and upper forms need only be performed once in one subroutine; the forward and back substitutions are accomplished with a separate subroutine which is called for each distinct force vector.

The algorithm for obtaining the decomposition is based on the structure displayed by taking the product of [L] and [U]:

$$\begin{bmatrix} L_{11} & 0 & 0 & \cdots \\ L_{21} & L_{22} & 0 & \cdots \\ L_{31} & L_{32} & L_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 1 & U_{12} & U_{13} & \cdots \\ 0 & 1 & U_{23} & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{3.5-9}$$

The result of multiplying the first row of [L] by the columns of [U] is

$$L_{11} = A_{11}$$

Solve f

$$
\begin{aligned}
L_{11}U_{12} &= A_{12} && \text{Solve f} \\
L_{11}U_{13} &= A_{13} && \text{Solve f} \\
&\vdots && \vdots \\
L_{11}U_{1n} &= A_{1n} && \text{Solve f}
\end{aligned}
$$

Similarly, the result of multiplying the second row of [L] by the columns of [U] is

$$
\begin{aligned}
L_{21} &= A_{21} && \text{Solve f} \\
L_{21}U_{12} + L_{22} &= A_{22} && \text{Solve f} \\
L_{21}U_{13} + L_{22}U_{23} &= A_{23} && \text{Solve f} \\
&\vdots && \vdots \\
L_{21}U_{1n} + L_{22}U_{2n} &= A_{2n} && \text{Solve f}
\end{aligned}
$$

The procedure is repeated for the remaining rows of [L]. Standard subroutines are available for obtaining this decomposition. Normally, separate storage is not used for the matrices [L] and [U]. Instead, the 1's on the diagonal of [U] are understood to exist and the remaining components of [L] and [U] are stored in the space originally occupied by [A] so the original matrix is destroyed. This replacement can be done as the procedure advances because data for subsequent steps is not lost. After the decomposition, the entries in the space originally occupied by [A] are

$$
[A] = \begin{bmatrix} L_{11} & U_{12} & U_{13} & \cdots & U_{1n} \\ L_{21} & L_{22} & U_{23} & \cdots & U_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \tag{3.5-12}
$$

In the process of obtaining a solution, {y} is stored in {b} so the original vector {b} is lost as well.

When obtaining numerical solutions, one frequently needs to solve [A]{x} = {b} for a large number of {b}'s. The procedure is to do one call to a subroutine that performs the **LU decomposition** of [A]. Then the solution for each {b} is obtained by calling another subroutine which performs the forward and back substitutions that provide the solution.

Pivots

In the LU decomposition, divisions by L_{ii} are required to obtain certain components of [U]. The first two diagonal terms are

$$\begin{aligned} L_{11} &= A_{11} = \det[A_{11}] \\ L_{22} &= A_{22} - L_{21}U_{12} = A_{22} - \frac{A_{21}A_{12}}{A_{11}} \\ &= \frac{1}{A_{11}} \det \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \end{aligned} \tag{3.5-13}$$

Similar expressions hold for subsequent diagonal terms. Since the nonzero value for each L_{ii} is crucial to the success of the approach, L_{ii} is called a **pivot**.

Theorem: (proof omitted for the sake of brevity)

Let $[A]^{(k)}$ denote the principal minor matrix made from the first k rows and columns of [A], i.e.,

$$[A]^{(1)} = [A_{11}], \quad [A]^{(2)} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad \cdots \quad , \ [A]^{(n)} = [A]$$

Assume $\det\,[A]^{(k)} \neq 0$ for k = 1, 2, ..., n - 1. Then the LU decomposition exists, is unique and

$$\det\,[A] = L_{11}L_{22} \ldots L_{nn} \tag{3.5-14}$$

Theorem: (Sylvester's Criterion)

A matrix [A] is positive definite if and only if $L_{ii} > 0$ for all i.

Proof: See Dahlquist, Björck, and Anderson [1974], page 163.

Theorem:

If [A] is symmetric and positive definite, then

$$|A_{ij}|^2 \le A_{ii}A_{jj} \tag{3.5-15}$$

Proof: Reorder any two rows and columns so that A_{ii} becomes A_{11} and A_{jj} becomes A_{22} and apply Sylvester's Criterion. Note: Interchanging 2 rows introduces a minus sign for the resulting determinant, as does interchanging 2 columns. Therefore, the interchange of 2 rows and 2 columns does not change the sign of the determinant. **QED**

Partial Pivoting

Suppose the factorization has occurred to the point that U_{ij} and L_{ji} have been determined with i = 1, ..., k - 1 and j = 1, ..., n. At the k'th step, suppose further that L_{kk} = 0 (or approximately zero). A possible solution is to interchange row k with one of the succeeding rows k* with k* > k. One criterion is to choose the row k* with the largest value $|A_{k^*k}|$ and then try to determine L_{kk} again. The procedure of only looking at one column in the rows for which k* > k as the need arises is called **partial pivoting**.

Interchanging rows corresponds to interchanging equations. The order of the variables in {x} is not changed but the ordering of the components in {b} is changed. If this ordering information is important, as it would be if multiple cases are to be solved with one decomposition, then the ordering information must be preserved. In fact, what is occurring is a multiplication of each term in the equation by an elementary matrix [E] for interchanging rows:

$$[E][A]\{x\} = [E]\{b\} \tag{3.5-16}$$

Complete Pivoting

Suppose the stage is reached such that $L_{kk} = 0$. Now instead of searching the terms in column k for A_{k^*k} for k* > k for the maximum value of $|A_{k^*k}|$, the search is expanded to seek the maximum value of $|A_{k^*l^*}|$ such that $k^*, l^* \geq k$. This procedure is called **complete pivoting**. Then both a row and a column may have to be interchanged. The interchange of a column implies that the ordering of the solution vector is changed. The fact that columns of the components of [U] already obtained are interchanged causes no problems.

In practice, partial pivoting is generally satisfactory and complete pivoting is hardly ever used. Pivoting is not required if:

(i) the matrix [A] is diagonally dominant, or
(ii) the matrix [A] is symmetric and positive definite.

A matrix [A] is **diagonally dominant** [Forsythe and Moler, 1967; page 15] if

$$|A_{ii}| \geq \sum_{j \neq i} |A_{ij}| \qquad \text{for all } i \tag{3.5-17}$$

with inequality for at least one i. In words, the absolute value of each component on the diagonal is greater than or equal to the sum of the absolute values of all other components in the corresponding row. Note that there is no implication concerning positive definiteness. Necessary, but not sufficient, conditions for positive definiteness of symmetric matrices are given by (3.4-13) and (3.4-14).

An Elementary Example of an LU Decomposition:

Suppose

$$[A] = \begin{bmatrix} 2 & 2 & 4 \\ 0 & 0 & 4 \\ 2 & 1 & 6 \end{bmatrix}$$

The first part of the decomposition yields $L_{11} = 2$, $U_{12} = 1$, $U_{13} = 2$ and from the next stage $L_{12} = 0$, $L_{22} = 0$. We see there is a problem because $L_{22} = 0$. At this stage the matrix [A] contains the following terms:

$$[A] = \begin{bmatrix} 2 & 1 & 2 \\ 0 & 0 & 4 \\ 2 & 1 & 6 \end{bmatrix}$$

With k = 2 there is only one other possibility and that is k* = 3. For partial pivoting the second and third rows are interchanged to obtain

$$[A]^* = \begin{bmatrix} 2 & 1 & 2 \\ 2 & 1 & 6 \\ 0 & 0 & 4 \end{bmatrix}$$

Now the decomposition proceeds with $L_{21} = 2$, $L_{22} = -1$, $U_{23} = -2$ and $L_{31} = 0$, $L_{32} = 0$, $L_{33} = 4$. The original matrix contains the components of the decomposition

$$[A]^{**} = \begin{bmatrix} 2 & 1 & 2 \\ 2 & -1 & -2 \\ 0 & 0 & 4 \end{bmatrix}$$

As a check, perform the operation

$$[L][U] = \begin{bmatrix} 2 & 0 & 0 \\ 2 & -1 & 0 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} 1 & 1 & 2 \\ 0 & 1 & -2 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 2 & 4 \\ 2 & 1 & 6 \\ 0 & 0 & 4 \end{bmatrix}$$

which is the matrix [A] with the last two rows interchanged.

Application of LU Decomposition to Obtain the Inverse

Suppose the LU decomposition has been performed. Use the forward and backward substitution part n times to solve the sequence

$$[A]\,\{x\}^i = \{I\}^i \qquad i = 1, ..., n \tag{3.5-18}$$

Then the inverse consists of the matrix formed from the columns $\{x\}^i$:

$$[A]^{-1} = \left[\{x\}^1 \;\; \{x\}^2 \cdots \{x\}^n\right] \tag{3.5-19}$$

which is true because

$$\begin{aligned} [A][A]^{-1} &= \left[\{[A]\{x\}^1\} \;\; \{[A]\{x\}^2\} \cdots \; \{[A]\{x\}^n\}\right] \\ &= \left[\{I\}^1 \;\; \{I\}^2 \;\; \cdots \;\; \{I\}^n\right] \\ &= [I] \end{aligned} \tag{3.5-20}$$

The use of the LU decomposition is a much more convenient approach than the use of the cofactor matrix if it is necessary to obtain the inverse of [A].

3.5.4 Cholesky Decomposition

If [A] is symmetric and positive definite, then there exists a lower triangular matrix [G] with positive diagonal entries such that $[A] = [G][G]^T$. This is the **Cholesky decomposition** and [G] is the **Cholesky triangle**. [Golub and van Loan, 1983; page 88]. Note that this decomposition is a special case of a LU decomposition because $[G]^T$ is upper triangular. The decomposition can be shown by constructing [G]. Consider the indicial form $[A] = [G][G]^T$:

$$A_{ij} = \sum_{k=1}^{n} G_{ik} G^T_{kj} = \sum_{k=1}^{n} G_{ik} G_{jk} = \sum_{k=1}^{\min(i,\, j)} G_{ik} G_{jk} \tag{3.5-21}$$

The summation on k only continues to the minimum of i and j because [G] is lower triangular and terms to the right of the diagonal are zero. Consider j = 1:

$$A_{i1} = G_{i1}G_{11} + G_{i2}G_{12} + G_{i3}G_{13} + \cdots \tag{3.5-22}$$

But $G_{12} = 0$, $G_{13} = 0$, ..., because [G] is lower triangular. Therefore

$$A_{i1} = G_{i1}G_{11} \tag{3.5-23}$$

Now, if we first set i = 1, and then consider i > 1, we obtain

$$G_{11} = \sqrt{A_{11}} \quad \text{and} \quad G_{i1} = A_{i1} / G_{11} \quad \text{for} \quad i > 1 \tag{3.5-24}$$

Thus, the first column of [G] has been obtained. Next consider the result of setting j = 2 in (3.5-21), i.e.,

$$A_{i2} = G_{i1}G_{21} + G_{i2}G_{22} + G_{i3}G_{23} + \cdots \tag{3.5-25}$$

But $G_{23} = 0$, ..., because [G] is lower triangular. Therefore (3.5-25) reduces to

$$A_{i2} = G_{i1}G_{21} + G_{i2}G_{22} \tag{3.5-26}$$

Now, if we set i = 1, we find

$$A_{12} = G_{11}G_{21} + G_{12}G_{22} \tag{3.5-27}$$

But $G_{12} = 0$ and $A_{12} = A_{21}$ so (3.5-27) is just a repeat of (3.5-24) with i = 2. Setting i = 2 yields

$$A_{22} = G_{21}G_{21} + G_{22}G_{22} \tag{3.5-28}$$

which can be rewritten as

$$G_{22} = \sqrt{A_{22} - G_{21}G_{21}} \tag{3.5-29}$$

Now set i > 2 in (3.5-26) to obtain

$$G_{i2} = (A_{i2} - G_{i1}G_{21})/G_{22} \qquad \text{for } i > 2 \tag{3.5-30}$$

and the second column is completed. The next step is to set j = 3 with i = 3 and i > 3 as separate steps in (3.5-21). Continue for the remaining values of j until all components of [G] are obtained.

Modified Cholesky Decomposition

If [A] is symmetric and nonsingular, then there exists a lower triangular matrix [G] with one's on the diagonal and a diagonal matrix [D] with nonzero entries such that $[A] = [G][D][G]^T$. This is also a Cholesky decomposition, modified to eliminate the need for determining square roots. Next, the matrices [G] and [D] are established by direct construction using the indicial notation:

$$A_{ij} = \sum_{k,l=1}^{n} G_{ik} D_{kl} G^T_{lj} = \sum_{k=1}^{n} G_{ik} D_{kk} G^T_{kj}$$
$$= \sum_{k=1}^{\min(i,j)} G_{ik} G_{jk} D_{kk} \qquad (3.5\text{-}31)$$

in which the triangular property of [G] is used in specifying the limits on the sum. Set j = 1 in (3.5-31). The result is

$$A_{i1} = G_{i1} G_{11} D_{11} \qquad (3.5\text{-}32)$$

Now, in addition, let i = 1 to obtain $A_{11} = (G_{11})^2 D_{11}$. Choose $G_{11} = 1$. Then $D_{11} = A_{11}$ and for the remaining values of i, we have

$$G_{i1} = \frac{A_{i1}}{D_{11}} \qquad i = 2, ..., n \qquad (3.5\text{-}33)$$

Next, consider j = 2 in (3.5-31) to obtain

$$A_{i2} = G_{i1} G_{21} D_{22} + G_{i2} G_{22} D_{22} \qquad (3.5\text{-}34)$$

With i = 1, the equation yields nothing new. However, i = 2 results in

$$A_{22} = G_{21} G_{21} D_{11} + G_{22} G_{22} D_{22} \qquad (3.5\text{-}35)$$

As before, we are free to choose $G_{22} = 1$. Then

$$D_{22} = A_{22} - (G_{21})^2 D_{11} = A_{22} - \frac{(A_{21})^2}{A_{11}} \qquad (3.5\text{-}36)$$

For the remaining values of i in (3.5-34), the result is

$$G_{i2} = \frac{1}{D_{22}} [A_{i2} - G_{i1} G_{21} D_{11}] \qquad i = 3, ..., n \qquad (3.5\text{-}37)$$

The formulas for j = 1 and j = 2 suggest the following rather elementary algorithm for obtaining the components of [G]:

```
Do 20  j = 1, n
       G(j,j) = 1
       D(j,j) = A(j,j)
```

```
          Do 5  k = 1, j-1
                D(j,j)=D(j,j) - G(j,k)*G(j,k)*D(k,k)
  5       Continue
          Do 15  i = j+1, n
                G(i,j) = A(i,j)
                Do 10, k = 1, j - 1
                      G(i,j) = G(i,j) - G(i,k)*G(j,k)*D(k,k)
 10             Continue
                G(i,j) = G(i,j)/D(j,j)
 15       Continue
 20  Continue
```

The determinant of [A] becomes

$$\det[A] = \det[G]\det[D]\det[G] = \prod_{i=1}^{n} D_{ii} \tag{3.5-38}$$

To obtain the final form of (3.5-38), we note that [G] is a triangular matrix, so that its determinant is the product of the diagonal terms. However, [G] has one's on the diagonal so det[G] =1.

3.5.5 QR Decomposition

Suppose [A] = [Q][R] where [R] is upper triangular and [Q] is orthogonal. With this **QR decomposition** the linear algebraic problem [A]{x} = {b} can be separated into the following steps: first [Q]{y} = {b}, and then {y} = [R]{x}. The solution for {y} is simply $\{y\} = [Q]^T\{b\}$ and {x} is solved by a back substitution.

The matrix [R] can be obtained through **Givens orthogonalization** in which a series of rotation matrices are used (see the example in Subsection 3.4.3). An alternative approach is to obtain [Q] through **Householder orthogonalization** in which a series of reflection matrices (see the example in Subsection 3.4.3) are used [Strang, 1988; page 373]. Then $[R] = [Q]^T[A]$.

QR decomposition is mathematically equivalent to using the Gram-Schmidt process to obtain an orthonormal basis from the columns of [A]. Denote the columns of [Q] by $\{Q\}^i$. Recall that the Gram-Schmidt process is the following. The initial step is to construct the first column of [Q] by normalizing the first column of [A]:

$$\{Q\}^1 = \frac{\{A\}^1}{|\{A\}^1|} \tag{3.5-39}$$

Now, move on to the second column of [A]. Remove the $\{Q\}^1$ component:

$$\{Q\}^{*2} = \{A\}^2 - (<Q>^1 \{A\}^2)\{Q\}^1 \tag{3.5-40}$$

Next, normalize according to

$$\{Q\}^2 = \frac{\{Q\}^{*2}}{|\{Q\}^{*2}|} \tag{3.5-41}$$

Then, remove the first and second components from the third column of [A]:

$$\{Q\}^{*3} = \{A\}^3 - (<Q>^1 \{A\}^3)\{Q\}^1 - (<Q>^2 \{A\}^3)\{Q\}^2 \tag{3.5-42}$$

This is followed by normalization again to obtain the third column of [Q]:

$$\{Q\}^3 = \frac{\{Q\}^{*3}}{|\{Q\}^{*3}|} \tag{3.5-43}$$

Proceed in a similar manner for the remaining columns to obtain the complete matrix [Q] whose columns form a set of orthonormal vectors so that [Q] is an orthogonal matrix. To show that [R] is upper triangular consider the construction

$$\begin{aligned}[Q][R] &= \begin{bmatrix}\{Q\}^1 & \{Q\}^2 & \cdots & \{Q\}^n\end{bmatrix}\begin{bmatrix} R_{11} & R_{12} & R_{13} & \cdots \\ 0 & R_{22} & R_{23} & \cdots \\ 0 & 0 & R_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \\ &= \begin{bmatrix}\{A\}^1 & \{A\}^2 & \cdots & \{A\}^n\end{bmatrix}\end{aligned} \tag{3.5-44}$$

With matrix multiplication, the component equations yield the following:

$$\begin{array}{lll} R_{11}\{Q\}^1 = \{A\}^1 & \text{or} & R_{11} = \langle Q\rangle^1\{A\}^1 \\ R_{12}\{Q\}^1 + R_{22}\{Q\}^2 = \{A\}^2 & \text{or} & R_{12} = \langle Q\rangle^1\{A\}^2 \quad R_{22} = \langle Q\rangle^2\{A\}^2 \\ \quad\vdots & & \end{array} \tag{3.5-45}$$

We have stated that [R] is upper triangular. To confirm this structure, suppose one assumes the existence of a nonzero term R_{21}. The above approach yields

$$R_{21} = \langle Q\rangle^2\{A\}^1 \tag{3.5-46}$$

But $\{Q\}^2$ was constructed to be orthogonal to $\{A\}^1$ so that R_{21} is indeed zero. A similar arguement holds for the other terms below the diagonal in [R]. Note that if the rank of

[A] is $r < n$, then only r nonzero vectors $\{Q\}^i$ will be obtained from the Gram-Schmidt process. Also

$$\det[A] = \det[Q]\det[R] = \pm\prod_{i=1}^{n} R_{ii} \tag{3.5-47}$$

3.6 MISCELLANEOUS TOPICS

3.6.1 Contravariant and Covariant Bases

Given a matrix $[A]_{nxn}$, suppose the vectors formed from the columns of [A], which we have previously labeled $\{A\}^i$, are defined to be a **contravariant basis**. Define a **covariant basis** $\{A\}_i$ such that

$$\langle A \rangle^i \{A\}_j = \delta_{ij} \qquad i,j = 1,...,n \tag{3.6-1}$$

Suppose the covariant basis is known. Define a matrix [B] whose rows consist of the covariant basis. Then, by taking the product

$$\begin{aligned}
[B][A] &= \begin{bmatrix} \langle A \rangle_1 \\ \langle A \rangle_2 \\ \cdots \\ \langle A \rangle_n \end{bmatrix} \begin{bmatrix} \{A\}^1 & \{A\}^2 & \cdots & \{A\}^n \end{bmatrix} \\
&= \begin{bmatrix} \langle A \rangle_1\{A\}^1 & \langle A \rangle_1\{A\}^2 & \cdots & \langle A \rangle_1\{A\}^n \\ \langle A \rangle_2\{A\}^1 & \langle A \rangle_2\{A\}^2 & \cdots & \langle A \rangle_2\{A\}^n \\ \vdots & \vdots & \ddots & \vdots \\ \langle A \rangle_n\{A\}^1 & \langle A \rangle_n\{A\}^2 & \cdots & \langle A \rangle_n\{A\}^n \end{bmatrix} \\
&= \begin{bmatrix} \{I\}^1 & \{I\}^2 & \cdots & \{I\}^n \end{bmatrix} \\
&= [I]
\end{aligned} \tag{3.6-2}$$

we see that the covariant basis forms the row space of $[A]^{-1}$. It also illustrates an alternative method for viewing the inverse matrix. Consider the linear algebraic problem $[A]\{x\} = \{b\}$. The solution is

$$\{x\} = [A]^{-1}\{b\} = \begin{bmatrix} \langle A \rangle_1 \\ \langle A \rangle_2 \\ \vdots \\ \langle A \rangle_n \end{bmatrix} \{b\} \tag{3.6-3}$$

with the components given by

$$x_i = \langle A \rangle_i \{b\} \tag{3.6-4}$$

This is just another way of writing Cramer's Rule.

3.6.2 Sherman-Morrison Formula

For a given matrix [A], suppose the inverse, $[A]^{-1}$, is known. When solving nonlinear problems, it is often necessary to obtain the inverse to a matrix

$$[B] = \left[[A] + \{u\}<v>\right] \tag{3.6-5}$$

which is a rank-one modification to [A]. For arbitrary vectors {u} and {v}, the Sherman-Morrison Formula provides this inverse:

$$[B]^{-1} = [A]^{-1} - \frac{[A]^{-1}\{u\} < v > [A]^{-1}}{1 + < v > [A]^{-1}\{u\}} \tag{3.6-6}$$

To verify the formula, multiply by the expression for [B] given in (3.6-5) and perform the matrix multiplications as summarized in the following steps:

$$\begin{aligned}
&\left[[A] + \{u\} < v >\right]^{-1}\left[[A] + \{u\} < v >\right] \\
&= [A]^{-1}[A]\,[A]^{-1}\{u\} < v > \\
&\quad - \frac{1}{1 + < v > [A]^{-1}\{u\}}\left[[A]^{-1}\{u\} < v > [A]^{-1}[A] + [A]^{-1}\{u\} < v > [A]^{-1}\{u\} < v >\right] \\
&= [I] + [A]^{-1}\{u\} < v > \\
&\quad - \frac{1}{1 + < v > [A]^{-1}\{u\}}\left[[A]^{-1}\{u\} < v > + [A]^{-1}\{u\}(< v > [A]^{-1}\{u\})^* < v >\right] \\
&= [I] + [A]^{-1}\{u\} < v > \\
&\quad - \frac{1}{1 + < v > [A]^{-1}\{u\}}\left[[A]^{-1}\{u\} < v >\right]\left(1 + (< v > [A]^{-1}\{u\})\right)^* \\
&= [I]
\end{aligned}$$

The key step is to identify and separate the scalar identified as ()* within the product of several terms. This formula is used in Newton-Raphson algorithms for solving the nonlinear algebraic problem and in the theory of plasticity.

3.6.3 Sherman-Morrison-Woodbury Formula

Suppose the modification to the original matrix [A] is now greater than rank 1 as reflected in the matrix [B] given as follows:

$$[B] = [A] + [U][V]^T \tag{3.6-7}$$

Again, suppose the inverse, $[A]^{-1}$, is available and it is desired to obtain the inverse, $[B]^{-1}$. The **Sherman-Morrison-Woodbury Formula** states that if the two matrices [U] and [V] meet the restriction that $[I] + [V]^T[A]^{-1}[U]$ is nonsingular, then

$$[B]^{-1} = [A]^{-1} - [A]^{-1}[U]\big[[I] + [V]^T[A]^{-1}[U]\big]^{-1}[V]^T[A]^{-1} \tag{3.6-8}$$

Note the similarity to the formula for the inverse of the rank one modification. The verification is also similar as the following steps show:

$$\big[[A] + [U][V]^T\big]^{-1}\big[[A] + [U][V]^T\big]$$

$$= [A]^{-1}[A] + [A]^{-1}[U][V]^T$$

$$- [A]^{-1}[U]\big[[I] + [V]^T[A]^{-1}[U]\big]^{-1}[V]^T[A]^{-1}[A]^*$$

$$- [A]^{-1}[U]\big[[I] + [V]^T[A]^{-1}[U]\big]^{-1}[V]^T[A]^{-1}[U][V]^T$$

Continuing with the matrix multiplications, we obtain

$$\big[[A] + [U][V]^T\big]^{-1}\big[[A] + [U][V]^T\big]$$

$$= [I] + [A]^{-1}[U][V]^T$$

$$- [A]^{-1}[U]\big[[I] + [V]^T[A]^{-1}[U]\big]^{-1}\big[[I] + [V]^T[A]^{-1}[U]\big][V]^T$$

$$= [I] + [A]^{-1}[U][V]^T - [A]^{-1}[U][I][V]^T$$

$$= [I]$$

The key point is to perform the following substitutions for the term identified with the asterisk:

$$[V]^T[A]^{-1}[A] = [V]^T[I] = [I][V]^T$$

The need for this formula can arise in connection with the tangent tensor for elasto-plasticity in which the yield surface is a composite of several surfaces.

3.7 CONCLUDING REMARKS

This chapter provides a compilation of the aspects of vector and matrix theory of importance to the field of computational mechanics. Most often used are those relationships and definitions associated with square matrices. Included are basic solution algorithms for the linear algebraic problem which are the essence also of algorithms for nonlinear problems, a topic not included here. The chapter concludes with special topics that arise in special situations such as plasticity.

3.8 EXERCISES

1. Write a matrix subroutine for each of the following operations:
   (i) multiplication of a matrix by a scalar,
   (ii) summation of two matrices,
   (iii) interchange of two rows in a matrix,
   (iv) interchange of two columns in a matrix,
   (v) multiplication of two matrices of arbitrary size,
   (vi) the inner product of two vectors, and
   (vii) the "magnitude" of a vector.

For each case demonstrate that your subroutine works with simple examples worked by hand.

2. Without creating space for a second matrix, write a subroutine that replaces a square matrix with its transpose. Demonstrate that your program works with an example.

3. Use the appropriate subroutines developed in Problems 1 and 2 on two example square matrices to illustrate the equation $\left[[A][B]\right]^T = [B]^T[A]^T$.

4. With the use of appropriate subroutines from Problem 1 show that

$$[A]\{x\} = x_1\{A\}_1 + x_2\{A\}_2 + ...$$

5. Construct a symmetric matrix $[A]_{4x4}$. For each of the following, construct an elementary matrix, [E], (and perform the matrix multiplication using your subroutines) which:

   (i) scales the third column by a factor of 5,
   (ii) interchanges rows 2 and 4,
   (iii) interchanges columns 2 and 4, and
   (iv) interchanges both columns 2 and 4 and rows 2 and 4.

For part (iv) confirm that the result is still a symmetric matrix. Prove the general result that if [A] is symmetric, and the same rows and columns are interchanged, the resulting matrix is symmetric?

6. Write a subroutine for solving a matrix equation based on the LU decomposition (without pivoting). As part of the procedure obtain the determinant of the matrix. Show that your program works with the following procedure:

(i) Assume a solution vector, $\{x\}^a$, and determine a right-hand vector,

$$\{b\} = [A]\{x\}^a$$

(ii) Solve the matrix equation using your algorithm. Suppose your solution is $\{x\}$.

(iii) Obtain the following two measures of error involving the inner product:

$$\varepsilon_1 = \frac{\left|\{x\} - \{x\}^a\right|}{\left|\{x\}^a\right|} \qquad \text{and} \qquad \varepsilon_2 = \frac{\left|[A]\{x\} - \{b\}\right|}{\left|\{b\}\right|}$$

(a) Perform the sequence of steps for 3x3 and 6x6 matrices of your choice. Which measure of error do you think is most appropriate for general problems?

(b) Now perform the sequence on Hilbert matrices, [H], which are matrices with components $H_{ij} = \frac{1}{i+j-1}$. Examples are:

$$[H]_{2x2} = \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} \end{bmatrix}, \qquad [H]_{3x3} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \end{bmatrix}$$

Note that if $b_i = \sum_{j=1}^{n} H_{ij}$, then the exact solution to $[H]\{x\} = \{b\}$ is $\{x\} = \begin{Bmatrix} 1 \\ 1 \\ \vdots \end{Bmatrix}$. Do the cases n = 2, 3,... up to one higher than the dimension for which you can obtain reasonable answers for your machine. Discuss your results with the understanding that Hilbert matrices are known to be notoriously ill-conditioned, a concept discussed in the next chapter.

7. Write a subroutine for solving a matrix equation based on the Cholesky decomposition of a symmetric, positive definite matrix that does not require square roots. Show that your program works with elementary examples in a manner similar to that outlined in Problem 6.

8. Repeat Problem 6 using iterative refinement which is described next.

Suppose $\{x\}^{(1)}$ is the solution to the linear algebraic problem $[A]\{x\} = \{b\}$ obtained by Gaussian elimination. Because of round-off, the equation will not be satisfied exactly. Let $\{r\}^{(1)}$ be the residual where

$$\{r\}^{(1)} = \{b\} - [A]\{x\}^{(1)} \qquad \text{(i)}$$

For an improved solution, solve

$$\{r\}^{(1)} = [A]\{\Delta x\}^{(2)} \tag{ii}$$

for $\{\Delta x\}^{(2)}$. Subtract corresponding terms (i) - (ii) to obtain theoretically

$$\{0\} = [A]\{x\}^{(2)} \qquad \{x\}^{(2)} = \{x\}^{(1)} + \{\Delta x\}^{(2)}$$

In a practical application, there will still be a residual so the process is repeated in a process called **iterative refinement**. The procedure is summarized as follows:

1. Solve $[A]\{x\}^{(1)} = \{b\}$ for $\{x\}^{(1)}$. Let i denote an iterative count starting with i = 1.
2. Determine $\{r\}^{(i)} = \{b\} - [A]\{x\}^{(i)}$.
3. Check to see if the residual meets an error criterion. If the criterion is met stop; otherwise proceed to the next step.
4. Solve $[A]\{\Delta x\}^{(i)} = \{r\}^{(i)}$ for $\{\Delta x\}^{(i)}$.
5. Obtain an improved solution by taking the sum $\{x\}^{(i+1)} = \{x\}^{(i)} + \{\Delta x\}^{(i)}$.
6. Increment i by one and return to Step 2.

With the assumption that the linear algebraic equation is solved using single-precision arithmetic, this procedure provides meaningful improvements only if the residual in Step 2 is obtained using double precision.