NUMERICAL SOLUTIONS OF LINEAR ALGEBRAIC EQUATIONS

PHY 311 — NUMERICAL ANALYSIS

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CONTENTS

1 INTRODUCTION

Various problems in physics can be expressed as systems of linear algebraic equations. The solutions of a set of linear algebraic equations represents quantities of interest in physical problems. A system of m linear algebraic equations in n unknowns has the following general form,

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$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots\cdots\cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \cdots\cdots\cdots + a_{2n}x_n &= b_2 \\
&\cdots \\
&\cdots \\
a_{m1}x_1 + a_{m2}x_2 + \cdots\cdots\cdots + a_{mn}x_n &= b_m
\end{aligned} \tag{1}
$$

Here $a_{11} \cdots\cdots a_{mn}$ and $b_1 \cdots\cdots b_m$ are coefficients of the linear equations and in the present course we consider only systems of n linear equations with n variables containing real valued coefficients.

2 LU DECOMPOSITION METHOD

Given a set of n linear equations in n variables, One can write a matrix equation of the form AX = B where A and B are the matrices containing the coefficients and X is a column matrix whose entries are the n solutions of the set of equations. The LU decomposition method involves decomposing the coefficient matrix A into a product of lower and upper triangular matrices and using this decomposition to solve the corresponding set of linear equations in a straightforward manner. The procedure for a set of three equations in three variables is illustrated below.

$$
\begin{aligned}
a_1x_1 + a_2x_2 + a_3x_3 &= b_1 \\
a_4x_1 + a_5x_2 + a_5x_3 &= b_2 \\
a_7x_1 + a_8x_2 + a_9x_3 &= b_3
\end{aligned} \tag{2}
$$

The above set of linear eqautions can be written as a matrix equation,

$$\mathrm{AX} = \mathrm{B} \tag{3}$$

The coefficient matrices and the matrix X are given by:

$$\mathrm{A} = \begin{bmatrix} a_1 & a_2 & a_3 \\ a_4 & a_5 & a_6 \\ a_7 & a_8 & a_9 \end{bmatrix} \qquad \mathrm{X} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \mathrm{B} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

One can decompose the matrix A into a product of a lower triangular matrix L and an upper triangular matrix U. We choose convenient general forms of L and U matrices. (Note: LU decomposition is possible only if the matrix A is non-singular).

$$\mathrm{A} = \mathrm{LU} \tag{4}$$

$$i.e.\quad \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \times \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} \tag{5}$$

The decomposition can be carried out by calculating the entries of the lower and upper triangular matrices. Multiplying the L and U matrices and comparing the entries with the matrix A, we obtain the values of $l_{11} \cdots\cdots\cdot l_{22}$ and $u_{11} \cdots\cdots\cdot u_{33}$.

$$u_{11} = a_{11} \qquad u_{12} = a_{12} \qquad u_{13} = a_{13} \tag{6}$$

$$l_{21} = \frac{a_{21}}{a_{11}} \qquad l_{31} = \frac{a_{31}}{a_{11}} \tag{7}$$

$$u_{22} = a_{22} - \frac{a_{21}}{a_{11}}a_{12} \qquad u_{23} = a_{23} - \frac{a_{21}}{a_{11}}a_{13} \tag{8}$$

$$l_{32} = \frac{a_{32} - \frac{a_{31}}{a_{11}}a_{12}}{u_{22}} \tag{9}$$

Once the matrix A is decomposed, we can rewrite equation (2) as

$$\mathrm{LUX} = \mathrm{B} \tag{10}$$

Let us set

$$\mathrm{UX} = \mathrm{Y} \tag{11}$$

Where Y is a matrix of unknowns, $\mathrm{Y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$. Now equation (9) becomes

$$\mathrm{LY} = \mathrm{B} \tag{12}$$

This matrix equation is equivalent to the following set of linear equations

$$\begin{aligned} y_1 &= b_1 \\ l_{21}y_1 + y_2 &= b_2 \\ l_{31}y_1 + l_{32}y_2 + y_3 &= b_3 \end{aligned} \tag{13}$$

The above set of equations are solved by forward substitution and one obtains the values of $y_1, y_2$and y_3. These set of values are now used to solve the set of equations corresponding to UX = Y, i.e the set

$$\begin{aligned} u_{11}x_1 + u_{12}x_2 + u_{13}x_3 &= y_1 \\ u_{22}x_2 + u_{23}x_3 &= y_2 \\ u_{33}x_3 &= y_3 \end{aligned} \tag{14}$$

These are solved by *back-substituting* the value of x_3 to obtain x_2 and x_1, which are the required solutions of the set of linear equations (2).

2.1 *Exercise problems*

2.1.1. Solve the following set of equations using LU-decomposition method.
2x + 3y + z = 9, x + 2y + 3z = 6, 3x + y + 2z = 8 .

2.1.2. Find the solutions of the following set of linear equations using LU-decomposition method.
3x + 2y + 4z = 7, 2x + y + z = 7, x + 3y +5z = 2 .

2.1.3. Factorize the matrix $A = \begin{bmatrix} 1 & 1 & 1 \\ 4 & 3 & -1 \\ 3 & 5 & 3 \end{bmatrix}$ into a product of lower and upper triangular matrices and find it's inverse.

3 GAUSS ELIMINATION

The Gauss elimination method is a numerical method of solving linear equations. In this section we shall see how this method is applied to solve a system of n linear equations in n variables. The system has the general form,

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots\cdots\cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots\cdots\cdots + a_{2n}x_n &= b_2 \\ &\cdots \\ &\cdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots\cdots\cdots + a_{nn}x_n &= b_n \end{aligned} \tag{15}$$

The solution of the system of equations (15) involves finding n quantities $x_1, x_2, x_3 \cdots\cdots x_n$ such that all the n equations are simultaneously satisfied. This is a non-trivial task when the number of unknowns is large and we have to resort to solving the set numerically.

In the Gauss elimination method, the number of unknowns $[x_1, x_2, \cdots\cdots x_n]$ is reduced sequentially in each equation till one obtains a linear equation involving a single unknown x_n. The value of x_n is *back-substituted* to the preceding equation (which will be a linear equation in two variables) to obtain the solution x_{n-1}. Carrying out this process repeatedly, one obtains numerical values of all the unknowns. The method is illustrated below.

Step 1: Elimination of unknowns. The first equation in the set is known as the *Pivot equation* and the first element of the pivot equation is known as the *Pivot element*. In order to eliminate the first unknown from an equation, we shall subtract the pivot equation multiplied by a carefully chosen constant from the equation.

(Eqn) - [constant](pivot eqn) = (New eqn with one unknown eliminated)

choosing $\frac{a_{21}}{a_{11}}$ to eliminate x_1 from the second equation, we have

$$\begin{aligned} a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n - \frac{a_{21}}{a_{11}} \times [a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n] \\ = b_2 - \frac{a_{21}}{a_{11}} b_1 \end{aligned} \tag{16}$$

$$\begin{aligned} \Rightarrow \left[a_{22} - a_{12}\frac{a_{21}}{a_{11}}\right] x_2 + \left[a_{23} - a_{13}\frac{a_{21}}{a_{11}}\right] x_3 + \cdots\cdots \left[a_{2n} - a_{1n}\frac{a_{21}}{a_{11}}\right] x_n \\ = \left[b_2 - b_1\frac{a_{21}}{a_{11}}\right] \end{aligned} \tag{17}$$

Re-labelling the coefficients,

$$a'_{22}x_2 + a'_{23}x_3 + \cdots\cdots + a'_{2n}x_n = b'_2 \tag{18}$$

Now the unknown x_1 is successfully eliminated from the second equation. Carrying out the same process for all the succeeding equations in (15) we obtain the reduced set of equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots\cdots\cdots\cdots + a_{1n}x_n &= b_1 \\ a'_{22}x_2 + a'_{23}x_3 + \cdots\cdots + a'_{2n}x_n &= b'_2 \\ a'_{32}x_2 + a'_{33}x_3 + \cdots\cdots + a'_{3n}x_n &= b'_3 \\ &\cdots \\ &\cdots \\ a'_{n2}x_2 + a'_{n3}x_3 + \cdots\cdots + a'_{nn}x_n &= b'_n \end{aligned} \tag{19}$$

Now, we shall use the second equation as the pivot equation in order to eliminate the first term in the third and succeeding equations. for the third equation ($a'_{32}x_2 + a'_{33}x_3 + \cdots\cdots + a'_{3n}x_n = b'_3$) we can multiply the second equation ($a'_{22}x_2 + a'_{23}x_3 + \cdots\cdots + a'_{2n}x_n = b'_2$) by $\left(\frac{a'_{32}}{a'_{22}}\right)$ and subtract it from the third to get, after relabelling the coefficients

$$a''_{33}x_3 + a''_{34}x_4 + \cdots\cdots\cdots\cdots a''_{3n}x_n = b''_3$$

Proceeding in a similar manner for all the equations which succeed the third equation, we arrive at the reduced set of equations

$$\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots\cdots\cdots\cdots\cdots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \cdots\cdots\cdots\cdots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + a''_{34}x_4 + \cdots\cdots + a''_{3n}x_n &= b''_3 \\
&\cdots \\
&\cdots \\
a''_{n3}x_3 + a''_{n4}x_4 + \cdots\cdots + a''_{nn}x_n &= b''_n
\end{aligned} \tag{20}$$

Proceeding in this manner, we can eliminate upto the $(n-1)th$ unknown in the n^{th} equation and obtain the set

$$\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots\cdots\cdots\cdots\cdots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \cdots\cdots\cdots\cdots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + a''_{34}x_4 + \cdots\cdots + a''_{3n}x_n &= b''_3 \\
&\cdots \\
&\cdots \\
a^{n-1}_{nn}x_n &= b^{n-1}_n
\end{aligned} \tag{21}$$

From the last equation, one obtains a numerical value for the unknown x_n

$$\left[x_n = \frac{b^{n-1}_n}{a^{n-1}_{nn}}\right] \tag{22}$$

Step 2: Back-substitution. Having obtained a solution for x_n, one can back-substitute it's numerical value into the preceding equation and solve for the unknown x_{n-1}. Similarly one can back-substitute these numerical values to obtain x_{n-2} and proceeding in this fashion one can obtain all the solutions $x_1, x_2, x_3 \cdots\cdots x_n$ of the set of n equations.

3.1 *Pivoting*

In the Gauss elimination method the first linear equation appearing in the set of equations (15) is known as the *pivot equation* and it's first element is known as the *pivot element*. The Gauss elimination method fails if the pivot element is zero and if it is a very small number compared to the other coefficients appearing in the set, then large errors are introduced in the numerical calculation of the solutions. To avoid this problem, we can adopt a method of rearranging the equations known as ***pivoting***.

Pivoting a set of equations involves interchanging the first row of the set (a linear equation) with any other row whose first element is non zero and large. This is known as ***partial pivoting***. If such a coefficient is not available as the first element in any row, then one may search for a suitable coefficient in any other column or row and modify the set of equations accordingly. This method is known as ***complete pivoting***.

An illustrative example of partial pivoting: A set of linear equations in two variables

$$0.000312x_1 + 0.006023x_2 = 0.003328$$
$$0.500000x_1 + 0.894200x_2 = 0.947100$$

Interchanging the rows,

$$0.500000x_1 + 0.894200x_2 = 0.947100$$
$$0.000312x_1 + 0.006023x_2 = 0.003328$$

The new set with pivot element equal to 0.5 can be solved numerically using Gauss elimination.

3.2 *Exercise problems*

3.2.1 Solve the set of linear equations using Gauss elimination method.

$6x + y + z = 20, \quad x + 4y - z = 6, \quad x - y + 5z = 7$

3.2.2 Solve the set of linear equations using Gauss elimination method with pivoting.

$3x + 2y + 4z = 7, \quad 2x + y + z = 7, \quad x + 3y + 5z = 2$

4 GAUSS-JORDAN METHOD

The Gauss-Jordan method is a modification of the Gauss elimination method. In this method when an unknown is eliminated, it is eliminated from all equations and *back-substitution* is not required. The following example is illustrative.

A set of three linear equations in three vriables is

$$\begin{aligned} 2x + y + z &= 10 \\ 3x + 2y + 3z &= 18 \\ x + 4y + 9z &= 16 \end{aligned} \tag{23}$$

Eliminating the first term in the second and third equations,

$$\begin{aligned} 2x + y + z &= 10 \\ 0.5y + 1.5z &= 3 \\ 3.5y + 8.5z &= 11 \end{aligned} \tag{24}$$

Now, eliminating y from the first and third equations, we obtain $x - z = 2$ and $z = 5$. The system of equations reduces to

$$\begin{aligned} x - z &= 2 \\ y + 3z &= 6 \\ z &= 5 \end{aligned} \tag{25}$$

Solving the first two equations using the value of z, the required solutions $[x = 7, y = -9, z = 5]$ are obtained.

4.1 *Exercise problems*

3.2.1 Solve the set of linear equations using Gauss-Jordan method.

$10x + 2y + z = 9, \quad 2x + 20y - 2z = -44, \quad -2x + 3y + 10z = 22$

3.2.2 Solve the set of linear equations given in problem 3.2.1 using Gauss-Jordan method.

5 BIBLIOGRAPHY

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