Chap. 6

Solution of Linear and Nonlinear Equations

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Simultaneous Linear Equations I

- Simultaneous set of linear equation:
  - One can solve the equation by using paper and a pen!
  - But if there are many variables, then the procedure is very tedious.
    - Moreover, humans are slow and prone to error in such tedious calculations.

Example: four simultaneous equations with four variables, w, x, y and z.

$$\begin{aligned} 2w + x + 4 + z &= -4, \\ 3w + 4x - y - z &= 3, \\ w - 4x + y + 5z &= 9, \\ 2w - 2x + y + 3z &= 7 \end{aligned} \tag{1}$$

In matrix form

$$\begin{pmatrix} 2 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}. \tag{2}$$

Simultaneous Linear Equations II

Alternatively, in a shorthand form:

$$\mathbf{A}\mathbf{x} = \mathbf{v}, \tag{3}$$

where $\mathbf{x} = (w, x, y, z)$ and the matrix $\mathbf{A}$ and vector $\mathbf{v}$ take the appropriate values. Then find the solution:

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{v}. \tag{4}$$

But the problem is finding $\mathbf{A}^{-1}$ is not so trivial using computer.

Gauss-Jordan Elimination

- The most straightforward method to find the solution of Eq. (3).
- Two rules for Gauss-Jordan elimination:
  1. If we multiply any row of the matrix $\mathbf{A}$ by any constant, and we multiply the corresponding row of the vector $\mathbf{v}$ by the same constant, then the solution does not change.
  2. If we add to or subtract from any row of $\mathbf{A}$ a multiple of any other row, and we do the same for the vector $\mathbf{v}$, then the solution does not change.

Exmaple:Eq. (2) I

As for an example, let's try to solve Eq. (2) by hand:

1. Divide the first row by the top-left element of the matrix:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3 \\ 9 \\ 7 \end{pmatrix}. \tag{5}$$

2. Subtract 3 times the first row from the second row:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 2.5 & -7 & -2.5 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 9 \\ 9 \\ 7 \end{pmatrix}. \tag{6}$$

Exmaple:Eq. (2) II

3. Subtract the first row from the third one, and also subtract 2 times the first row from the fourth:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 2.5 & -7 & -2.5 \\ 0 & -4.5 & -1 & 4.5 \\ 0 & -3 & -3 & 2 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 9 \\ 11 \\ 11 \end{pmatrix}. \tag{7}$$

4. Divide the second row by 2.5:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 1 & -2.8 & -1 \\ 0 & -4.5 & -1 & 4.5 \\ 0 & -3 & -3 & 2 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3.6 \\ 11 \\ 11 \end{pmatrix}. \tag{8}$$

Exmaple:Eq. (2) III

5. Subtract -4.5 times the second row from the third, and -3 times the second row from the fourth:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 1 & -2.8 & -1 \\ 0 & 0 & -13.6 & 0 \\ 0 & 0 & -11.4 & -1 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3.6 \\ 27.2 \\ 21.8 \end{pmatrix}. \tag{9}$$

6. Divide the third row by -13.6:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 1 & -2.8 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -11.4 & -1 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3.6 \\ -2 \\ 21.8 \end{pmatrix}. \tag{10}$$

Exmaple:Eq. (2) IV

7. Subtract -11.4 times third row from the fourth:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 1 & -2.8 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3.6 \\ -2 \\ -1 \end{pmatrix}. \tag{11}$$

8. Divide the fourth row by -1:

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 1 & -2.8 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3.6 \\ -2 \\ 1 \end{pmatrix}. \tag{12}$$

By definition, Eq. (12) has the same solution with Eq. (2), but the matrix is now upper triangular.

Backsubstitution I

- To find the final solution of Eq. (2) we now use the process of backsubstitution.
- Suppose we have any set of equations of the form:

$$\begin{pmatrix} 1 & a_{01} & a_{02} & a_{03} \\ 0 & 1 & a_{12} & a_{13} \\ 0 & 0 & 1 & a_{23} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ v_3 \end{pmatrix}. \tag{13}$$

- Eq. (13) can be written as:

$$w + a_{01}x + a_{02}y + a_{03}z = v_0, \tag{14}$$

$$x + a_{12}y + a_{13}z = v_1, \tag{15}$$

$$y + a_{23}z = v_2, \tag{16}$$

$$z = v_3. \tag{17}$$

Backsubstitution II

1. From Eq. (17):
   $$z = v_3 \tag{18}$$
2. From Eq. (16)
   $$y = v_2 - a_{23}z \tag{19}$$
3. From Eq. (15)
   $$x = v_1 - a_{12}y - a_{13}z \tag{20}$$
4. From Eq. (14)
   $$w = v_0 - a_{01}x - a_{02}y - a_{03}z \tag{21}$$

- Applying Eqs. (18)-(21) we obtain:

$$w = 2, \quad x = -1, \quad , y = -2, \quad , z = 1. \tag{22}$$

Example 6.1: I

Guassian elimination for Eq. (2):

```
from numpy import array, empty

A=array([[2,1,4,1],
    [3,4,-1,-1],
    [1,-4,1,5],
    [2,-2,1,3]],float)

v=array([-4,3,9,7],float)
N=len(v)

# Gaussian Elimination
for m in range(N):
    # Divide by the diagonal element
    div=A[m,m]
    A[m,:]/=div
    v[m]/=div

    # Subtract fro the lower rows
    for i in range(m+1,N):
        mult=A[i,m]
        A[i,:]-=mult*A[m,:]
        v[i]-=mult*v[m]

# Backsubtraction
```

Example 6.1: II

```
x=empty(N,float)
for m in range(N-1,-1,-1):
    x[m]=v[m]
    for i in range(m+1,N):
        x[m]-=A[m,i]*x[i]

print(x)
```

Pivoting I

Now let's consider the equations:

$$\begin{pmatrix} 0 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}. \tag{23}$$

- Here the first element of the first row is zero!
- This causes a problem to apply Gauss-Jordan elimination.
  - Divide by zero is not allowed.

Pivoting II

Pivoting

Exchange rows:

$$\begin{pmatrix} 3 & 4 & -1 & -1 \\ 0 & 1 & 4 & 1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 3 \\ -4 \\ 9 \\ 7 \end{pmatrix}. \tag{24}$$

Partial Pivoting

With partial pivoting, we consider rearranging the rows at each stage.

- When we get to the mth row, we compare it to all lower rows, looking at the value each row has in its mth elements and finding the one such value that is the farthest from zero–either positive or negative.
- If the row containing this winning value is not currently mth row, then we move it up to mth place by swapping it with the current mth row.

Example–Exercise6.2 I

Solve Eq. (23) using Gauss-Jordan elimination with partial pivoting.

```
from numpy import array, empty

A=array([[0,1,4,1],
    [3,4,-1,-1],
    [1,-4,1,5],
    [2,-2,1,3]],float)

v=array([-4,3,9,7],float)
N=len(v)

# Gaussian Elimination
for m in range(N):
    # Applying partial pivoting
    pivot_max=abs(A[m,m])
    pivot_point=m
    for i in range(m+1,N):
        pivot_tmp=abs(A[i,m])
        if pivot_tmp>pivot_max:
            pivot_point,pivot_max=i,pivot_tmp
    if m!=pivot_point:
        for i in range(N):
            A[m,i],A[pivot_point,i]=A[pivot_point,i],A[m,i]
        v[m],v[pivot_point]=v[pivot_point],v[m]
```

Example–Exercise6.2 II

```
    print(A)
    input()
    # Divide by the diagonal element
    div=A[m,m]
    A[m,:]/=div
    v[m]/=div

    # Subtract fro the lower rows
    for i in range(m+1,N):
        mult=A[i,m]
        A[i,:]-=mult*A[m,:]
        v[i]-=mult*v[m]

# Backsubtraction
x=empty(N,float)
for m in range(N-1,-1,-1):
    x[m]=v[m]
    for i in range(m+1,N):
        x[m]-=A[m,i]*x[i]

print(x)
```

Gauss-Jordan Elimination in Matrix Form I

- Basically based on the Gauss-Jordan elimination method.
- Powerful when we have to solve many different sets of equations $\mathbf{A}\mathbf{x} = \mathbf{v}$ with the same matrix $\mathbf{A}$ but different right-hand sides $\mathbf{v}$.
    - Repeating Gauss-Jordan elimination would be time-consuming.

Suppose we have a 4×4 matrix

$$\mathbf{A} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix} \tag{25}$$

The Gauss-Jordan elimination is written as a matrix form:
Step 1:

$$\frac{1}{a_{00}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a_{10} & a_{00} & 0 & 0 \\ -a_{20} & 0 & a_{00} & 0 \\ -a_{30} & 0 & 0 & a_{00} \end{pmatrix} \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} 1 & b_{01} & b_{02} & b_{03} \\ 0 & b_{11} & b_{12} & b_{13} \\ 0 & b_{21} & b_{22} & b_{23} \\ 0 & b_{31} & b_{32} & b_{33} \end{pmatrix} \tag{26}$$

Gauss-Jordan Elimination in Matrix Form II

Define a *lower triangular* matrix $\mathbf{L}_0$ as

$$\mathbf{L}_0 = \frac{1}{a_{00}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a_{10} & a_{00} & 0 & 0 \\ -a_{20} & 0 & a_{00} & 0 \\ -a_{30} & 0 & 0 & a_{00} \end{pmatrix} \tag{27}$$

Step 2:

$$\frac{1}{b_{11}} \begin{pmatrix} b_{11} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -b_{21} & b_{11} & 0 \\ 0 & -b_{31} & 0 & b_{11} \end{pmatrix} \begin{pmatrix} 1 & b_{01} & b_{02} & b_{03} \\ 0 & b_{11} & b_{12} & b_{13} \\ 0 & b_{21} & b_{22} & b_{23} \\ 0 & b_{31} & b_{32} & b_{33} \end{pmatrix} = \begin{pmatrix} 1 & c_{01} & c_{02} & c_{03} \\ 0 & 1 & c_{12} & c_{13} \\ 0 & 0 & c_{22} & c_{23} \\ 0 & 0 & c_{32} & c_{33} \end{pmatrix} \tag{28}$$

Define another lower triangular matrix $\mathbf{L}_1$ as

$$\mathbf{L}_1 = \frac{1}{b_{11}} \begin{pmatrix} b_{11} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -b_{21} & b_{11} & 0 \\ 0 & -b_{31} & 0 & b_{11} \end{pmatrix} \tag{29}$$

Gauss-Jordan Elimination in Matrix Form III

Step 3:

$$\frac{1}{c_{22}}\begin{pmatrix} c_{22} & 0 & 0 & 0 \\ 0 & c_{22} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -c_{32} & c_{22} \end{pmatrix}\begin{pmatrix} 1 & c_{01} & c_{02} & c_{03} \\ 0 & 1 & c_{12} & c_{13} \\ 0 & 0 & c_{22} & c_{23} \\ 0 & 0 & c_{32} & c_{33} \end{pmatrix} = \begin{pmatrix} 1 & d_{01} & d_{02} & d_{03} \\ 0 & 1 & d_{12} & d_{13} \\ 0 & 0 & 1 & d_{23} \\ 0 & 0 & 0 & d_{33} \end{pmatrix} \tag{30}$$

And define $\mathbf{L}_2$ as

$$\mathbf{L}_2 = \frac{1}{c_{22}}\begin{pmatrix} c_{22} & 0 & 0 & 0 \\ 0 & c_{22} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -c_{32} & c_{22} \end{pmatrix} \tag{31}$$

Step 4:

$$\frac{1}{d_{33}}\begin{pmatrix} d_{33} & 0 & 0 & 0 \\ 0 & d_{33} & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & d_{01} & d_{02} & d_{03} \\ 0 & 1 & d_{12} & d_{13} \\ 0 & 0 & 1 & d_{23} \\ 0 & 0 & 0 & d_{33} \end{pmatrix} = \begin{pmatrix} 1 & u_{01} & u_{02} & u_{03} \\ 0 & 1 & u_{12} & u_{13} \\ 0 & 0 & 1 & u_{23} \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{32}$$

Gauss-Jordan Elimination in Matrix Form IV

Define $\mathbf{L}_3$ as

$$\mathbf{L}_3 = \frac{1}{d_{33}} \begin{pmatrix} d_{33} & 0 & 0 & 0 \\ 0 & d_{33} & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{33}$$

Step 1-Step 4 are mathematically written as

$$\mathbf{L}_3\mathbf{L}_2\mathbf{L}_1\mathbf{L}_0\mathbf{A}$$

Therefore, we solve our original set of equations $\mathbf{A}\mathbf{x} = \mathbf{v}$ by multiplying $\mathbf{L}_3\mathbf{L}_2\mathbf{L}_1\mathbf{L}_0$ as

$$\mathbf{L}_3\mathbf{L}_2\mathbf{L}_1\mathbf{L}_0\mathbf{A}\mathbf{x} = \mathbf{L}_3\mathbf{L}_2\mathbf{L}_1\mathbf{L}_0\mathbf{v} \tag{34}$$

Then apply the backsubstitution.

LU Decomposition I

In practice, we don't need to have all four matrix $\mathbf{L}_0$, $\mathbf{L}_1$ $\mathbf{L}_2$, and $\mathbf{L}_3$.

- Define two matrices:

$$\mathbf{L} = \mathbf{L}_0^{-1}\mathbf{L}_1^{-1}\mathbf{L}_2^{-1}\mathbf{L}_3^{-1}, \qquad \mathbf{U} = \mathbf{L}_3\mathbf{L}_2\mathbf{L}_1\mathbf{L}_0\mathbf{A} \tag{35}$$

- Note that $\mathbf{U}$ is the upper triangular matrix (right-hand side of Eq. (32)).
- Multiplying $\mathbf{L}$ and $\mathbf{U}$ gives

$$\mathbf{LU} = \mathbf{A} \tag{36}$$

- Form the original set of equations, $\mathbf{Ax} = \mathbf{v}$,

$$\mathbf{LUx} = \mathbf{v} \tag{37}$$

- Note that $\mathbf{L}$ is lower triangular matrix.

LU Decomposition II

- Consider the matrix $\mathbf{L}_0$ for example:

$$\mathbf{L}_0 = \frac{1}{a_{00}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a_{10} & a_{00} & 0 & 0 \\ -a_{20} & 0 & a_{00} & 0 \\ -a_{30} & 0 & 0 & a_{00} \end{pmatrix} \tag{38}$$

- Inverse of $\mathbf{L}_0$ is

$$\mathbf{L}_0^{-1} = \begin{pmatrix} a_{00} & 0 & 0 & 0 \\ a_{10} & 1 & 0 & 0 \\ a_{20} & 0 & 1 & 0 \\ a_{30} & 0 & 0 & 1 \end{pmatrix}. \tag{39}$$

It can be easily verified by showing $\mathbf{L}_0\mathbf{L}_0^{-1} = \mathbf{I}$, where $\mathbf{I}$ is an identity matrix (or more precisely see Boas's book).

LU Decomposition III

- Similarly,

$$\mathbf{L}_1^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b_{11} & 0 & 0 \\ 0 & b_{21} & 1 & 0 \\ 0 & b_{31} & 0 & 1 \end{pmatrix} \quad \mathbf{L}_2^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_{22} & 0 \\ 0 & 0 & c_{32} & 1 \end{pmatrix} \quad \mathbf{L}_c^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & d_{33} \end{pmatrix}$$

- Multiplying them all together:

$$\mathbf{L} = \mathbf{L}_0^{-1}\mathbf{L}_1^{-1}\mathbf{L}_2^{-1}\mathbf{L}_3^{-1} = \begin{pmatrix} a_{00} & 0 & 0 & 0 \\ a_{10} & b_{11} & 0 & 0 \\ a_{20} & b_{21} & c_{22} & 0 \\ a_{30} & b_{31} & c_{32} & d_{33} \end{pmatrix} \tag{41}$$

- Not only is $\mathbf{L}$ is lower triangular, but its elements are easily obtained through Gauss-Jordan elimination.

LU Decomposition-Backsubtraction I

To find a rule for backsubstitution, let's consider a 3×3 matrix $\mathbf{A}$.

- The LU decomposition of $\mathbf{A}$ looks like:

$$\mathbf{A} = \begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} l_{00} & 0 & 0 \\ l_{10} & l_{11} & 0 \\ l_{20} & l_{21} & l_{22} \end{pmatrix} \begin{pmatrix} u_{00} & u_{01} & u_{02} \\ 0 & u_{11} & u_{12} \\ 0 & 0 & u_{22} \end{pmatrix}. \tag{42}$$

- Then the linear equations $\mathbf{A}\mathbf{x} = \mathbf{v}$ becomes

$$\begin{pmatrix} l_{00} & 0 & 0 \\ l_{10} & l_{11} & 0 \\ l_{20} & l_{21} & l_{22} \end{pmatrix} \begin{pmatrix} u_{00} & u_{01} & u_{02} \\ 0 & u_{11} & u_{12} \\ 0 & 0 & u_{22} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \end{pmatrix}. \tag{43}$$

- Define a new vector $\mathbf{y}$ as

$$\begin{pmatrix} u_{00} & u_{01} & u_{02} \\ 0 & u_{11} & u_{12} \\ 0 & 0 & u_{22} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \end{pmatrix}. \tag{44}$$

LU Decomposition-Backsubtraction II

- Then Eq. (43) becomes

$$\begin{pmatrix} l_{00} & 0 & 0 \\ l_{10} & l_{11} & 0 \\ l_{20} & l_{21} & l_{22} \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \end{pmatrix}. \tag{45}$$

- From the first line of Eq. (45), $l_{00}y_0 = v_0$. Thus

$$y_0 = \frac{v_0}{l_{00}}. \tag{46}$$

- From the second line of Eq. (45), $l_{10}y_0 + l_{11}y_1 = v_1$, or

$$y_1 = \frac{v_1 - l_{10}y_0}{l_{11}}. \tag{47}$$

- From the third line of Eq. (45) gives

$$y_2 = \frac{v_2 - l_{20}y_0 - l_{21}y_1}{l_{22}}. \tag{48}$$

LU Decomposition-Backsubtraction III

General Representation of $\mathbf{y}$

$$y_i = \frac{v_i - \sum_{j=0}^{i-1} l_{ij} y_j}{l_{ii}}. \tag{49}$$

- Applying partial pivoting is also trivial.

However, the simplest way to implement LU decomposition and backsubstitution is to use the `solve` function in `numpy.linalg` package like this:

```
from numpy.linalg import solve
x=solve(A,v)
```

LU Decomposition: Example I

Solve Eq. (23) using LU decomposition with partial pivoting.

```
from numpy import array,zeros, empty,copy,dot
from numpy.linalg import solve

A=array([[0,1,4,1],
    [3,4,-1,-1],
    [1,-4,1,5],
    [2,-2,1,3]],float)
v=array([-4,3,9,7],float)
N=len(v)
L=zeros([N,N],float)
U=empty([N,N],float)
U=copy(A)
print("A=",A)
print("U=",U)


# Gaussian Elimination with LU decomposition
for m in range(N):
    # Applying partial pivoting
    pivot_max=abs(U[m,m])
    pivot_point=m
    for i in range(m+1,N):
        pivot_tmp=abs(U[i,m])
        if pivot_tmp>pivot_max:
```

LU Decomposition: Example II

```
            pivot_point,pivot_max=i,pivot_tmp
    if m!=pivot_point:
        for i in range(N):
            U[m,i],U[pivot_point,i]=U[pivot_point,i],U[m,i]
            L[m,i],L[pivot_point,i]=L[pivot_point,i],L[m,i]
            A[m,i],A[pivot_point,i]=A[pivot_point,i],A[m,i]
        v[m],v[pivot_point]=v[pivot_point],v[m]

    L[m:,m]=U[m:,m]

    # Divide by the diagonal element
    div=U[m,m]
    U[m,:]/=div

    # Subtract from the lower rows
    for i in range(m+1,N):
        mult=U[i,m]
        U[i,:]-=mult*U[m,:]

print()
print("After GE with LUD")
print("U=",U)
print()
print("L=",L)
print()
```

LU Decomposition: Example III

```
print("A=",A)
print()
print("LU=",dot(L,U))

# Backsubtraction
y=empty(N,float)
for m in range(N):
    y[m]=v[m]
    for i in range(m):
        y[m]-=L[m,i]*y[i]
    y[m]/=L[m,m]

x=empty(N,float)
for m in range(N-1,-1,-1):
    x[m]=y[m]
    for i in range(m+1,N):
        x[m]-=U[m,i]*x[i]
    x[m]/=U[m,m]
print("\n")
print("x=",x)
print("solve(A,v)=",solve(A,v))
```

Calculating the Inverse of a Matrix I

Inverse of matrix:

$$\mathbf{A}^{-1} = \frac{1}{\det \mathbf{A}} \mathbf{C}^{T} \tag{50}$$

where C_{ij} is cofactor of a_{ij} (see the mathematical physics textbook).

- But calculating the determinants are time consuming and prone to make large error.
- Apply the method to solve simultaneous linear equations.
- Consider a form

$$\mathbf{A}\mathbf{X} = \mathbf{V}. \tag{51}$$

- Now, $\mathbf{X}$ and $\mathbf{V}$ are $N \times N$ matrix as well as $\mathbf{A}$.
- If $\mathbf{V} = \mathbf{I}$, then $\mathbf{X}$ is the inverse matrix of $\mathbf{A}$.

Calculating the Inverse of a Matrix II

Calculating the Inverse of a Matrix

Now we have to solve a set of N simultaneous linear equations:

$$\mathbf{A}\mathbf{X}_j = \mathbf{V}_j, \tag{52}$$

where $j = 0, 1, \cdots, N-1$.

- $\mathbf{X}_j$ is the jth column of matrix $\mathbf{X}$.
- $\mathbf{V}_j$ is the jth column of matrix $\mathbf{V}$.
- We set $\mathbf{V} = \mathbf{I}$.
- Then we can apply the Gauss-Jordan elimination or LU decomposition method for each column vector $\mathbf{X}_j$ and $\mathbf{V}_j$.
- By combining $\mathbf{X}_j$'s we can obtain $\mathbf{X} = \mathbf{A}^{-1}$.

Of course we can also use `inv` function in `numpy.linalg` package as:

```
from numpy.linalg import inv
X=inv(A)
```

Inverse Matrix: Example I

Find $\mathbf{A}^{-1}$ in Eq. (23) using LU decomposition with partial pivoting.

```
from numpy import array,zeros,empty,copy,dot
from numpy.linalg import inv

A=array([[0,1,4,1],
     [3,4,-1,-1],
     [1,-4,1,5],
     [2,-2,1,3]],float)
n=A.shape
N=n[1]
L=zeros([N,N],float)
U=empty([N,N],float)
U=copy(A)
V=zeros([N,N],float)
for m in range(N):
    V[m,m]=1.0

print("A=",A)
print("U=",U)
print("V=",V)
print("inv(A)=",inv(A))    # for comparison

# Gaussian Elimination with LU decomposition
for m in range(N):
    # Applying partial pivoting
```

Inverse Matrix: Example II

```
    pivot_max=abs(U[m,m])
    pivot_point=m
    for i in range(m+1,N):
        pivot_tmp=abs(U[i,m])
        if pivot_tmp>pivot_max:
            pivot_point,pivot_max=i,pivot_tmp
    if m!=pivot_point:
        for i in range(N):
            U[m,i],U[pivot_point,i]=U[pivot_point,i],U[m,i]
            L[m,i],L[pivot_point,i]=L[pivot_point,i],L[m,i]
            A[m,i],A[pivot_point,i]=A[pivot_point,i],A[m,i]
            V[m,i],V[pivot_point,i]=V[pivot_point,i],V[m,i]

    L[m:,m]=U[m:,m]

    # Divide by the diagonal element
    div=U[m,m]
    U[m,:]/=div

    # Subtract from the lower rows
    for i in range(m+1,N):
        mult=U[i,m]
        U[i,:]-=mult*U[m,:]

# Now we have L and U
```

Inverse Matrix: Example III

```
Y=empty([N,N],float)
for j in range(N):        # for each column
    for m in range(N):          # for each row
        Y[m,j]=V[m,j]
        for i in range(m):
            Y[m,j]-=L[m,i]*Y[i,j]
        Y[m,j]/=L[m,m]

X=empty([N,N],float)
for j in range(N):
    for m in range(N-1,-1,-1):
        X[m,j]=Y[m,j]
        for i in range(m+1,N):
            X[m,j]-=U[m,i]*X[i,j]
        X[m,j]/=U[m,m]

print("\n")
print("X=",X)
```

Tridiagonal Matrices: Trigonal Matrix Algorithm or Thomas Algorithm

A special case that arise often in physics problems is the solution of $\mathbf{A}\mathbf{x} = \mathbf{v}$ when the matrix $\mathbf{A}$ is tridiagonal:

$$\mathbf{A} = \begin{pmatrix} a_{00} & a_{01} & 0 & 0 & 0 \\ a_{10} & a_{11} & a_{12} & 0 & 0 \\ 0 & a_{21} & a_{22} & a_{23} & 0 \\ 0 & 0 & a_{32} & a_{33} & a_{34} \\ 0 & 0 & 0 & a_{43} & a_{44} \end{pmatrix}. \tag{53}$$

- The matrix has nonzero elements only along the diagonal and immediately above and below it.
- Simple Gauss-Jordan elimination is a good choice for solving the problem.
  - Quick
  - pivoting is typically not used
    - Thus, the programming is straightforward.
  - We do not need to go through the entire Gauss-Jordan elimination process.
    - Each row only need to be subtracted from the single row immediately below it – and not all lower rows – to make the matrix triangular.

Illustration: How to Make the Matrix Triangular I

Consider a 4×4 matrix:

$$\mathbf{A} = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 3 & 4 & -5 & 0 \\ 0 & -4 & 3 & 5 \\ 0 & 0 & 1 & 3 \end{pmatrix} \tag{54}$$

1. Step 1: Divide the first row by 2, then subtract 3 times the result from the second row:

$$\begin{pmatrix} 1 & 0.5 & 0 & 0 \\ 0 & 2.5 & -5 & 0 \\ 0 & -4 & 3 & 5 \\ 0 & 0 & 1 & 3 \end{pmatrix} \tag{55}$$

Illustration: How to Make the Matrix Triangular II

2. Step 2: Divide the second row by 2.5 and subtract -4 times the result from the third row:

$$\begin{pmatrix} 1 & 0.5 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & -5 & 5 \\ 0 & 0 & 1 & 3 \end{pmatrix} \tag{56}$$

3. Step:3 Divide the third row by -5 and subtract it from the fourth row:

$$\begin{pmatrix} 1 & 0.5 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 4 \end{pmatrix} \tag{57}$$

Illustration: How to Make the Matrix Triangular III

4. Step 4: Divide the fourth row by 4 ,then we obtain upper triangular matrix:

$$\begin{pmatrix} 1 & 0.5 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{58}$$

- Note that **green** colored elements are not changed when subtracting some constant multiple of the above row.
- Use this fact to reduce the computing time.

Illustration: Backsubstitution I

The matrix form after the Gauss-Jordan elimination:

$$\begin{pmatrix} 1 & a_{01} & 0 & 0 \\ 0 & 1 & a_{12} & 0 \\ 0 & 0 & 1 & a_{23} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ v_3 \end{pmatrix}. \tag{59}$$

Solution:

$$x_3 = v_3 \tag{60}$$
$$x_2 = v_2 - a_{23}x_3 \tag{61}$$
$$x_1 = v_1 - a_{12}x_2 \tag{62}$$
$$x_0 = v_0 - a_{01}x_1. \tag{63}$$

This algorithm is known as trigonal matrix algorithm or Thomas algorithm.

- Note that the **cyan** colored elements do not work anything in the .
- They just become 0.
  - Just keep in mind this and never use the **cyan** colored elements during the back substitution to reduce computing time.

Banded Matrix

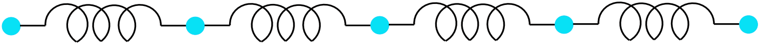
The matrix $\mathbf{A}$ is banded, if it is similar to a trigonal matrix but can have more than one nonzero elements to either side of the diagonal, like this:

$$\mathbf{A} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & 0 & 0 & 0 & 0 \\ a_{10} & a_{11} & a_{12} & a_{13} & 0 & 0 & 0 \\ a_{20} & a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 \\ 0 & a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & 0 \\ 0 & 0 & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ 0 & 0 & 0 & a_{53} & a_{54} & a_{55} & a_{56} \\ 0 & 0 & 0 & 0 & a_{64} & a_{65} & a_{66} \end{pmatrix} \tag{64}$$

- The method to solve such equation is also similar to that for triangular matrix.
- But the backsubstitution is more complicated.
  - Such complication makes the calculation little bit slower than that for triangular matrix.
  - But still be faster than the general algorithm such as `solve` in `numpy.linalg` package.

Example 6.2: Vibration in a One-Dimensional System I

Suppose we have a set of N identical masses in a row, joined by identical linear spring as:



We ignore gravity for simplicity.

- Let ζ_i be the displacement of the ith mass relative to its equilibrium position.
- Newton's equation:

$$m\frac{d^2\zeta_i}{dt^2} = k(\zeta_{i+1} - \zeta_i) + k(\zeta_{i-1} - \zeta_i) + F_i, \tag{65}$$

  where m is the mass and k is the spring constant.
- F_i represents any external force acting on mass i.

Example 6.2: Vibration in a One-Dimensional System II

- The masses at the two ends:

$$m\frac{d^2\zeta_1}{dt^2} = k(\zeta_2 - \zeta_1) + F_1, \tag{66}$$

$$m\frac{d^2\zeta_N}{dt^2} = k(\zeta_{N-1} - \zeta_N) + F_N, \tag{67}$$

- Assume that $F_1 = Ce^{i\omega t}$ and $F_i = 0$ for all $i > 1$.
- By assuming that the solution $\zeta_i = x_i e^{i\omega t}$ we obtain the N-coupled linear equations:

$$\begin{aligned} -m\omega^2 x_1 &= k(x_2 - x_1) + C, &(68)\\ -m\omega^2 x_i &= k(x_{i+1} - x_i) + k(x_{i-1} - x_i), &(69)\\ -m\omega^2 x_N &= k(x_{N-1} - x_N), &(70) \end{aligned}$$

where i is in the range $2 \le i \le N - 1$.

Example 6.2: Vibration in a One-Dimensional System III

- Rearrange Eqs. (68)-(70):

$$\begin{aligned} (\alpha - k)x_1 - kx_2 &= C, & (71)\\ \alpha x_i - k_{i-1} - kx_{i+1} &= 0, & (72)\\ (\alpha - k)x_N - kx_{N-1} &= 0, & (73) \end{aligned}$$

  where $\alpha = 2k - m\omega^2$.

- In matrix form:

$$\begin{pmatrix} (\alpha-k) & -k & & & & \\ -k & \alpha & -k & & & \\ & -k & \alpha & -k & & \\ & & \ddots & \ddots & \ddots & \\ & & & -k & \alpha & -k \\ & & & & -k & (\alpha-k) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix} = \begin{pmatrix} C \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}. \quad (74)$$

Solve Eq. (74) with $m = 1$, $k = 6$, and $\omega = 2$.

Example 6-2: Solution I

Direct transform of Step1-Step5:

```
from numpy import zeros, empty
from pylab import plot, show
from numpy.linalg import solve

# Constants
N=26
C=1.0
m=1.0
k=6.0
omega=2.0
alpha=2*k-m*omega**2

# Set up the initial values of the array
A=zeros([N,N],float)
for i in range(N-1):
    A[i,i]=alpha
    A[i,i+1]=-k
    A[i+1,i]=-k

A[0,0]-=k
A[N-1,N-1]=alpha-k

v=zeros(N,float)
v[0]=C
```

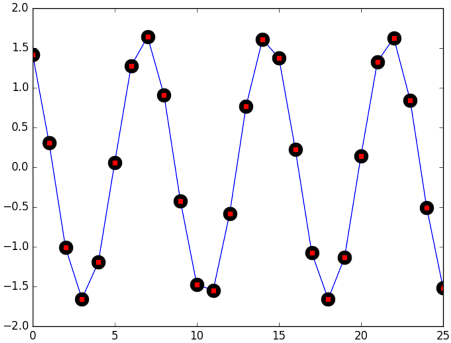
Example 6-2: Solution II

```
# To compare the results with numpy.linalg
xx=solve(A,v)

# Peform The Gauss-Jordan Elimination
for i in range(N-1):
  # Divide row i by its diagonal element
  div=A[i,i]
  A[i,i+1]/=div
  v[i]/=div

  # Now subtract it from the next row down
  if i==N-2:
    n=2
  else:
    n=3
  a_tmp=A[i+1,i]
  for j in range(n):
    A[i+1,i+j]-=A[i,i+j]*a_tmp
  v[i+1]-=a_tmp*v[i]

# Divide the last element of v by the last diagonal element
v[N-1]/=A[N-1,N-1]

# Backsubstitution
```

Example 6-2: Solution III

```
x=empty(N, float)
x[N-1]=v[N-1]
for i in range(N-2,-1,-1):
    x[i]=v[i]-A[i,i+1]*x[i+1]

# Plot the results
plot(x)
plot(x,"ko",ms=15.0)
plot(xx,"rs")
show()
```

Example 6-2: Solution IV



Example 6-2: Modified Version I

Applying the cyan and red colored parts:

```
from numpy import zeros, empty
from pylab import plot, show
from numpy.linalg import solve

# Constants
N=26
C=1.0
m=1.0
k=6.0
omega=2.0
alpha=2*k-m*omega**2

# Set up the initial values of the array
A=zeros([N,N],float)
for i in range(N-1):
  A[i,i]=alpha
  A[i,i+1]=-k
  A[i+1,i]=-k

A[0,0]-=k
A[N-1,N-1]=alpha-k

v=zeros(N,float)
v[0]=C
```

Example 6-2: Modified Version II

```
xx=solve(A,v)

# Peform The Gauss-Jordan Elimination
for i in range(N-1):
  # Divide row i by its diagonal element
  A[i,i+1]/=A[i,i]
  v[i]/=A[i,i]

  # Now subtract it from the next row down
  A[i+1,i+1]-=A[i+1,i]*A[i,i+1]
  v[i+1]-=A[i+1,i]*v[i]

# Divide the last element of v by the last diagonal element
v[N-1]/=A[N-1,N-1]

# Backsubstitution
x=empty(N,float)
x[N-1]=v[N-1]
for i in range(N-2,-1,-1):
  x[i]=v[i]-A[i,i+1]*x[i+1]

# Plot the results
plot(x)
plot(x,"ko")
```

Example 6-2: Modified Version III

```
plot(xx,"rs")
show()
```

Eigenvalues and Eigenvectors

- Eigenvalue problems are common in physics.
  - Mechanics
  - Electromagnetism
  - Quantum mechanics
  - etc.
- Most eigenvalue problems in physics concern real symmetric matrix or Hermitian matrix when complex numbers are involved.
- Focus on a real symmetric matrix $\mathbf{A}$.
- The eigenvector $\mathbf{v}$ satisfies:

  $$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}, \tag{75}$$

  where λ is the corresponding eigenvalue.
- For $N \times N$ matrix, there are N eigenvectors, $\mathbf{v}_1$, $\mathbf{v}_2$, $\cdots$, $\mathbf{v}_N$ with eigenvalues λ_1. λ_2, $\cdots$, λ_N.
- Eigenvectors for symmetric matrix are orthogonal and we will assume they are normalized, i.e., $\mathbf{v}_i \cdot \mathbf{v}_j = \delta_{ij}$. Here δ_{ij} is Kronecker delta.

QR Decomposition

- Let $\mathbf{V}$ be an $N \times N$ matrix whose ith column corresponds to the ith eigenvector $\mathbf{v}_i$.
- In a matrix form Eq. (75) can be written as

$$\mathbf{AV} = \mathbf{VD}, \tag{76}$$

where $\mathbf{D}$ is the diagonal matrix with the eigenvalues λ_i as its diagonal entries.

- Note that the matrix $\mathbf{V}$ is orthogonal, thus $\mathbf{V}^T = \mathbf{V}^{-1}$, so $\mathbf{V}^T\mathbf{V} = \mathbf{V}\mathbf{V}^T = \mathbf{I}$.

QR Decomposition

- Like the LU decomposition, rewrite the matrix $\mathbf{A}$ as the product $\mathbf{QR}$, i.e.,

$$\mathbf{A} = \mathbf{QR} \tag{77}$$

- $\mathbf{Q}$: an orthogonal matrix
- $\mathbf{R}$: upper-triangular matrix

Mathematics on QR Decomposition I

- Suppose we have some way to calculate the matrices $\mathbf{Q}$ and $\mathbf{R}$.
- Let $\mathbf{A}$ be a real symmetric matrix then $\mathbf{A}$ can be written as:

$$\mathbf{A} = \mathbf{Q}_1\mathbf{R}_1 \tag{78}$$

- Multiplying on the left by $\mathbf{Q}^T$, we get

$$\mathbf{Q}_1^T\mathbf{A} = \mathbf{Q}_1^T\mathbf{Q}_1\mathbf{R}_1 = \mathbf{R}_1, \tag{79}$$

  where we use the fact that $\mathbf{Q}_1$ is orthogonal.
- Let us define a new matrix

$$\mathbf{A}_1 = \mathbf{R}_1\mathbf{Q}_1. \tag{80}$$

- Combining Eqs. (79) and (80), we have

$$\mathbf{A}_1 = \mathbf{Q}_1^T\mathbf{A}\mathbf{Q}_1. \tag{81}$$

- Decompose $\mathbf{A}_1$ as $\mathbf{A}_1 = \mathbf{Q}_2\mathbf{R}_2$, then $\mathbf{R}_2 = \mathbf{Q}_2^T\mathbf{A}_1$.

Mathematics on QR Decomposition II

- Define a new matrix $\mathbf{A}_2$ as

$$\mathbf{A}_2 = \mathbf{R}_2\mathbf{Q}_2 = \mathbf{Q}_2^T\mathbf{A}_1\mathbf{Q}_2 = \mathbf{Q}_2^T\mathbf{Q}_1^T\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2 \qquad (82)$$

- Repeat the process up to total k steps then

$$\begin{aligned}
\mathbf{A}_1 &= \mathbf{Q}_1^T\mathbf{A}\mathbf{Q}_1, && (83)\\
\mathbf{A}_2 &= \mathbf{Q}_2^T\mathbf{Q}_1^T\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2, && (84)\\
\mathbf{A}_3 &= \mathbf{Q}_3^T\mathbf{Q}_2^T\mathbf{Q}_1^T\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2\mathbf{Q}_3, && (85)\\
&\vdots && (86)\\
\mathbf{A}_k &= (\mathbf{Q}_k^T\cdots\mathbf{Q}_1^T)\mathbf{A}(\mathbf{Q}_1\cdots\mathbf{Q}_k). && (87)
\end{aligned}$$

- As one continue this process long enought, the matrkx $\mathbf{A}_k$ become diagonal.
  - The off-diagonal elements get smaller and smaller the more iterations of the process on do until they eventually reach zero– or as close to zero as makes no difference.
  - With given accuracy we can obtain diagonalized matrix $\mathbf{A}_k$.

Mathematics on QR Decomposition III

- The matrix $\mathbf{A}_k$ approximates a diagonal matrix $\mathbf{D}$ in Eq. (76)

- Let us define the additional matrix:

$$\mathbf{V} = \mathbf{Q}_1\mathbf{Q}_2\cdots\mathbf{Q}_k = \prod_{i=1}^{k}\mathbf{Q}_i \tag{88}$$

- Then from Eq. (87) we have

$$\mathbf{D} = \mathbf{A}_k = \mathbf{V}^T\mathbf{A}\mathbf{V}. \tag{89}$$

- Multiplying on the left by $\mathbf{V}$:

$$\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{D}, \tag{90}$$

which is exactly the same form of Eq. (76).

Algorithm for QR Decomposition

QR Decomposition

1. Create an $N \times N$ matrix $\mathbf{V}$ to hold the eigenvectors.
2. Initialize $\mathbf{V}$ to be equal to the identity matrix $\mathbf{I}$.
3. Choose a target accuracy ϵ for off-diagonal elements of the eigenvalue matrix.
4. Calculate the QR decomposition $\mathbf{A} = \mathbf{QR}$.
5. Update $\mathbf{A}$ to the new value $\mathbf{A} = \mathbf{RQ}$.
6. Multiply $\mathbf{V}$ on the right by $\mathbf{Q}$.
7. Check the off-diagonal elements of $\mathbf{A}$. If they are all less than ϵ, we are done. Otherwise go back to step 4.

In `numpy.linalg` package, `eigh()` and `eigvalsh()` functions are also available for the general purpose.

How to Calculate $\mathbf{Q}$ and $\mathbf{R}$ I

Given $N \times N$ matrix $\mathbf{A}$ we can compute the QR decomposition as follows:

- Let us think of the matrix as a set of N column vectors $\mathbf{a}_0, \mathbf{a}_1, \cdots, \mathbf{a}_{N-1}$.

$$\mathbf{A} = \begin{pmatrix} | & | & | & \cdots \\ \mathbf{a}_0 & \mathbf{a}_1 & \mathbf{a}_2 & \cdots \\ | & | & | & \cdots \end{pmatrix}. \tag{91}$$

- Define two new set of vectors $\mathbf{u}_0, \cdots, \mathbf{u}_{N-1}$ and $\mathbf{q}_0, \cdots, \mathbf{q}_{N-1}$ as follows (Gram-Schmidt Orthogonalization):

$$\begin{aligned} \mathbf{u}_0 &= \mathbf{a}_0, & \mathbf{q}_0 &= \frac{\mathbf{u}_0}{|\mathbf{u}_0|} \\ \mathbf{u}_1 &= \mathbf{a}_1 - (\mathbf{q}_0 \cdot \mathbf{a}_1)\mathbf{q}_0, & \mathbf{q}_1 &= \frac{\mathbf{u}_1}{|\mathbf{u}_1|} \\ \mathbf{u}_2 &= \mathbf{a}_2 - (\mathbf{q}_0 \cdot \mathbf{a}_2)\mathbf{q}_0 - (\mathbf{q}_1 \cdot \mathbf{a}_2)\mathbf{q}_1, & \mathbf{q}_2 &= \frac{\mathbf{u}_2}{|\mathbf{u}_2|} \end{aligned}$$

and so forth.

How to Calculate $\mathbf{Q}$ and $\mathbf{R}$ II

- General form:

$$\mathbf{u}_i = \mathbf{a}_i - \sum_{j=0}^{i-1} (\mathbf{q}_j \cdot \mathbf{a}_i)\mathbf{q}_j, \qquad \mathbf{q}_i = \frac{\mathbf{u}_i}{|\mathbf{u}_i|}$$

- Then $\mathbf{A}$ becomes:

$$\mathbf{A} = \begin{pmatrix} | & | & | & \cdots \\ \mathbf{a}_0 & \mathbf{a}_1 & \mathbf{a}_2 & \cdots \\ | & | & | & \cdots \end{pmatrix} = \begin{pmatrix} | & | & | & \cdots \\ \mathbf{q}_0 & \mathbf{q}_1 & \mathbf{q}_2 & \cdots \\ | & | & | & \cdots \end{pmatrix} \begin{pmatrix} |\mathbf{u}_0| & \mathbf{q}_0 \cdot \mathbf{a}_1 & \mathbf{q}_0 \cdot \mathbf{a}_2 & \cdots \\ 0 & |\mathbf{u}_1| & \mathbf{q}_1 \cdot \mathbf{a}_2 & \cdots \\ 0 & 0 & |\mathbf{u}_2| & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

- The resulting $\mathbf{Q}$ and $\mathbf{R}$ have the form:

$$\mathbf{Q} = \begin{pmatrix} | & | & | & \cdots \\ \mathbf{q}_0 & \mathbf{q}_1 & \mathbf{q}_2 & \cdots \\ | & | & | & \cdots \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} |\mathbf{u}_0| & \mathbf{q}_0 \cdot \mathbf{a}_1 & \mathbf{q}_0 \cdot \mathbf{a}_2 & \cdots \\ 0 & |\mathbf{u}_1| & \mathbf{q}_1 \cdot \mathbf{a}_2 & \cdots \\ 0 & 0 & |\mathbf{u}_2| & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Example I

Find the eigenvalues and eigenvectors of the square matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 4 & 8 & 4 \\ 4 & 2 & 3 & 7 \\ 8 & 3 & 6 & 9 \\ 4 & 7 & 9 & 2 \end{pmatrix}$$

```
import numpy as np
from numpy.linalg import eigh

A=np.array([[1,4,8,4],[4,2,3,7],[8,3,6,9],[4,7,9,2]],float)

#  Just for comparison
xx,VV=eigh(A)

print("==== Result using numpy.linalg ====")
print("xx=",xx)
print("VV=",VV)

# Implementation of QR decomposition
epsilon=1.0e-10
n=A.shape
```

Example II

```
N=n[1]

V=np.zeros([N,N],float)
U=np.empty([N,N],float)
Q=np.empty([N,N],float)
R=np.empty([N,N],float)
# Initialize V
for i in range(N):
  V[i,i]=1.0

delta=1.0
while delta>epsilon:
  for i in range(N):
    U[:,i]=A[:,i]
    if i>0:
      for j in range(i):
        U[:,i]-=(np.dot(Q[:,j],A[:,i])*Q[:,j])
    magU=np.dot(U[:,i],U[:,i])**(1/2)
    Q[:,i]=U[:,i]/magU

  # Computing R matrix
  for j in range(N):
    for k in range(N):
      if j>k:
        R[j,k]=0
```

Example III

```
      elif j==k:
        R[j,k]=np.dot(U[:,j],U[:,j])**(1/2)
      else:
        R[j,k]=np.dot(Q[:,j],A[:,k])

  #print("R=",R)
  A=np.dot(R,Q)
  V=np.dot(V,Q)
  delta=0.0
  for j in range(N):
    for k in range(N):
      if j<k:
        if delta<abs(A[j,k]):
          delta=abs(A[j,k])
  #print("delta=",delta)
  #input()
x=np.empty(N,float)
for i in range(N):
  x[i]=A[i,i]

print("\n=== Result obtained from my QR decomposition code ===")
print("x=",x)
print(V)
```