MATRICES

5.1 INTRODUCTION

We come across matrices while we deal with a set of linear equations or when we need to rotate vectors. In chemistry the use of matrices is really wide spread as we deal with wave functions of atoms and molecules all the time. The energy levels of these systems turn out to be the eigenvalues of appropriate matrices. In the present chapter we will deal with the problem of finding the determinant and inverse of a matrix. For eigenvalues, we will use public domain software that will be introduced in chapter 8. For getting the eigenvalues of a matrix, we need to find the roots of polynomial equations and shall also consider this problem here.

5.2 MATRIX INVERSION

The problem of matrix multiplication has already been considered in chapter 3. The inverse of a square matrix A is defined through the equation.

$$A^{-1}A = AA^{-1} = I \qquad (5.1)$$

where I is the identity matrix. The inverse of the matrix exists only if the determinant of the matrix is non-zero.

$$I = \begin{bmatrix} 1 & 0 & 0 & . & . \\ 0 & 1 & 0 & . & . \\ 0 & 0 & 1 & . & . \\ . & . & . & . & . \\ . & . & . & . & 1 \end{bmatrix} \ldots\ldots\ldots\ldots (5.2)$$

If the elements of the matrix A are denoted by a_{ij}, then the elements of the inverse matrix are given by

$(A^{-1})_{ij}$ = cofactor of the element a_{ji} / (determinant of matrix A) (5.3)

Where the cofactor of an element a_{ji} is the determinant of the matrix that results when the j^{th} row and the i^{th} column of matrix A is removed resulting in matrix of order $(n-1)\times(n-1)$. If A is 4×4 matrix,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \quad (5.4)$$

Then the cofactor of a_{32} is

$$\begin{bmatrix} a_{11} & a_{13} & a_{14} \\ a_{21} & a_{23} & a_{24} \\ a_{41} & a_{43} & a_{44} \end{bmatrix} \times (-1)^{i+j} \quad (5.5)$$

The determinant of matrix A is defined as

$\det A = \sum_{k=1}^{n_1} a_{ik} C_{ik}$ for i= 1…n (5.6)

Where C_{ik} is the cofactor of element a_{ik}. From equation (5.6) we see that the matrix can be expanded by taking any row or any column. For solving a linear equations such as

$$A\vec{X} = \vec{Y} \quad (5.7)$$

Where $\vec{X}, \vec{Y}$ are $(n \times 1)$ vectors, the following solution

$$\vec{Y} = A^{-1}\vec{X} \quad (5.8)$$

can be obtained only if the determinant of matrix A is not zero.

5.3 THE ELIMINATION METHOD

To find the inverse, we need several elementary operations on matrices and the means of performing these operations by the use of elementary matrices. The first operation denoted by $E_i(c)$which multiplies the ithrow of the matrix by a constant c. this is accomplished by using the elementary matrix

$$E_i(c) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \leftarrow i^{th}\ row \quad (5.9)$$

The second operation is the exchange of row 'i' with row 'k' and this is accomplished by performing the multiplication of a matrix A on its leftby a modified identity matrix (I) in which i^{th} and j^{th} rows are interchanged. To interchange the second and forth rows of matrix A, we need to multiply A from the left by E_{24} which is given by

$$E_{24} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \quad (5.10)$$

The third elementary operation is multiplication of a row, say kth row by a constant c and adding it to the ith row. Such a matrix is denoted by E_{ik} (c). e.g. to add c times the 5th row to the second row of a 5×5 matrix, we use

$$E_{25}\ (c) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & c \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad (5.11)$$

The matrices that operate on A are also operated on I so that we get A^{-1}, as follows.

$E_n \ldots. E_k, E_{k-1} \ldots.E_1, A = I$ (5.12)

$\therefore E_n \ldots. E_k, E_{k-1} \ldots.E_1 = A^{-1}$(5.13)

Therefore operate the sequence E_n ……..E_1 on I to get A^{-1}.

The summary of the three elementary operations is

1) $E_i(c)$: multiply i^{th} row by c :i^{th}row of I multiplied by c.
2) E_{ik}: Interchange rows i and k : rows i and k of I interchanged.
3) $E_{ik}(c)$: Replace i^{th}row byi^{th} row + c times k^{th}row : row i of I replaced by row i + c times row k.

e.g. $A' = \begin{bmatrix} a_{11}' & a_{12}' & a_{13}' \\ a_{21}' & a_{22}' & a_{23}' \\ a_{31}' & a_{32}' & a_{33}' \end{bmatrix} =$

$$\begin{bmatrix} 1 & 0 & c \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} + ca_{31} & a_{12} + ca_{32} & a_{13} + ca_{33} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = E_{13}(c)A$$

5.4 THE GAUSS ELIMAINATION ALGORITHM

The algorithm for matrix inversion by elimination is k^{th} stage among the stages 1….n

(i) Normalization of element a_{kk} by multiplying the k^{th} row by a_{kk}^{-1}. If $a_{kk} = 0$, replace k^{th} row by row imax and vice versa such thatimax>k.

(ii) Zeroing the off diagonal elements of col k by replacing row i ($i \neq k$) by suitable combinations of row i and k. These two steps are shown below. The superscripts (k), (k-1),..etc indicate the stages or steps in the matrix inversion process.

$$\left.\begin{array}{c} a_{kj}{}^{(k)} = \dfrac{a_{kj}{}^{(k-1)}}{a_{kk}{}^{(k-1)}} \;;\quad b_{kj}{}^{(k)} = \dfrac{b_{kj}{}^{(k-1)} \curvearrowleft \; stages}{a_{kk}{}^{(k-1)}} \\ a_{ij}{}^{(k)} = a_{ij}{}^{(k-1)} - a_{ik}{}^{(k-1)} a_{kj}{}^{(k)} \;;\; b_{ij}{}^{(k)} = b_{ij}{}^{(k-1)} - a_{ik}{}^{(k-1)} b_{kj}{}^{(k)} \\ (i \neq k) \quad (i \neq k) \end{array}\right\} j = 1,2 \ldots n$$

after n stages, $A^{(n)} = I$ and $B^{(n)} = A^{-1}$

Initially, $A^{(o)} = A$ and $B^{(o)} = I$

5.5A NUMERICAL EXAMPLE

A numerical example is given below.

1) Step/Stage 0: initial matrices A and I

$$A = \begin{bmatrix} 4 & 8 & 2 & 1 \\ 1 & 5 & 3 & 8 \\ 2 & 7 & 1 & 4 \\ 3 & 8 & 2 & 1 \end{bmatrix} \qquad B = I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

2) Stage 1:
   a) Divide the first row by 4.
   b) Subtract the new first row from the second row.
   c) Subtract 2 times new first row from the third row, E_{31} (-2) and
   d) E_{41} (-3).
   e) Repeat these operations on B to get $B^{(1)}$.

$$A^{(1)} = \begin{bmatrix} 1 & 2 & 1/2 & 1/4 \\ 0 & 3 & 5/2 & 31/4 \\ 0 & 3 & 0 & 7/2 \\ 0 & 2 & 1/2 & 1/4 \end{bmatrix} B^{(1)} = \begin{bmatrix} 1/4 & 0 & 0 & 0 \\ -1/4 & 1 & 0 & 0 \\ -1/2 & 0 & 1 & 0 \\ -3/4 & 0 & 0 & 1 \end{bmatrix}$$

3) Stage 2:
   a) Divide the second row by 3, E_2 (1/3).
   b) Subtract two times the new second row from first row. E_{12} (-2)
   c) E_{32} (-3).
   d) E_{42} (-2).

$$A^{(2)} = \begin{bmatrix} 1 & 0 & -76 & -59/12 \\ 0 & 1 & 5/6 & 31/12 \\ 0 & 0 & -15/6 & -17/4 \\ 0 & 0 & -7/6 & -15/12 \end{bmatrix} B^{(2)} = \begin{bmatrix} 5/12 & -2/3 & 0 & 0 \\ -1/12 & 1/3 & 0 & 0 \\ -3/12 & -1 & 1 & 0 \\ -7/12 & -2/3 & 0 & 1 \end{bmatrix}$$

4) Stage 3:
   a) E_3 (-6/15).
   b) E_{13} (7/6).
   c) E_{23} (-6/5).
   d) E_{43} (7/6).

$$A^{(3)} = E_{43}\left(\frac{7}{6}\right) E_{23}\left(\frac{-6}{5}\right) E_{13}\left(\frac{7}{6}\right) E_3\left(\frac{-6}{15}\right) A^{(2)}$$

$$A^{(3)} = \begin{bmatrix} 1 & 0 & 0 & -44/15 \\ 0 & 1 & 0 & 7/6 \\ 0 & 0 & 1 & 17/10 \\ 0 & 0 & 0 & -44/15 \end{bmatrix} B^{(3)} = \begin{bmatrix} 8/15 & 3/15 & -7/15 & 0 \\ -1/6 & 0 & 1/3 & 0 \\ 1/10 & 6/15 & -6/15 & 0 \\ -7/15 & -1/5 & -7/15 & 1 \end{bmatrix}$$

5) Stage 4:
   a) E_4 (-15/44)
   b) E_{14} (44/15)
   c) E_{24} (-7/6)
   d) E_{34} (-17/10)

$$B^{(4)} = E_{34}\left(\frac{-17}{10}\right) E_{24}\left(\frac{7}{6}\right) E_{14}\left(\frac{44}{15}\right) E_4\left(\frac{-15}{44}\right) B^{(3)}$$

$$A^{(4)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} B^{(4)} = \begin{bmatrix} 1 & 0 & 0 & -1 \\ -31/88 & -7/88 & 13/88 & 35/88 \\ -15/88 & 25/88 & -59/88 & 51/88 \\ 7/44 & 3/44 & 7/44 & -15/44 \end{bmatrix}$$

$$\det A = 1\,.\ a_{11}{}^{(0)}.\,a_{22}{}^{(1)}.\,a_{33}{}^{(2)}.\,a_{44}{}^{(3)}$$

$$= 1\,.4\,.3\,.\left(-\frac{15}{6}\right).\left(-\frac{44}{15}\right) = 88$$

To obtain the determinant of the matrix we need to take the product of intermediate diagonal values, i.e.

$$\det A = 1\,.\; a_{11}{}^{(0)}.\,a_{22}{}^{(1)}.\,a_{33}{}^{(2)}.\,a_{44}{}^{(3)}$$

$$= 1\,.4\,.3\,.\left(-\frac{15}{6}\right).\left(-\frac{44}{15}\right) = 88 \quad (5.14)$$

The general formula is

$$\det = \prod_{i=1}^{n} a_{ii}{}^{(n-1)}$$

This follows from the properties of the products of determinants of matrices and the fact that the determinants of all elementary matrices have a value of unity. In the case of matrices where the determinant is zero, special care has to be taken to isolate the diagonal terms which are likely to be zero.

5.7 THE PROGRAM FOR MATRIX INVERSION

```
programmatinv
c       warning: This is for strictly nonsingular matrices
c       for N other than 4, change the values of N and the data file
c       original matrix elements a(i,j), inverse matrix elements b(i,j)
dimension a(25,25), b(25,25),aold(25,25)
open(unit=11,file='input1.dat')
open(unit=12,file='output.dat')
         N=4
cc      this value of N can be read from a file too and the program can be
cc      generalized ot any matrix of size less than equal to 25 x 25.
read(11,*)((a(i,j),j=1,N),i=1,N)
c       matrix is read row wise, i.e. a11,a12,...a2n
cdef         eps=0.00000001
ine the identity matrix B(3)=I
doi=1,N
do j=1,N
aold(i,j)= a(i,j)
b(i,j)=0.0
if (i.eq.j)then
b(i,j)=1.0
end if
end do
end do
cloacate the maximum magnitude of a(i,k) on or below the main
cdigonal
det=1.0
do 450 k=1,N
c      test for singular matrix
c      warning: This is for strictly nonsingular matrices
c      stop if div = 0.0
div = a(k,k)
if(abs(div).lt.eps) go to 960
det = det * div
do 380 j= 1,N
a(k,j) = a(k,j)/div
aold(k,j) = a(k,j)
380 b(k,j) = b(k,j)/div
c       replace each row by suitable linear combination with pivot row
c
do 430 j  = 1,N
do 430 i = 1,N
if (i.ne.k) then
amult = aold(i,k)
a(i,j) = a(i,j)- amult * a(k,j)
b(i,j) = b(i,j)- amult * b(k,j)
end if
```

```
 430   continue
write(*,*) k
c        the matrix aold retains the old values of a so that
c        correct substractions are done
do 440 ii = 1,N
do 440 jj = 1,N
440 aold(ii,jj) = a(ii,jj)
  450 continue
  900    format(2x, 6E12.5)
cwrite inverse matrix and determinant
write(12,*) 'determinant=',det
write(12,*)'the elements of the inverse matrix are'
write(12,200)((b(i,j),j=1,N),i=1,N)
write(12,*)'the modified original matrix is'
write(12,200)((a(i,j),j=1,N),i=1,N)
200 format(1x,4e15.6)
960write(12,*)'the matrix is singular'
End
```

5.8 MATRIX DIAGONALIZATION

Consider the following multiplication of matrix A and $\vec{X}$

$$A.\vec{X} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -2 \\ 2 \end{bmatrix} = 2\begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad (5.15)$$

$$\text{Or} \quad A\,\overrightarrow{X} = \lambda\overrightarrow{X} \quad (5.16)$$

In this case, the multiplication of $\overrightarrow{X}$ by A gives a constant number λtimes of vector $\overrightarrow{X}$. It is like elongating or contracting the vector $\overrightarrow{X}$. In the above equation, λ is called the eigenvalue of A and $\overrightarrow{X}$ is an eigenvector of A. Finding all the eigenvalues and eigenvectors of A is the process of diagonalization of the matrix A.

To get each eigenvector, substitute the corresponding eigenvalue in Eq (5.17).

$A\vec{X} - \lambda\vec{X} = (A - \lambda I)\vec{X}$ (5.17)

If $B = (A - \lambda I)$, then $\det(B)$ has to be zero for nontrivial (nonzero) solution of eigenvector $\vec{X}$

$$\therefore \det(B) = \det(A - \lambda I) = 0 \quad (5.18)$$

For an n × n matrix, $\det(A - \lambda I)$ is an nth order polynomial in λ and the n roots of this polynomial are the n eigenvalues. By substituting each eigenvalue in Eq (5.17) we can obtain the eigenvector corresponding to that eigenvalue. For the matrix in Eq (5.15), the determinant of (5.18) is

$$\det\begin{pmatrix} a_{11} - \lambda & a_{12} \\ a_{21} - \lambda & a_{22} \end{pmatrix} = \begin{vmatrix} 1 - \lambda & -1 \\ -1 & 1 - \lambda \end{vmatrix} = 0 \quad (5.19)$$

Or $\lambda^2 - 2\lambda + 1 - 1 = \lambda^2 - 2\lambda = \lambda(\lambda - 2) = 0$ (5.20)

The two eigenvalues are $\lambda = 0$ and $\lambda = 2$.

,

We have

$$\begin{pmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{pmatrix}\begin{pmatrix} X_{11} \\ X_{21} \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} X_{11} \\ X_{21} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (5.21)$$

$$X_{11} - X_{21} = 0$$

$-X_{11} + X_{21} = 0$ (5.22)

Or $X_{11} = X_{12}$ and we can take the first eigenvector to be

$$\begin{pmatrix} X_{11} \\ X_{21} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (5.23)$$

We could take any multiple of $\begin{pmatrix}1\\1\end{pmatrix}$ but it is preferable to keep the simplest form.

For the second eigenvector, use the second value of λ, i.e. $\lambda_2 = 2$,

$$\begin{pmatrix}a_{11}-\lambda & a_{12}\\ a_{21} & a_{22}-\lambda\end{pmatrix}\begin{pmatrix}X_{12}\\X_{22}\end{pmatrix} = \begin{pmatrix}1-2 & -1\\ -1 & 1-2\end{pmatrix}\begin{pmatrix}X_{12}\\X_{22}\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix} \quad (5.24)$$

Or $\begin{matrix}-X_{12} - X_{22} = 0\\ -X_{12} - X_{22} = 0\end{matrix}$ (5.25)

Or $X_{12} = -X_{22}$

Or $\begin{pmatrix}X_{12}\\X_{22}\end{pmatrix} = \begin{pmatrix}1\\-1\end{pmatrix}$ (5.26)

The matrix of eigenvectors is

$$X = \begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \quad (5.27)$$

The inverse of this matrix, X^{-1} is

$$X^{-1} = \begin{pmatrix}1/2 & 1/2\\ 1/2 & -1/2\end{pmatrix} \quad (5.28)$$

It is very easy to see that

$$X^{-1}AX = \begin{pmatrix}1/2 & 1/2\\ 1/2 & -1/2\end{pmatrix}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = \begin{pmatrix}0 & 0\\ 0 & 2\end{pmatrix} \quad (5.29)$$

In general, for a matrix A that can be diagonalized, the above transformation (called the similarity transformation) results in the diagonal form of the matrix A wherein the diagonal values of the matrix are the eigenvalues and all the off diagonal elements are zero.

$$X^{-1}AX = A_D, \qquad A_D = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & . & \dots\dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \lambda_n \end{pmatrix} \quad (5.30)$$

The n[th] order polynomial for the determinant of $|A - \lambda I|$ can be factored as follows

$$P_n(\lambda) = \lambda^n + b_1\lambda^{n-1} + \cdots + b_{n-1}\lambda + b_n = (\lambda - \lambda_1)(\lambda - \lambda_2)\dots.(\lambda - \lambda_n) = 0 \quad (5.31)$$

This is a rather involved problem to program and we will illustrate a method to find the largest eigenvalue. We would like to reemphasize and reiterate that the numerical methods used in these chapters are illustrative and by no means the best methods. The main purpose is to give a practical experience and illustrations in numerical techniques and an enthusiastic learner is encouraged to peruse books/materials that specialize in sophisticated numerical analysis.

5.11 EIGENVALUE OF THE LARGEST MAGNITUDE

Let A be a square matrix with n distinct eigenvalues such that$|\gamma_1| > |\gamma_2| > \cdots \dots \dots .. > |\gamma_n|$. (Please note that the symbol$\gamma$is used in place λ that was used earlier). Here $\gamma_1, \gamma_2 \dots \dots \dots \dots . \gamma_n$ are the eigenvalues. Since the eigenvalues are distinct, the corresponding eigenvectors $V_1, V_2, \dots \dots V_n$ are linearly independent and satisfythe relations

$$AV_i = \gamma_i V_i, \quad i = 1, \dots \dots . n, \text{with} \sum_{i=1,n} c_i V_i = 0 \text{ only if all } c_i = 0 \quad (5.32)$$

In the language of vectors, any arbitrary vector X_0 in n-dimensional space can be expressed as a linear combination of these n linearly independent eigenvectors. This is called the vector span theorem. This is a generalization of the three dimensional case wherein any three dimensional vector can be written as $x\hat{\imath} + y\hat{\jmath} + z\hat{k}$, a linear combination of unit vectors$\hat{\imath}, \hat{\jmath}and\hat{k}$.

$\therefore X_0 = C_1V_1 + C_2V_2 \dots\dots + C_nV_n$ (5.33)

Multiply X_0 successively (of course from the left side!) by $A, A^2 \dots\dots A^k$ to get

$$AX_0 = C_1AV_1 + C_2AV_2 \dots\dots + C_nAV_n$$

$$AX_0 = C_1\gamma_1V_1 + C_2\gamma_2V_2 \dots\dots + C_n\gamma_nV_n \quad (5.34)$$

Similarly

$A^2X_0 = C_1{\gamma_1}^2V_1 + C_2{\gamma_2}^2V_2 \dots\dots + C_n{\gamma_n}^nV_n$ (5.35)

$A^kX_0 = C_1{\gamma_1}^kV_1 + C_2{\gamma_2}^kV_2 \dots\dots + C_n{\gamma_n}^kV_n$ (5.36)

$= {\gamma_1}^k[\, C_1V_1 + C_2(\frac{\gamma_2}{\gamma_1})^kV_2 + \dots\dots + C_n(\frac{\gamma_n}{\gamma_1})^kV_n]$ (5.37)

As 'k' becomes large all $\frac{\gamma_i}{\gamma_1}$ $(i = 2, \dots., n)$ become small and we get

$$A^kX_0 = C_1{\gamma_1}^kV_1 \quad (5.38)$$

And $$A^{k+1}X_0 = C_1{\gamma_1}^{k+1}V_1 \quad (5.39)$$

i.e. for large k we have

$$\gamma_1 = (A^{k+1}X_0)_i/(A^kX_0)_i \forall\, i = 1, \dots\dots n \quad (5.40)$$

A simple way to do the above operations without actually taking powers of A is given below.

Let an arbitrary 'normalized' vector ${X_0}^t$ be given by

$${X_0}^t = [1, X_{20}, X_{30}, \dots X_{n0}] \quad (5.41)$$

Here ${X_0}^t$ is the transpose of the column vector X_0 and thus written as a row vector. The meaning of this "normalized" is that the first value$X_{10} = 1$.

We then have

$$AX_0 = AX_0 = Y_1 = m_1 X_1$$

$$\frac{1}{m_1} A^2 X_0 = AX_1 = Y_2 = m_2 X_2$$

$$\frac{1}{m_1 m_2} A^3 X_0 = AX_2 = Y_3 = m_3 X_3$$

$$\frac{1}{m_{k-1} \ldots\ldots m_1} A^k X_0 = AX_{k-1} = Y_k = m_k X_k \text{(5.42)}$$

$$\frac{1}{m_k \ldots\ldots m_1} A^{k+1} X_0 = AX_k = Y_{k+1} = m_{k+1} X_{k+1}$$

Here, ${Y_k}^t = [Y_{1k}, Y_{2k}, \ldots . Y_{nk}]$and ${X_k}^t = [1, X_{1k}, X_{2k}, \ldots . X_{nk}]$

By using Eq (5.40) and the above equation, we get

$$Y_{k+1} = \frac{1}{m_k \ldots\ldots m_1} A^{k+1} X_0 = \frac{1}{m_k \ldots\ldots m_1} \gamma_1^{k+1} C_1 V_1 \text{(5.43)}$$

$$X_k = \frac{1}{m_k \ldots\ldots m_1} A^k X_0 = \frac{1}{m_k \ldots\ldots m_1} \gamma_1^k C_1 V_1 \text{(5.44)}$$

By taking the ratio of the first components of Y_{k+1} and X_k, we get

$$\frac{Y_{1,k+1}}{X_{1,k+1}} = \frac{\frac{1}{m_k \ldots\ldots m_1} \gamma_1^{k+1} C_1 V_1}{\frac{1}{m_k \ldots\ldots m_1} \gamma_1^k C_1 V_1} = \gamma_1 \text{(5.45)}$$

Since $X_{1,k+1} = 1$, we have

$Y_{1,k+1} = \gamma_1$(5.46)

The eigenvector X_{k+1} which is the 'normalized' eigenvector corresponding to γ_1 is

$$X_{k+1} = \frac{1}{m_{k+1}, m_k \ldots m_1} A^{k+1} X_0 = \frac{1}{m_k \ldots m_1} \gamma_1^{k+1} C_1 V_1 \quad (5.47)$$

As $X_{1k} = 1, Y_{1k} = m_k$ and the recursion formulae to be used in the computer program are

$$AX_{k-1} = Y_k \quad (5.48a)$$

$$X_k = \frac{1}{Y_{1k}} Y_k \quad (5.48b)$$

The program to calculate γ_1 and V_4 is given below. Do write the algorithm and flow chart for the same problem of finding the largest eigenvalue and the eigenvector corresponding to it.

```
programlargeig
c     calculates iteratevely the largest eigenvalues and eigenvector
dimension a(20,20),x(20),y(20)
c     the maximum number of iterations=Kmax usually about 50
 n=4
cgeneralalise thisprogram to N > 4 up to a value of 20.
eps=0.0001
kmax=300
open(unit=23,file='input1.dat')
read(23,*) ((a(i,j),j=1,n),i=1,n)
c     setup the initial eigenvector X0=(1,0,....0)and y0=(0,0..0)
doi=2,n
x(i)=0.0
end do
x(1)=1.0
gamold=1.0
gamnew=1.0
kk=1
100 do 110 i=1,n
110 y(i)=0.0
doi=1,n
do j=1,n
y(i)=y(i)+a(i,j)*x(j)
end do
end do
write(*,*) kk,gamnew,(x(k),k=1,n)
```

```
gamnew=y(1)
doi=1,n
x(i)=y(i)/gamnew
end do
if((abs(gamnew-gamold)).lt.eps) then
write (*,*)'gamnew=',gamnew
write (*,*)'eigenvector is'
write (*,*) (x(i),i=1,n)
stop
else
kk=kk+1
gamold=gamnew
if (kk.lt.kmax) then
go to 100
else
write(*,*) 'the solution doesnot converge'
stop
end if
end if
end
```

5.12 SUMMARY

In the present chapter, we have described different aspects of matrix operations. A computationally simple method of matrix inversion was explored using elementary matrices that can multiply a given row by a constant, or exchange rows or columns or add multiples of a given row to another row. Eigenvalue methods were also described and a program to estimate the largest Eigenvalue of a square matrix and its corresponding eigenvector was also outlined.

PROBLEMS

1. Write a program to perform the following tasks on the arrays A(100, 100) and B(100, 100)

   a. Sum a row.

   b. Determine the maximum value within each array.

c. Transpose an array. The transposed array (B) is the original array (A) with rows and columns switched.

d. Subtract each element in the array B from the corresponding element of the A array. Have the results returned in the A array. In general, this can be represented as A (I, J) = A (I, J) – B(I, J).

2. Write a program to solve the following equations using Cramer's rule

I. $-2x + 3y = 8$

$3x - y = -5$

II. $2x - y + 3z = -3$

$-x - y + 3z = -6$

$x - 2y - z = -2$