NUMERICAL RECIPES

Example Book (FORTRAN) Second Edition

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Preface

This Numerical Recipes Example Book (FORTRAN) is designed to accompany the text and reference book Numerical Recipes in FORTRAN: The Art of Scientific Computing, Second Edition, by William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery (Cambridge University Press, 1992). In that volume, the algorithms and methods of scientific computation are developed in considerable detail, starting with basic mathematical analysis and working through to actual implementation in the form of FORTRAN subroutines. The routines in Numerical Recipes in FORTRAN: The Art of Scientific Computing, numbering more than 300, are meant to be incorporated into user applications; they are subroutines (or functions), not stand-alone programs.

It often happens, when you want to incorporate somebody else's procedure into your own application program, that you first want to see the procedure demonstrated on a simple example. Prose descriptions of how to use a procedure (even those in Numerical Recipes) can occasionally be inexact. There is no substitute for an actual, FORTRAN demonstration program that shows exactly how data are fed to a procedure, how the procedure is called, and how its results are unloaded and interpreted.

Another not unusual case occurs when you have, for one seemingly good purpose or another, modified the source code in a "foreign" procedure. In such circumstances, you might well want to test the modified procedure on an example known previously to have worked correctly, before letting it loose on your own data. There is the related case where procedure source code may have become corrupted, e.g., lost some lines or characters in transmission from one machine to another, and a simple revalidation test is desirable.

These are the needs addressed by this Numerical Recipes Example Book. Divided into chapters identically with Numerical Recipes in FORTRAN: The Art of Scientific Computing, this book contains FORTRAN source programs that exercise and demonstrate all of the Numerical Recipes subroutines and functions. The programs are commented, and each is also prefaced by a short description of what it does, and of which Numerical Recipes routines it exercises. In many cases where the demonstration programs require input data, that data is also printed in this book. In some cases, where the demonstration programs are not "self-validating," sample output is also shown.

Necessarily, in the interests of clarity, the Numerical Recipes procedures and functions are demonstrated in simple ways. A consequence is that the demonstration programs in this book do not usually test all possible regimes of input data, or even all lines of procedure source code. The demonstration programs in this book were by no means the only validating tests that the Numerical Recipes procedures and functions

were required to pass during their development. The programs in this book were used during the later stages of the production of Numerical Recipes in FORTRAN: The Art of Scientific Computing to maintain integrity of the source code, and in this role were found to be invaluable.

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CONTENTS

	Preface
1.	Preliminaries
2.	Solution of Linear Algebraic Equations
3.	Interpolation and Extrapolation
4.	Integration of Functions
5.	Evaluation of Functions
6.	Special Functions
7.	Random Numbers
8.	Sorting
9.	Root Finding and Nonlinear Sets of Equations
10.	Minimization and Maximization of Functions
11.	Eigensystems
12.	Fast Fourier Transform
13.	Fourier and Spectral Applications
14.	Statistical Description of Data
15.	Modeling of Data
16.	Integration of Ordinary Differential Equations
17.	Two Point Boundary Value Problems
18.	Integral Equations and Inverse Theory
19.	Partial Differential Equations
20.	Less-Numerical Algorithms
	Index of Demonstrated Subroutines

Chapter 1: Preliminaries

The routines in Chapter 1 of Numerical Recipes are introductory and less general in purpose than those in the remainder of the book. This chapter's routines serve primarily to expose the book's notational conventions, illustrate control structures, and perhaps to amuse. You may even find them useful. We hope that you will use badluk for no serious purpose.

* * * *

Subroutine flmoon calculates the phases of the moon, or more exactly, the Julian day and fraction thereof on which a given phase will occur or has occurred. The program xflmoon asks the present date and compiles a list of upcoming phases. We have compared the predictions to lunar tables, with happy results. Shown are the results of a test run, which you may replicate as a check. In this program, notice that we have set TZONE (the time zone) to -5.0 to signify the five hour separation of the Eastern Standard time zone from Greenwich, England. Our convention requires you to use negative values of TZONE if you are west of Greenwich, as we are. The Julian day results are converted to calendar dates through the use of caldat, which appears later in the chapter. The fractional Julian day and time zone combine to form a correction that can possibly change the calendar date by one day.

Date			Tim	e(EST)	Phase
12	9	1992	7	P M	full moon
12	16	1992	2	PM	last quarter
12	23	1992	8	PM	new moon
12	31	1992	10	PM	first quarter
1	8	1993	8	AM	full moon
1	14	1993	11	PM	last quarter
1	22	1993	1	PM	new moon
1	30	1993	6	PM	first quarter
2	6	1993	7	PM	full moon
2	13	1993	10	AM	last quarter
2	21	1993	8	AM	new moon
3	1	1993	11	AM	first quarter
3	8	1993	5	AM	full moon
3	14	1993	11	PM	last quarter
3	23	1993	2	AM	new moon
3	30	1993	11	P M	first quarter
4	6	1993	2	P M	full moon
4	13	1993	3	PM	last quarter
4	21	1993	6	PM	new moon
4	29	1993	8	AM	first quarter

```
2
```

```
PROGRAM xflmoon
C
      driver for routine flmoon
      REAL TZONE
      PARAMETER (TZONE=-5.0)
      REAL frac, timzon
      INTEGER i, im, id, iy, ifrac, istr, j1, j2, julday, n, nph
      CHARACTER phase(4)*15,timstr(2)*3
      DATA phase/'new moon', 'first quarter',
            'full moon', 'last quarter'/
      DATA timstr/' AM', ' PM'/
      write(*,*) 'Date of the next few phases of the moon'
      write(*,*) 'Enter today''s date (e.g. 12,15,1992)'
      timzon=TZONE/24.0
      read(*,*) im,id,iy
C
      approximate number of full moons since January 1900
      n=12.37*(iy-1900+(im-0.5)/12.0)
      nph=2
      j1=julday(im,id,iy)
      call flmoon(n,nph,j2,frac)
      n=n+nint((j1-j2)/29.53)
      write(*,'(/1x,t6,a,t19,a,t32,a)') 'Date','Time(EST)','Phase'
      do 11 i=1,20
        call flmoon(n,nph,j2,frac)
        ifrac=nint(24.*(frac+timzon))
        if (ifrac.lt.0) then
          j2=j2-1
          ifrac=ifrac+24
        endif
        if (ifrac.ge.12) then
          j2=j2+1
          ifrac=ifrac-12
          ifrac=ifrac+12
        if (ifrac.gt.12) then
          ifrac=ifrac-12
          istr=2
        else
          istr=1
        endif
        call caldat(j2,im,id,iy)
        write(*,'(1x,2i3,i5,t20,i2,a,5x,a)') im,id,iy,
             ifrac, timstr(istr), phase(nph+1)
        if (nph.eq.3) then
          nph=0
          n=n+1
        else
          nph=nph+1
        endif
11
      continue
```

The function julday, our exemplar of the if control structure, converts calendar dates to Julian dates. Not many people know the Julian date of their birthday or any other convenient reference point, for that matter. To remedy this, we offer a list of checkpoints, which appears at the end of this chapter as the file DATES.DAT. The

program xjulday lists the Julian date for each historic event for comparison. Then it allows you to make your own choices for entertainment.

```
PROGRAM xjulday
C
      driver for julday
      INTEGER i, im, id, iy, julday, n
      CHARACTER txt*40, name(12)*15
      DATA name/'January', 'February', 'March', 'April', 'May', 'June',
           'July', 'August', 'September', 'October', 'November',
           'December'/
      open(7,file='DATES.DAT',status='OLD')
      read(7,'(a)') txt
      read(7,*) n
      write(*,'(/1x,a,t12,a,t17,a,t23,a,t37,a/)') 'Month','Day','Year',
           'Julian Day', 'Event'
      do 11 i=1,n
        read(7,'(i2,i3,i5,a)') im,id,iy,txt
        write(*,'(1x,a10,i3,i6,3x,i7,5x,a)') name(im),id,iy,
             julday(im,id,iy),txt
11
      continue
      close(7)
      write(*,'(/1x,a/)') 'Month,Day,Year (e.g. 1,13,1905)'
      do 12 i=1,20
        write(*,*) 'MM,DD,YYYY'
        read(*,*) im,id,iy
        if (im.lt.0) stop
        write(*,'(1x,a12,i8/)') 'Julian Day: ',julday(im,id,iy)
12
      continue
      END
```

The next program in *Numerical Recipes* is badluk, an infamous code that combines the best and worst instincts of man. We include no demonstration program for badluk, not just because we fear it, but also because it is self-contained, with sample results appearing in the text.

Chapter 1 closes with routine caldat, which illustrates no new points, but complements julday by doing conversions from Julian day number to the month, day, and year on which the given Julian day began. This offers an opportunity, grasped by the demonstration program xcaldat, to push dates through both julday and caldat in succession, to see if they survive intact. This, of course, tests only your authors' ability to make mistakes backwards as well as forwards, but we hope you will share our optimism that correct results here speak well for both routines. (We have checked them a bit more carefully in other ways.)

```
PROGRAM xcaldat

C driver for routine caldat
INTEGER i,im,imm,id,idd,iy,iyy,iycopy,j,julday,n
CHARACTER name(12)*10

C check whether CALDAT properly undoes the operation of JULDAY
DATA name/'January','February','March','April','May',

* 'June','July','August','September','October',

* 'November','December'/
open(7,file='DATES.DAT',status='OLD')
read(7,*)
read(7,*)
read(7,*)
vrite(*,'(/1x,a,t40,a)') 'Original Date:','Reconstructed Date:'
```

```
write(*,'(1x,a,t12,a,t17,a,t25,a,t40,a,t50,a,t55,a/)')
* 'Month','Day','Year','Julian Day','Month','Day','Year'
do 11 i=1,n
    read(7,'(i2,i3,i5)') im,id,iy
    iycopy=iy
    j=julday(im,id,iycopy)
    call caldat(j,imm,idd,iyy)
    write(*,'(1x,a,i3,i6,4x,i9,6x,a,i3,i6)') name(im),id,
    * iy,j,name(imm),idd,iyy

11 continue
    END
```

Appendix

File DATES.DAT:

```
List of dates for testing routines in Chapter 1
16 entries
12 31
      -1 End of millennium
         1 One day later
10 14 1582 Day before Gregorian calendar
10 15 1582 Gregorian calendar adopted
01 17 1706 Benjamin Franklin born
04 14 1865 Abraham Lincoln shot
04 18 1906 San Francisco earthquake
05 07 1915 Sinking of the Lusitania
07 20 1923 Pancho Villa assassinated
05 23 1934 Bonnie and Clyde eliminated
07 22 1934 John Dillinger shot
04 03 1936 Bruno Hauptman electrocuted
05 06 1937 Hindenburg disaster
07 26 1956 Sinking of the Andrea Doria
06 05 1976 Teton dam collapse
05 23 1968 Julian Day 2440000
```

Chapter 2: Linear Algebraic Equations

Numerical Recipes Chapter 2 begins the "true grit" of numerical analvsis by considering the solution of linear algebraic equations. This is done first by Gauss-Jordan elimination (gauss), and then by LU decomposition with forward and backsubstitution (ludcmp and lubksb). Several linear systems of special form, represented by tridiagonal, band diagonal, cyclic, Vandermonde, and Toeplitz matrices, may be treated with subroutines tridag, bandec, cyclic, vander, and toeplz respectively. Cholesky decomposition (choldc and cholsl) is the preferred method for symmetric positive definite systems. QR decomposition (qrdcmp) is less efficient than LU decomposition in general; however, the ease with which it is updated (qrupdt) if the system is changed slightly makes it useful in certain applications. For singular or nearly singular matrices the best choice is singular value decomposition with backsubstitution (svdcmp and svbksb). Linear systems with relatively few non-zero coefficients, so-called "sparse" matrices, are handled by routine linbcg. A suite of routines for manipulating general sparse matrices, sprsax, sprstx, etc., is provided.

* * * *

gaussj performs Gauss-Jordan elimination with full pivoting to find the solution of a set of linear equations for a collection of right-hand side vectors. The demonstration routine xgaussj checks its operation with reference to a group of test input matrices printed at the end of this chapter as file MATRX1.DAT. Each matrix is subjected to inversion by gaussj, and then multiplication by its own inverse to see that a unit matrix is produced. Then the solution vectors are each checked through multiplication by the original matrix and comparison with the right-hand side vectors that produced them.

```
PROGRAM xgaussj

C driver for routine gaussj
INTEGER MP,NP
PARAMETER(MP=20,NP=20)
INTEGER j,k,1,m,n
REAL a(NP,NP),b(NP,MP),ai(NP,NP),x(NP,MP)
REAL u(NP,NP),t(NP,MP)
CHARACTER dummy*3
open(7,file='MATRX1.DAT',status='old')

10 read(7,'(a)') dummy
if (dummy.eq.'END') goto 99
read(7,*)
read(7,*)
read(7,*)
```

```
read(7,*) ((a(k,1), l=1,n), k=1,n)
      read(7,*)
      read(7,*) ((b(k,1), k=1,n), l=1,m)
      save Matrices for later testing of results
C
      do 13 l=1,n
        do 11 k=1,n
          ai(k,1)=a(k,1)
        continue
        do 12 k=1,m
          x(1,k)=b(1,k)
12
        continue
13
      continue
      invert Matrix
      call gaussj(ai,n,NP,x,m,MP)
      write(*,*) 'Inverse of Matrix A : '
      do 14 k=1,n
        write(*,'(1h,(6f12.6))') (ai(k,1), l=1,n)
14
      continue
C
      test Results
      check Inverse
      write(*,*) 'A times A-inverse (compare with unit matrix)'
     do 17 k=1,n
        do 16 l=1,n
         u(k,1)=0.0
         do 15 j=1,n
            u(k,1)=u(k,1)+a(k,j)*ai(j,1)
         continue
16
        continue
        write(*,'(1h,(6f12.6))') (u(k,1), l=1,n)
17
      continue
      check Vector Solutions
     write(*,*) 'Check the following vectors for equality:'
     write(*,'(t12,a8,t23,a12)') 'Original','Matrix*Sol''n'
       write(*,'(1x,a,i2,a)') 'Vector ',1,':'
       do 19 k=1,n
         t(k,1)=0.0
         do 18 j=1,n
           t(k,1)=t(k,1)+a(k,j)*x(j,1)
18
         write(*,'(8x,2f12.6)') b(k,1),t(k,1)
19
       continue
21
     write(*,*) 'Press RETURN for next problem:'
     read(*,*)
     goto 10
99
     close(7)
     END
```

The demonstration program for routine ludcmp relies on the same package of test matrices, but just performs an LU decomposition of each. The performance is checked by multiplying the lower and upper matrices of the decomposition and comparing with the original matrix. The array indx keeps track of the scrambling done by ludcmp to effect partial pivoting. We had to do the unscrambling here, but you will normally not be called upon to do so, since ludcmp is used with the routine

lubksb, which knows how to do its own descrambling.

```
PROGRAM xludcmp
C
       driver for routine ludcmp
       INTEGER NP
       PARAMETER (NP=20)
       INTEGER j,k,1,m,n,indx(NP),jndx(NP)
       REAL d, dum, a(NP, NP), x1(NP, NP), xu(NP, NP), x(NP, NP)
       CHARACTER txt*3
       open(7,file='MATRX1.DAT',status='old')
       read(7,*)
10
      read(7,*)
      read(7,*) n,m
      read(7,*)
      read(7,*) ((a(k,1), l=1,n), k=1,n)
      read(7,*)
      read(7,*) ((x(k,1), k=1,n), l=1,m)
C
      print out a-matrix for comparison with product of lower
      and upper decomposition matrices.
      write(*,*) 'Original matrix:'
      do 11 k=1,n
        write(*,'(1x,6f12.6)') (a(k,1), l=1,n)
11
      continue
      perform the decomposition
      call ludcmp(a,n,NP,indx,d)
C
      compose separately the lower and upper matrices
      do 13 k=1,n
        do 12 l=1,n
          if (l.gt.k) then
            xu(k,1)=a(k,1)
            x1(k,1)=0.0
          else if (1.1t.k) then
            xu(k,1)=0.0
            x1(k,1)=a(k,1)
          else
            xu(k,1)=a(k,1)
            x1(k,1)=1.0
          endif
12
        continue
13
C
      compute product of lower and upper matrices for
C
      comparison with original matrix.
      do 16 k=1,n
        indx(k)=k
        do 15 l=1,n
          x(k,1)=0.0
          do 14 j=1,n
            x(k,1)=x(k,1)+x1(k,j)*xu(j,1)
14
          continue
15
        continue
16
      write(*,*) 'Product of lower and upper matrices (unscrambled):'
      do 17 k=1,n
        dum=jndx(indx(k))
        jndx(indx(k))=jndx(k)
        jndx(k)=dum
17
      continue
```

```
do 19 k=1,n
       do 18 j=1,n
         if (jndx(j).eq.k) then
           write(*,'(1x,6f12.6)') (x(j,1), l=1,n)
         endif
       continue
18
     continue
19
     write(*,*) 'Lower matrix of the decomposition:'
     do 21 k=1,n
       write(*,'(1x,6f12.6)') (xl(k,1), l=1,n)
21
     write(*,*) 'Upper matrix of the decomposition:'
     do 22 k=1.n
       write(*,'(1x,6f12.6)') (xu(k,1), l=1,n)
22
     write(*,*) 'Press RETURN for next problem:'
     read(*,*)
     read(7,'(a3)') txt
     if (txt.ne.'END') goto 10
     close(7)
     END
```

Our example driver for lubksb makes calls to both ludcmp and lubksb in order to solve the linear equation problems posed in file MATRX1.DAT (see discussion of gaussj). The original matrix of coefficients is applied to the solution vectors to check that the result matches the right-hand side vectors posed for each problem. We apologize for using routine ludcmp in a test of lubksb, but ludcmp has been tested independently, and anyway, lubksb is nothing without this partner program, so a test of the combination is more to the point.

```
PROGRAM xlubksb
C
      driver for routine lubksb
      INTEGER NP
      PARAMETER (NP=20)
      REAL p,a(NP,NP),b(NP,NP),c(NP,NP),x(NP)
      INTEGER j,k,l,m,n,indx(NP)
      CHARACTER txt*3
      open(7,file='MATRX1.DAT',status='old')
      read(7,*)
10
      read(7,*)
      read(7,*) n,m
      read(7,*)
      read(7,*) ((a(k,1), l=1,n), k=1,n)
      read(7,*)
      read(7,*) ((b(k,1), k=1,n), l=1,m)
C
      save matrix a for later testing
      do 12 l=1,n
        do 11 k=1,n
          c(k,1)=a(k,1)
11
        continue
12
      continue
      do LU decomposition
      call ludcmp(c,n,NP,indx,p)
C
      solve equations for each right-hand vector
      do 16 k=1,m
```

```
do 13 1=1,n
         x(1)=b(1,k)
13
       continue
       call lubksb(c,n,NP,indx,x)
     test results with original matrix
       write(*,*) 'Right-hand side vector:'
       write(*,'(1x,6f12.6)') (b(1,k), l=1,n)
       write(*,*) 'Result of matrix applied to sol''n vector'
       do 15 l=1,n
         b(1,k)=0.0
         do 14 j=1,n
           b(1,k)=b(1,k)+a(1,j)*x(j)
14
         continue
15
       continue
       write(*,'(1x,6f12.6)') (b(1,k), l=1,n)
       16
     continue
     write(*,*) 'Press RETURN for next problem:'
     read(*,*)
     read(7,'(a3)') txt
     if (txt.ne.'END') goto 10
     close(7)
     END
```

Subroutine tridag solves linear equations with coefficients that form a tridiagonal matrix. We provide at the end of this chapter a second file of matrices MA-TRIX2.DAT for the demonstration driver. In all other respects, the demonstration program xtridag operates in the same fashion as xlubksb.

```
PROGRAM xtridag
C
      driver for routine tridag
      INTEGER NP
      PARAMETER (NP=20)
      INTEGER k,n
      REAL diag(NP), superd(NP), subd(NP), rhs(NP), u(NP)
      CHARACTER txt*3
      open(7,file='MATRX2.DAT',status='old')
      read(7,'(a3)') txt
10
      if (txt.eq.'END') goto 99
      read(7,*)
      read(7,*) n
      read(7,*)
      read(7,*) (diag(k), k=1,n)
      read(7,*)
      read(7,*) (superd(k), k=1,n-1)
      read(7,*)
      read(7,*) (subd(k), k=2,n)
      read(7,*)
      read(7,*) (rhs(k), k=1,n)
C
      carry out solution
      call tridag(subd,diag,superd,rhs,u,n)
      write(*,*) 'The solution vector is:'
      write(*,'(1x,6f12.6)') (u(k), k=1,n)
C
      test solution
      write(*,*) '(matrix)*(sol''n vector) should be:'
      write(*,'(1x,6f12.6)') (rhs(k), k=1,n)
      write(*,*) 'Actual result is:'
```

```
do 11 k=1,n
       if (k.eq.1) then
         rhs(k)=diag(1)*u(1) + superd(1)*u(2)
       else if (k.eq.n) then
         rhs(k)=subd(n)*u(n-1) + diag(n)*u(n)
         rhs(k)=subd(k)*u(k-1) + diag(k)*u(k)
             + superd(k)*u(k+1)
       endif
11
     continue
     write(*,'(1x,6f12.6)') (rhs(k), k=1,n)
     write(*,*) 'Press RETURN for next problem:'
     read(*,*)
     goto 10
99
     close(7)
     END
```

The demonstration program xbanmul forms a banded matrix, multiplies if by a vector using banmul, and compares the answer to the result of carrying out a full matrix multiplication.

```
PROGRAM xbanmul
      driver for routine banmul
       INTEGER NP, M1, M2, MP
      PARAMETER (NP=7,M1=2,M2=1,MP=M1+1+M2)
      INTEGER i,j,k
      REAL a(NP, MP), aa(NP, NP), ax(NP), b(NP), x(NP)
      do 12 i=1,M1
        do 11 j=1,NP
           a(j,i)=10*j+i
11
        continue
12
      continue
C
      lower band
      do 13 i=1,NP
        a(i,M1+1)=i
13
      continue
C
      diagonal
      do 15 i=1,M2
        do 14 j=1,NP
          a(j,M1+1+i)=0.1*j+i
14
        continue
15
      continue
C
      upper band
      do 17 i=1,NP
        do 16 j=1,NP
          k=i-M1-1
          if (j.ge.max(1,1+k).and.j.le.min(M1+M2+1+k,NP)) then
            aa(i,j)=a(i,j-k)
          else
            aa(i,j)=0.0
          endif
16
        continue
17
      continue
      do 18 i=1,NP
        x(i)=i/10.0
18
      continue
```

```
call banmul(a,NP,M1,M2,NP,MP,x,b)
do 21 i=1,NP
    ax(i)=0.0
    do 19 j=1,NP
        ax(i)=ax(i)+aa(i,j)*x(j)

19    continue
21    continue
    write(*,'(t8,a,t32,a)') 'Reference vector','banmul vector'
    do 22 i=1,NP
        write(*,'(t8,f12.4,t32,f12.4)') ax(i),b(i)

22    continue
    END
```

The sample program xbandec forms a random banded matrix A, a random vector x, and calculates $b = A \cdot x$. It then supplies A and b to bandec and banbks and compares the solution to the saved copy of x.

```
PROGRAM xbandec
C
      driver for routine bandec
      REAL ran1
      REAL a(7,4),x(7),b(7),al(7,2),d
      INTEGER indx(7)
      INTEGER i, idum, j
      idum=-1
      do 12 i=1,7
        x(i)=ran1(idum)
        do 11 j=1,4
          a(i,j)=ran1(idum)
11
        continue
12
      continue
      call banmul(a,7,2,1,7,4,x,b)
      do 13 i=1,7
        write(*,*) i,b(i),x(i)
13
      continue
      call bandec(a,7,2,1,7,4,al,2,indx,d)
      call banbks(a,7,2,1,7,4,al,2,indx,b)
      do 14 i=1.7
        write(*,*) i,b(i),x(i)
14
      continue
      stop
```

mprove is a short routine for improving the solution vector for a set of linear equations, providing that an LU decomposition has been performed on the matrix of coefficients. Our test of this function is to use ludcmp and lubksb to solve a set of equations specified in the DATA statements at the beginning of the program. The solution vector is then corrupted by the addition of random values to each component. mprove works on the corrupted vector to recover the original.

```
PROGRAM xmprove

driver for routine mprove
INTEGER N,NP
PARAMETER(N=5,NP=5)
INTEGER i,j,idum,indx(N)
REAL d,a(NP,NP),b(N),x(N),aa(NP,NP),ran3
DATA a/1.0,2.0,1.0,4.0,5.0,2.0,3.0,1.0,5.0,1.0,
```