PHYS4300 Numerical Methods and Scientific Computing

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HW 2
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Solution. *Problem 1.* This program takes in a matrix A, prints A, prints its LU decomposition, prints L with the solution for y in the matrix equation $Ly = B$ using forward substitution, prints U with the solution for x in the matrix equation $Ux = y$ using back substitution. The program then proceeds to use these methods to find the inverse of A by finding the columns of the inverse individually from iterations of the vector B and solving, and the $det(A)$. Here is the first segment of code.

```
[forestan@sirius ~/hw2]$ cat ludecom.C
//----------------------------
// We will write a program that performs LU decomposition on
// a predefined 5x5 matrix. We will write the original matrix, A.
// We will then write the LU decom matrix, L, U, LxU, the
// inverse of A=LU, and det(A).
//----------------------------
using namespace std;
#include <iostream>
#include <iomanip>
#include <math.h>
#include <cmath>

const int N=5;

void InitMat(double A[N][N], double B[N] ){
A[0][0] =   1.0;  A[0][1] =  7.0;  A[0][2] = 18.0;   A[0][3] = 4.0;  A[0][4] =
0.0; B[0] =   41;
A[1][0] =   6.0;  A[1][1] =  0.1;  A[1][2] =  7.0;   A[1][3] = 0.0;  A[1][4] =
2.0; B[1] =   -9;
A[2][0] =   0.0;  A[2][1] = -5.0;  A[2][2] = -6.0;   A[2][3] = 4.0;  A[2][4] =
3.0; B[2] =    8;
A[3][0] =  19.3;  A[3][1] =  3.0;  A[3][2] = -0.2;   A[3][3] =-0.4;  A[3][4] = -
5.0; B[3] =  3.7;
A[4][0] =   7.3;  A[4][1] = -2.0;  A[4][2] = 17.2;   A[4][3] = 5.4;  A[4][4] =
0.2; B[4] = -7.7;
}

void PrintMatVec(double A[N][N], double B[N]){
        int i,j;

        for(i=0;i<N;i++){cout << setw(8) << "A[" << i << ",.] =" << setw(8) << "
 ";
                for(j=0;j<N;j++){cout << setw(12) << A[i][j] << setw(12) << " ";
}

                 cout << "    " << setw(10) << "B[" << i << "] =" <<  B[i] <<  e
ndl;
        }
        }

void PrintMat(double A[N][N]){
        int i,j;

        for(i=0;i<N;i++){cout << setw(8) << "A[" << i << ",.] =" << setw(8) << "
 ";
                for(j=0;j<N;j++){cout << setw(12) << A[i][j] << setw(12) << " ";
}
                cout << " " << endl;
        }
        }
```

Here is the second.

```
void PrintMatInv(double I[N][N]){
        int i,j;

        for(i=0;i<N;i++){cout << setw(8) << "I[" << i << ",.] =" << setw(8) << "
 ";
                for(j=0;j<N;j++){cout << setw(12) << I[i][j] << setw(12) << " ";
}
                cout << " " << endl;
        }
        }


void LUdec(double A[N][N]){
        int i,j,k;

        for(j=0;j<N;j++){
                for(i=0;i<j+1;i++){if(i>0){for(k=0;k<i;k++){A[i][j]-=A[i][k]*A[k
][j];}}}
                if(j<N-1){for(i=j+1;i<N;i++){if(j>0){for(k=0;k<j;k++){A[i][j]-=A
[i][k]*A[k][j];}}
                        A[i][j]=A[i][j]/A[j][j];}}
        }
        }

void FSub(double L[N][N], double B[N], double x[N]){
        int i,j,k;

        for(i=0;i<N;i++){
                for(j=0;j<N;j++){
                if(i==j){L[i][j] = 1;}
                if(i<j){L[i][j] = 0;}
                }
        }
        cout << "For the Lower Triangular matrix L" << " " << endl;

        x[0]=B[0];
        for(k=0;k<N;k++){x[k]=B[k]; for(j=0;j<k;j++){x[k]=x[k]-L[k][j]*x[j];}}
        cout << " " << endl;
        for(i=0;i<N;i++){cout << setw(8) << "y[" << i << "] =" << " " << setw(8)
 << x[i] << endl;}
        }
```

The third segment.

```
void BSub(double U[N][N], double B[N], double x[N]){
        int i,j,k;

        for(i=0;i<N;i++){
               for(j=0;j<N;j++){if(i>j){U[i][j] = 0;}}
        }
        cout << "For the upper triangular matrix U" << " " << endl;
        if(U[N-1][N-1]==0){cout << "error" << endl; }
        x[N-1]=B[N-1]/U[N-1][N-1];
        for(k=N-2;-k<1;k--){x[k]=B[k];for(j=k+1;j<N;j++){x[k]=x[k]-U[k][j]*x[j];
}
          x[k]=x[k]/U[k][k];
        }
        cout << " " << endl;
        for(i=0;i<N;i++){cout << setw(8) << "x[" << i << "] =" << " " << setw(8)
 << x[i] << endl;}
        }

void test(double A[N][N], double B[N], double x[N], double o[N], double e[N]){
        int i,j,k;
        o[0]=0;

        InitMat(A,B);
        for(k=0;k<N;k++){for(i=0;i<N;i++){o[k]=o[k]+A[k][i]*x[i];}}
        for(k=0;k<N;k++){e[k]=B[k]-o[k];}

        cout << setw(8) << "A*x" << setw(12) << " " << "B" << " " << setw(15) <<
 "error" << endl;
        cout << setw(8) << "---" << setw(12) << " " << "---" << " " << setw(15)
<< "------" << endl;

        for(j=0;j<N;j++){cout << setw(8) << o[j] << setw(12) <<  " " <<  B[j] <<
 " " << setw(15) << e[j]  << endl;}

        cout << " " << endl;
        }

void LtimesU(double L[N][N], double U[N][N], double LU[N][N]){
        int i,j,k;

        for(i=0;i<N;i++){for(j=0;j<N;j++){for(k=0;k<N;k++){LU[i][j]+=L[i][k]*U[k
][j];}}}
        cout << "L times U" << " " << endl;
        }
```

The fourth segment.

```
void inverse(double A[N][N], double L[N][N], double U[N][N], double B[N], double
 y[N], double x[N], double I[N][N], double ID[N][N]){
        int i,j,q,k;
        cout << " " << endl;
        cout << " " << endl;
        cout << "Calculating the Inverse of A" << endl;
        for(i=0;i<N;i++){
                InitMat(L,B);
                for(j=0;j<N;j++){if(i==j){B[j]=1;}else{B[j]=0;}}
                cout << " " << endl;
                cout << setw(12) << "For B = " << " ";
                for(q=0;q<N;q++){cout << setw(6)  << B[q] << " ";}
                cout << " " << endl;
                LUdec(L);
                FSub(L,B,y);
                InitMat(U,B);
                LUdec(U);
                BSub(U,y,x);
                for(j=0;j<N;j++){I[j][i]=x[j];}
        }
        cout << "Inverse of A" << " " << endl;
        PrintMatInv(I);
        cout<< " " << endl;
        cout << "Test to see if AA^(-1) = 1." << " " << endl;
        InitMat(A,B);
        for(k=0;k<N;k++){
                for(i=0;i<N;i++){
                        for(j=0;j<N;j++){ID[i][k]+= A[i][j]*I[j][k];
        }
        }
        }
        for(i=0;i<N;i++){for(j=0;j<N;j++){if(ID[i][j]<1e-10){ID[i][j]=0;}}}
        cout << "A times its Inverse Yields" << " " << endl;
        PrintMat(ID);
        }

void det(double U[N][N], double B[N], double y[N], double x[N]){
        int i;
        double p;
        p=1;

        cout << " " << endl;
        cout << " " << endl;
        cout << "Calculating the determinant of A" << " " << endl;
        cout << " " << endl;
        InitMat(U,B);
        LUdec(U);
        BSub(U,y,x);
        for(i=0;i<N;i++){p*=U[i][i];}
        cout << " " << endl;
        cout << "The determinant of the matrix A is " << p << ".  " << endl;
        }
```

The fifth segment.

```
int main(){

double A[N][N], U[N][N], L[N][N], LU[N][N], B[N], y[N], x[N], o[N], e[N], I[N][N
], ID[N][N];
int i,j,k;
double M;

InitMat(L,B);
PrintMat(L);
cout << "LU Decomposition" << " " << endl;
LUdec(L);
PrintMat(L);
FSub(L,B,y);
cout << " " << endl;
PrintMatVec(L,B);
cout << " " << endl;
InitMat(U,B);
LUdec(U);
BSub(U,y,x);
cout << " " << endl;
test(A,B,x,o,e);
PrintMatVec(U,B);
cout << " " << endl;
LtimesU(L,U,LU);
PrintMat(LU);
inverse(A,L,U,B,y,x,I,ID);
det(U,B,y,x);
}
```

Here is the output for the program.

```
[forestan@sirius ~/hw2]$ g++ ludecom.C
[forestan@sirius ~/hw2]$ ./a.out
      A[0,.] =                1                7               18                4                0
      A[1,.] =                6              0.1                7                0                2
      A[2,.] =                0               -5               -6                4                3
      A[3,.] =             19.3                3             -0.2             -0.4               -5
      A[4,.] =              7.3               -2             17.2              5.4              0.2
LU Decomposition
      A[0,.] =                1                7               18                4                0
      A[1,.] =                6             -41.9             -101             -24                2
      A[2,.] =                0            0.119332          6.05251          6.86396          2.76134
      A[3,.] =             19.3             3.15274         -4.81995          31.1498          2.00402
      A[4,.] =              7.3              1.2673          2.27965         -0.289959         -8.04841
For the Lower Triangular matrix L

      y[0] =       41
      y[1] =     -255
      y[2] =  38.4296
      y[3] =  201.579
      y[4] = -12.9943

      A[0,.] =                1                0                0                0                0                B[0] =41
      A[1,.] =                6                1                0                0                0                B[1] =-9
      A[2,.] =                0            0.119332             1                0                0                B[2] =8
      A[3,.] =             19.3             3.15274         -4.81995             1                0                B[3] =3.7
      A[4,.] =              7.3              1.2673          2.27965         -0.289959             1                B[4] =-7.7

For the upper triangular matrix U

      x[0] = -0.268384
      x[1] =  6.39256
      x[2] = -1.60828
      x[3] =  6.36739
      x[4] =  1.61452

     A*x           B          error
     ---           ---        ------
      41           41             0
      -9           -9     3.55271e-15
       8            8             0
     3.7          3.7     7.54952e-14
    -7.7         -7.7     2.13163e-14

      A[0,.] =                1                7               18                4                0                B[0] =41
      A[1,.] =                0             -41.9             -101             -24                2                B[1] =-9
      A[2,.] =                0                0             6.05251          6.86396          2.76134          B[2] =8
      A[3,.] =                0                0                0             31.1498          2.00402          B[3] =3.7
      A[4,.] =                0                0                0                0             -8.04841          B[4] =-7.7

L times U
      A[0,.] =                1                7               18                4                0
      A[1,.] =                6              0.1                7                0                2
      A[2,.] =                0               -5               -6                4                3
      A[3,.] =             19.3                3             -0.2             -0.4               -5
      A[4,.] =              7.3               -2             17.2              5.4              0.2
```

Continuing.

```
Calculating the Inverse of A

    For B =      1     0     0     0     0
For the Lower Triangular matrix L

      y[0] =        1
      y[1] =       -6
      y[2] =  0.71599
      y[3] =  3.06751
      y[4] = -0.43894
For the upper triangular matrix U

      x[0] = -0.00361118
      x[1] = 0.125838
      x[2] = -0.0142845
      x[3] = 0.0949672
      x[4] = 0.0545374

    For B =      0     1     0     0     0
For the Lower Triangular matrix L

      y[0] =        0
      y[1] =        1
      y[2] = -0.119332
      y[3] = -3.72792
      y[4] = -2.07621
For the upper triangular matrix U

      x[0] = 0.0602669
      x[1] = 0.0251982
      x[2] = 0.0171355
      x[3] = -0.136273
      x[4] = 0.257965

    For B =      0     0     1     0     0
For the Lower Triangular matrix L

      y[0] =        0
      y[1] =        0
      y[2] =        1
      y[3] =  4.81995
      y[4] = -0.882064
For the upper triangular matrix U

      x[0] = 0.0236651
      x[1] = 0.0466196
      x[2] = -0.0522632
      x[3] = 0.147684
      x[4] = 0.109595
```

Finally,

```
    For B =      0     0     0     1     0
For the Lower Triangular matrix L

      y[0] =       0
      y[1] =       0
      y[2] =       0
      y[3] =       1
      y[4] = 0.289959
For the upper triangular matrix U

      x[0] = 0.0378237
      x[1] = 0.0330391
      x[2] = -0.0225989
      x[3] = 0.0344207
      x[4] = -0.0360269

    For B =      0     0     0     0     1
For the Lower Triangular matrix L

      y[0] =       0
      y[1] =       0
      y[2] =       0
      y[3] =       0
      y[4] =       1
For the upper triangular matrix U

      x[0] = -0.012053
      x[1] = -0.125299
      x[2] = 0.0476206
      x[3] = 0.00799349
      x[4] = -0.124248
Inverse of A
      I[0,.] =         -0.00361118            0.0602669            0.0236851            0.0378237           -0.012053
      I[1,.] =            0.125838            0.0251982            0.0466196            0.0330391           -0.125299
      I[2,.] =          -0.0142845            0.0171355           -0.0522632           -0.0225989            0.0476206
      I[3,.] =           0.0949672           -0.136273             0.147684             0.0344207            0.00799349
      I[4,.] =           0.0545374            0.257965             0.109595            -0.0360269           -0.124248

Test to see if AA^(-1) = 1.
A times its Inverse Yields
      A[0,.] =                   1                    0                    0                    0                    0
      A[1,.] =                   0                    1                    0                    0                    0
      A[2,.] =                   0                    0                    1                    0                    0
      A[3,.] =                   0                    0                    0                    1                    0
      A[4,.] =                   0                    0                    0                    0                    1

Calculating the determinant of A

For the upper triangular matrix U

      x[0] = -0.012053
      x[1] = -0.125299
      x[2] = 0.0476206
      x[3] = 0.00799349
      x[4] = -0.124248

The determinant of the matrix A is 63579.2.
```

□