3 The Direct Solution of a Set of Linear Equations

A typical example of a system of linear equations is:

$$\begin{array}{rcrcrcrcr} 2x_1 & + & 2x_2 & + & 0x_3 & + & 6x_4 & = & 8 \\ 2x_1 & + & x_2 & - & x_3 & + & x_4 & = & 1 \\ 3x_1 & - & x_2 & - & x_3 & + & 2x_4 & = & -3 \\ -x_1 & + & 2x_2 & + & 6x_3 & - & x_4 & = & 4 \end{array}$$

and is usually written in the notation:

$$A\underline{x} = \underline{b},$$

where A is an $n \times n$ matrix and $\underline{b}$ and $\underline{x}$ are column vectors of length n. Before looking at some methods for solving this general type of system we consider, first, some special systems of equations which are particularly easy to solve.

1) A **diagonal** system:

$$\begin{array}{rcrcrcr} 2x_1 & + & 0x_2 & + & 0x_3 & = & 6 \\ 0x_1 & - & 3x_2 & + & 0x_3 & = & -9 \\ 0x_1 & + & 0x_2 & - & x_3 & = & 5 \end{array}$$

2) An **upper triangular** system:

$$\begin{array}{rcrcrcr} 2x_1 & - & x_2 & + & 3x_3 & = & 11 \\ 0x_1 & + & x_2 & - & x_3 & = & 3 \\ 0x_1 & + & 0x_2 & - & 2x_3 & = & 4 \end{array}$$

3) A **lower triangular** system:

$$\begin{array}{rcrcrcr} -3x_1 & + & 0x_2 & + & 0x_3 & = & -6 \\ x_1 & + & 2x_2 & + & 0x_3 & = & -8 \\ 2x_1 & - & x_2 & + & 5x_3 & = & 9 \end{array}$$

These systems get their names because the matrix A in the system of equations is either a diagonal matrix, an upper triangular matrix or a lower triangular system. No matter what the size of the system, such sets of equations are very easy to solve. (Can you solve them?)

The basic idea behind any method for solving a general system of equations is to try and transform it into one or other of these simple systems.

3.1 The basic Gaussian elimination process

Consider the following method for solving:

$$\begin{array}{rcrcrcrcrl} 2x_1 & + & 2x_2 & + & 0x_3 & + & 6x_4 & = & 8 & \quad (1) \\ 2x_1 & + & x_2 & - & x_3 & + & x_4 & = & 1 & \quad (2) \\ 3x_1 & - & x_2 & - & x_3 & + & 2x_4 & = & -3 & \quad (3) \\ -x_1 & + & 2x_2 & + & 6x_3 & - & x_4 & = & 4 & \quad (4)\,. \end{array}$$

Leaving equation (1) and using it to eliminate x_1 from equations (2), (3), and (4) we get:

$$\begin{array}{lcccl} \text{new (2)} & \leftarrow & \text{old (2)} & - & (1.0) \times \text{old (1)} \\ \text{new (3)} & \leftarrow & \text{old (3)} & - & (1.5) \times \text{old (1)} \\ \text{new (4)} & \leftarrow & \text{old (4)} & - & (-0.5) \times \text{old (1)}\,. \end{array}$$

That is:

$$\begin{array}{rcrcrcrcrl} 2x_1 & + & 2x_2 & + & 0x_3 & + & 6x_4 & = & 8 & (1) \\ & - & x_2 & - & x_3 & - & 5x_4 & = & -7 & (2) \\ & - & 4x_2 & - & x_3 & - & 7x_4 & = & -15 & (3) \\ & & 3x_2 & + & 6x_3 & + & 2x_4 & = & 8 & (4)\,. \end{array}$$

Note. The 'new' set of equations has the same solution as the old set of equations.

Now, leaving equation (2) and using it to eliminate x_2 from equations (3) and (4) we get

$$\begin{array}{lcccl} \text{new (3)} & \leftarrow & \text{old (3)} & - & (4.0) \times \text{old (2)} \\ \text{new (4)} & \leftarrow & \text{old (4)} & - & (-3.0) \times \text{old (2)}\ . \end{array}$$

That is:

$$\begin{array}{rcrcrcrcrl} 2x_1 & + & 2x_2 & + & 0x_3 & + & 6x_4 & = & 8 & (1) \\ & - & x_2 & - & x_3 & - & 5x_4 & = & -7 & (2) \\ & & & & 3x_3 & + & 13x_4 & = & 13 & (3) \\ & & & & 3x_3 & - & 13x_4 & = & -13 & (4)\,. \end{array}$$

Finally, eliminating x_3 from (4) using (3) we get:

$$\text{new (4)} \quad \leftarrow \quad \text{old (4)} \quad - \quad (1.0) \times \text{old (3)}\ .$$

That is:

$$\begin{array}{rcrcrcrcrl} 2x_1 & + & 2x_2 & + & 0x_3 & + & 6x_4 & = & 8 & (1) \\ & - & x_2 & - & x_3 & - & 5x_4 & = & -7 & (2) \\ & & & & 3x_3 & + & 13x_4 & = & 13 & (3) \\ & & & & & - & 26x_4 & = & -26 & (4)\,. \end{array}$$

Thus we have transformed the original system to an upper triangular system (without changing the solution). It is now a simple task to solve this upper triangular system giving the solution: $x_4 = 1.0$, $x_3 = 0.0$, $x_2 - 2.0$, $x_1 = -1.0$. This process is usually called **Gaussian elimination with backward substitution.**

3.2 Gaussian elimination using augmented matrix notation

Using augmented matrix notation the set of equations

$$\begin{array}{rcrcrcrcr} 2x_1 & + & 2x_2 & & & + & 6x_4 & = & 8 \\ 2x_1 & + & x_2 & - & x_3 & + & x_4 & = & 1 \\ 3x_1 & - & x_2 & - & x_3 & + & 2x_4 & = & -3 \\ -x_1 & + & 2x_2 & + & 6x_3 & - & x_4 & = & 4 \end{array}$$

is represented by the augmented matrix $A^{(0)}$ given by:

$$A^{(0)} = \begin{bmatrix} 2 & 2 & 0 & 6 & 8 \\ 2 & 1 & -1 & 1 & 1 \\ 3 & -1 & -1 & 2 & -3 \\ -1 & 2 & 6 & -1 & 4 \end{bmatrix} = [A \mid \underline{b}] \, .$$

Using the first equation to eliminate x_1 from the other equations gives us the augmented system:

$$A^{(1)} = \begin{bmatrix} 2 & 2 & 0 & 6 & 8 \\ 0 & -1 & -1 & -5 & -7 \\ 0 & -4 & -1 & -7 & -15 \\ 0 & 3 & 6 & 2 & 8 \end{bmatrix},$$

where the second row is calculated using,

$$A_{2i}^{(1)} = A_{2i}^{(0)} - \left(\frac{A_{21}^{(0)}}{A_{11}^{(0)}} \right) A_{1i}^{(0)} \qquad \text{for } i = 1, 2, \cdots, n+1 = 5,$$

or

$$A_{2i}^{(1)} = A_{2i}^{(0)} - m_{21} A_{1i}^{(0)} \qquad \text{with } m_{21} = \left(\frac{A_{21}^{(0)}}{A_{11}^{(0)}} \right).$$

Generally, we obtain:

$$A_{pi}^{(1)} = A_{pi}^{(0)} - m_{p1} A_{1i}^{(0)} \qquad \text{with } m_{p1} = \left(\frac{A_{p1}^{(0)}}{A_{11}^{(0)}} \right)$$
$$\text{for } i = 1, 2, \cdots, n+1 = 5 \text{ and } p = 2, 3, \cdots, n = 4.$$

Using the new second equation, represented by the second row of the new augmented matrix $A^{(1)}$, to eliminate x_2 from the new third and fourth equations gives us the augmented matrix:

$$A^{(2)} = \begin{bmatrix} 2 & 2 & 0 & 6 & 8 \\ 0 & -1 & -1 & -5 & -7 \\ 0 & 0 & 3 & 13 & 13 \\ 0 & 0 & 3 & -13 & -13 \end{bmatrix},$$

where,

$$A_{pi}^{(2)} = A_{pi}^{(1)} - m_{p2} A_{2i}^{(1)} \qquad \text{with } m_{p2} = \left(\frac{A_{p2}^{(1)}}{A_{22}^{(1)}} \right)$$
$$\text{for } i = (1), 2, \cdots, n = 5 \qquad \text{and } p = 3, \cdots, n = 4.$$

Note: The case $i = 1$ is trivial and gives zero. For this reason, we usually write the 1 in brackets.

Finally, using the latest third equation, represented by the third row of $A^{(2)}$, to eliminate x_3 from the last equation we obtain:

$$A^{(3)} = \begin{bmatrix} 2 & 2 & 0 & 6 & 8 \\ 0 & -1 & -1 & -5 & -7 \\ 0 & 0 & 3 & 13 & 13 \\ 0 & 0 & 0 & -26 & -26 \end{bmatrix} = [U \mid \underline{r}],$$

where,

$$A^{(3)}_{4i} = A^{(2)}_{4i} - m_{43}A^{(2)}_{3i} \quad \text{with } m_{43} = \left(\frac{A^{(2)}_{43}}{A^{(2)}_{33}} \right) \quad \text{for } i = (1,2),3,4,5.$$

Again the cases $i = 1$ and $i = 2$ are trivial. As before, we now have an upper triangular matrix system and obtain the solution by solving:

$$U\underline{x} = \underline{r}.$$

If we want to solve the linear system with not one but **several different right-hand-sides,** i.e.

$$\begin{aligned} A\underline{x} &= \underline{b}, \\ A\underline{y} &= \underline{c}, \\ A\underline{z} &= \underline{d}, \end{aligned}$$

we form the augmented matrix:

$$A^{(0)} = [\ A \mid \ \underline{b} \mid \ \underline{c} \mid \ \underline{d}\ ]$$

which is an $n \times (n+3)$ matrix. We carry out the Gaussian elimination process to produce $A^{(n-1)}$ by computing

$$\begin{aligned} &\text{for } q = 1, 2, \cdots, n-1 \\ &\text{for } p = q+1, \cdots, n \\ &\text{for } i = (1, 2, \cdots, q-1), q, \cdots, n+3 \\ &\quad A^{(q)}_{pi} = A^{(q-1)}_{pi} - m_{pq}A^{(q-1)}_{qi}. \end{aligned}$$

Hence we obtain,

$$A^{(n-1)} = [\ U \mid \ \tilde{\underline{b}} \mid \ \tilde{\underline{c}} \mid \ \tilde{\underline{d}}\ ]$$

and then solve an upper triangular system for each right-hand-side.

$$U\underline{x} = \tilde{\underline{b}}, \quad U\underline{y} = \tilde{\underline{c}}, \quad U\underline{z} = \tilde{\underline{d}}.$$

3.3 An LU factorisation

Another way to solve a system of equations

$$A\underline{x} = \underline{b}$$

is to **factorise** A into the product of two matrices

$$A = LU$$

where L is a lower triangular matrix and U is an upper triangular matrix. We can then obtain $\underline{x}$ by solving

$$\begin{aligned} &1. \quad L\underline{y} = \underline{b}, \\ &2. \quad U\underline{z} = \underline{y}. \end{aligned}$$

Note that,

$$\begin{aligned} L\underline{y} &= \underline{b} \\ \therefore L\left(U\underline{z}\right) &= L\left(\underline{y}\right) = \underline{b} \\ \therefore (LU)\,\underline{z} &= \underline{b} \\ \therefore A\underline{z} &= \underline{b} \end{aligned}$$

Hence, we have $\underline{z} = \underline{x}$ provided that A is non singular.

There are two important questions:-

1. If A is non-singular can we always find an L and a U?
2. If L and U do exist, are they unique?

Unfortunately the answer to both these questions is NO! We shall return to this issue later. For now, we shall assume that the given matrix A does have an LU factorisation. In fact the factorisation will be **unique** if we specify that L has a **unit diagonal** i.e.

$$(L)_{ii} = 1 \text{ for } i = 1, 2, \cdots, n$$

For example, using the same 4×4 matrix as above, we write

$$A = \begin{bmatrix} 2 & 2 & 0 & 6 \\ 2 & 1 & -1 & 1 \\ 3 & -1 & -1 & 2 \\ -1 & 2 & 6 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix}$$

$$= \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} & l_{21}u_{14} + u_{24} \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} = LU.$$

Comparing the first row of LU with the first row of A we find that

$$u_{11} = 2,\ u_{12} = 2,\ u_{13} = 0,\ u_{14} = 6.$$

Comparing the second row of LU with the second row of A we find, after some trivial algebra, that

$$l_{21} = 1,\ u_{22} = -1,\ u_{23} = -1,\ u_{24} = -5.$$

The third row of LU gives,

$$\begin{aligned} A_{31} &= l_{31}u_{11}, \qquad \therefore l_{31} = 1.5 \\ A_{32} &= l_{31}u_{12} + l_{32}u_{22}, \qquad \therefore l_{32} = 4 \\ A_{33} &= l_{31}u_{13} + l_{32}u_{23} + u_{33}, \qquad \therefore u_{33} = 3 \\ A_{34} &= l_{31}u_{14} + l_{32}u_{24} + u_{34}, \qquad \therefore u_{34} = 13. \end{aligned}$$

Finally, comparing the fourth row of LU with the fourth row of A we find that:

$$l_{41} = -0.5,\ l_{42} = -3,\ l_{43} = 1,\ u_{44} = -26.$$

Thus

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1.5 & 4 & 1 & 0 \\ -0.5 & -3 & 1 & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 2 & 2 & 0 & 6 \\ 0 & -1 & -1 & -5 \\ 0 & 0 & 3 & 13 \\ 0 & 0 & 0 & -26 \end{bmatrix}.$$

You should note the similarity between U and the triangular matrix in $A^{(3)}$ above and compare the values of l_{ij} with the coefficients m_{ij}. We now solve

$$L\underline{y} = \underline{b} = \begin{bmatrix} 8 \\ 1 \\ -3 \\ 4 \end{bmatrix} \qquad \therefore \underline{y} = \begin{bmatrix} 8 \\ -7 \\ 13 \\ -26 \end{bmatrix}$$

and then solve

$$U\underline{x} = \underline{y} = \begin{bmatrix} 8 \\ -7 \\ 13 \\ -26 \end{bmatrix} \qquad \therefore \underline{x} = \begin{bmatrix} -1 \\ 2 \\ 0 \\ 1 \end{bmatrix}.$$

This final stage is exactly the same as solving $U\underline{x} = \underline{r}$ in the Gaussian elimination process. Moreover, the entries l_{ij} of the matrix L are identical to the m_{ij}. Thus the LU decomposition and Gaussian elimination are essentially the same process devised by a different mechanism.

3.4 Gaussian elimination with row interchanges

Consider the system of equations

$$\begin{array}{rcrcrcrl} 0x_1 & + & 3x_2 & - & x_3 & = & 1 & \quad (1) \\ x_1 & - & x_2 & - & 3x_3 & = & -4 & \quad (2) \\ 3x_1 & - & 3x_2 & + & x_3 & = & 8 & \quad (3) \end{array}$$

which has the augmented matrix

$$A^{(0)} = \begin{bmatrix} 0 & 3 & -1 & 1 \\ 1 & -1 & -3 & -4 \\ 3 & -3 & 1 & 8 \end{bmatrix}.$$

Standard Gaussian elimination **breaks down** because $\left(A^{(0)}\right)_{11} = 0$. That is, we cannot use equation (1) to eliminate x_1 from equations (2) and (3). If we interchange equations (1) and (3), we can use the new first equation to eliminate x_1 from the other two. That is

$$\begin{array}{rcrcrcr} 3x_1 & - & 3x_2 & + & x_3 & = & 8 \\ x_1 & - & x_2 & - & 3x_3 & = & -4 \\ 0x_1 & + & 3x_2 & - & x_3 & = & 1 \end{array}$$

$$\downarrow \text{Gaussian elimination (first stage)}$$

$$\begin{array}{rcrcrcr} 3x_1 & - & 3x_2 & + & x_3 & = & 8 \\ 0x_1 & - & 0x_2 & - & \frac{10}{3}x_3 & = & -\frac{20}{3} \\ 0x_1 & + & 3x_2 & - & x_3 & = & 1 \end{array}$$

Gaussian elimination breaks down again because we cannot use the second equation to eliminate x_2 from the third equation. However, if we perform another row interchange and swap equations (2) and (3) we get

$$\begin{array}{rcrcrcr} 3x_1 & - & 3x_2 & + & x_3 & = & 8 \\ & & 3x_2 & - & x_3 & = & 1 \\ & & & - & \frac{10}{3}x_3 & = & -\frac{20}{3} \end{array}$$

and the triangular system can now be simply solved.

Using augmented matrices, we write

$$A^{(0)} = \begin{bmatrix} 0 & 3 & -1 & 1 \\ 1 & -1 & -3 & -4 \\ 3 & -3 & 1 & 8 \end{bmatrix}.$$

Interchanging rows 1 and 3 we get

$$\begin{aligned} \tilde{A}^{(0)} &= \begin{bmatrix} 3 & -3 & 1 & 8 \\ 1 & -1 & -3 & -4 \\ 0 & 3 & -1 & 1 \end{bmatrix} \\ &= P_1 A^{(0)} \end{aligned}$$

where

$$P_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

is a 'permutation matrix.' The first stage of Gaussian elimination gives

$$\begin{aligned} A^{(1)} &= \begin{bmatrix} 3 & -3 & 1 & 8 \\ 0 & 0 & -\frac{10}{3} & -\frac{20}{3} \\ 0 & 3 & -1 & 1 \end{bmatrix} \\ &= M_1 \tilde{A}^{(0)} \end{aligned}$$

with

$$M_1 = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{3} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Interchanging rows 2 and 3 we get

$$\begin{aligned} \tilde{A}^{(1)} &= \begin{bmatrix} 3 & -3 & 1 & 8 \\ 0 & 3 & -1 & 1 \\ 0 & 0 & -\frac{10}{3} & -\frac{20}{3} \end{bmatrix} \\ &= P_2 A^{(1)} \end{aligned}$$

where

$$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

The second stage of Gaussian elimination gives

$$A^{(2)} = M_2 \tilde{A}^{(1)} = \tilde{A}^{(1)} \text{ with } M_2 = I,$$

since $m_{32} = \tilde{A}^{(1)}_{32} / \tilde{A}^{(1)}_{22} = 0$.

We note that

$$\begin{aligned} A^{(0)} &= [A \mid \underline{b}] \\ \tilde{A}^{(0)} &= [P_1 A \mid *] \\ A^{(1)} &= [M_1 P_1 A \mid *] \\ \tilde{A}^{(1)} &= [P_2 M_1 P_1 A \mid *] \\ A^{(2)} &= [M_2 P_2 M_1 P_1 A \mid *] \\ &= [U \mid *] \\ \therefore\ M_2 P_2 M_1 P_1 A &= U \\ \therefore\ A &= (M_2 P_2 M_1 P_1)^{-1} U \\ &= P_1^{-1} M_1^{-1} P_2^{-1} M_2^{-1} U. \end{aligned}$$

However, $P_1^{-1} = P_1$, $P_2^{-1} = P_2$ and

$$M_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad M_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Hence we have the factorisation,

$$\begin{aligned} A &= P_1 P_2 \left(P_2 M_1^{-1} P_2\right) M_2^{-1} U \\ &= QLU \end{aligned}$$

where

$$\begin{aligned} Q &= P_1 P_2 \\ L &= P_2 M_1^{-1} P_2 M_2. \end{aligned}$$

More generally, (for a set of 4 equations)

$$\begin{aligned} U &= M_3 P_3 M_2 P_2 M_1 P_1 A \\ A &= P_1 M_1^{-1} P_2 P_3 P_3 M_2^{-1} P_3 M_3^{-1} U \\ &= P_1 P_2 P_3 \left(P_3 P_2 M_1^{-1} P_2 P_3\right) \left(P_3 M_2^{-1} P_3\right) M_3^{-1} U \\ &= QLU \end{aligned}$$

where

$$\begin{aligned} Q &= P_1 P_2 P_3 \\ L &= \left(P_3 P_2 M_1^{-1} P_2 P_3\right) \left(P_3 M_2^{-1} P_3\right) M_3^{-1}. \end{aligned}$$

Also note, if $P_i = I$ for all i (i.e. no row interchanges)

$$\begin{aligned} A &= M_1^{-1} M_2^{-1} M_3^{-1} U \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ m_{21} & 1 & 0 & 0 \\ m_{31} & m_{32} & 1 & 0 \\ m_{41} & m_{42} & m_{43} & 1 \end{bmatrix} [U] \\ &= LU \end{aligned}$$

as before.

Although we shall not prove this, we have the following result.

If A is a **non-singular** matrix then $A\underline{x} = \underline{b}$ can always be reduced to the upper triangular system $U\underline{x} = \underline{y}$ provided that we allow for the possibility of **row interchanges.**

Or, equivalently:

Every non-singular matrix A can be factorised into

$$A = QLU$$

where

Q	is a permutation matrix
L	is a lower triangular matrix
U	is an upper triangular matrix.

However, this factorisation is **NOT unique.** We have to make a number of decisions

1. When do we do a row interchange?
2. Which rows do we interchange?

The answer to *when do we do a row interchange* seems obvious, namely when $A_{pp}^{(p-1)} = 0$ and the Gaussian Elimination process breaks down. However, that rule ignores the fact that in practice the computation will be done by computer and rounding errors will be present in the calculations.

Example

If the above system of three equations is solved working to three significant figures, i.e. using three digit decimal floating point numbers, the first augmented matrix $A^{(0)}$ is

$$A^{(0)} = \begin{bmatrix} 0 & 3 & -1 & 1 \\ 1 & -1 & -3 & -4 \\ 3 & -3 & 1 & 8 \end{bmatrix}.$$

Interchanging rows 1 and 3 because $A_{11}^{(0)} = 0$ gives

$$\tilde{A}^{(0)} = \begin{bmatrix} 3 & -3 & 1 & 8 \\ 1 & -1 & -3 & -4 \\ 0 & 3 & -1 & 1 \end{bmatrix}.$$

Eliminating the first column

$$m_{21} = \tilde{A}_{21}^{(0)}/\tilde{A}_{11}^{(0)} = 0.333$$
$$m_{31} = 0$$

giving

$$A^{(1)} = \begin{bmatrix} 3 & -3 & 1 & 8 \\ * & -0.001 & -3.33 & -6.66 \\ * & 3 & -1 & 1 \end{bmatrix}.$$

No interchange is required since $A_{22}^{(1)} \neq 0$. Eliminating the second column

$$m_{32} = -3000$$

giving

$$A^{(2)} = \begin{bmatrix} 3 & -3 & 1 & 8 \\ * & -0.001 & -3.33 & -6.66 \\ * & * & -9990 & -20000 \end{bmatrix}.$$

Solving this triangular system gives

$$x_1 = 2.00,\ x_2 = 0.00,\ x_3 = 2.00$$

but the exact answer is $[3, 1, 2]^T$. Thus this simple method for choosing when to do a row interchange can give the wrong answer.

3.5 Gaussian elimination with partial pivoting

Gaussian elimination with partial pivoting is a method that automates the decision on when to do row interchanges in the following way. At each stage of the Gaussian elimination process, the column

$$\begin{bmatrix} A_{pp}^{(p-1)} \\ \vdots \\ A_{np}^{(p-1)} \end{bmatrix}$$

is scanned and the first element of maximum modulus is found. That is we find I as the smallest value in $p \leq I \leq n$ such that

$$\left| A_{Ip}^{(p-1)} \right| \geq \left| A_{ip}^{(p-1)} \right| \quad \text{for } i = p, p+1, \cdots, n.$$

We then interchange the Ith and the pth rows. Thus we do an interchange at every stage of the Gaussian elimination process except when I turns out to be equal to p.

Consider the following example in which the first augmented matrix $A^{(0)}$ is

$$A^{(0)} = \begin{bmatrix} 1 & -1 & -1 & 2 & 6 \\ 0 & 4 & 4 & -1 & -13 \\ 2 & 2 & 1 & -3 & -6 \\ 1 & 0 & -2 & 1 & 4 \end{bmatrix}.$$

The first pivotal element is in the third row so we interchange rows 1 and 3

$$\tilde{A}^{(0)} = \begin{bmatrix} 2 & 2 & 1 & -3 & -6 \\ 0 & 4 & 4 & -1 & -13 \\ 1 & -1 & -1 & 2 & 6 \\ 1 & 0 & -2 & 1 & 4 \end{bmatrix}.$$

Eliminating the first column gives,

$$A^{(1)} = \begin{bmatrix} 2 & 2 & 1 & -3 & -6 \\ * & 4 & 4 & -1 & -13 \\ * & -2 & -\frac{3}{2} & \frac{7}{2} & 9 \\ * & -1 & -\frac{5}{2} & \frac{5}{2} & 7 \end{bmatrix}.$$

The second pivotal element is in the second row, no interchange is required. Eliminating the second column gives,

$$A^{(2)} = \begin{bmatrix} 2 & 2 & 1 & -3 & -6 \\ * & 4 & 4 & -1 & -13 \\ * & * & \frac{1}{2} & 3 & \frac{5}{2} \\ * & * & -\frac{3}{2} & \frac{9}{4} & \frac{15}{4} \end{bmatrix}.$$

The third pivotal element is in the fourth row, we interchange rows 3 and 4

$$\tilde{A}^{(2)} = \begin{bmatrix} 2 & 2 & 1 & -3 & -6 \\ * & 4 & 4 & -1 & -13 \\ * & * & -\frac{3}{2} & \frac{9}{4} & \frac{15}{4} \\ * & * & \frac{1}{2} & 3 & \frac{5}{2} \end{bmatrix}.$$

Eliminating the third column gives,

$$A^{(3)} = \begin{bmatrix} 2 & 2 & 1 & -3 & -6 \\ * & 4 & 4 & -1 & -13 \\ * & * & -\frac{3}{2} & \frac{9}{4} & \frac{15}{4} \\ * & * & * & \frac{15}{4} & \frac{15}{4} \end{bmatrix}.$$

Solving the upper triangular matrix system using back substitution gives the solution

$$x = [1, -2, -1, 1]^T.$$

3.6 Cholesky's method

Cholesky's method is a method for solving a linear system of equations $A\underline{x} = \underline{b}$ for the special case when A is a **symmetric positive definite matrix.** That is when

1. $A^T = A$

2. All the eigenvalues of A are positive.

Such systems occur in a very wide range of important applications usually associated with a 'minimum energy principle'. Cholesky's method relies on the following result.

Any **symmetric positive definite** matrix A can be factorised into

$$A = DD^T$$

where D is a **lower triangular** matrix.

Thus to solve

$$\begin{bmatrix} 1 & -3 & 4 \\ -3 & 34 & -17 \\ 4 & -17 & 18 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 9 \\ 38 \\ 25 \end{bmatrix},$$

we have

$$DD^T = \begin{bmatrix} d_{11} & 0 & 0 \\ d_{21} & d_{22} & 0 \\ d_{31} & d_{32} & d_{33} \end{bmatrix} \begin{bmatrix} d_{11} & d_{21} & d_{31} \\ 0 & d_{22} & d_{32} \\ 0 & 0 & d_{33} \end{bmatrix}.$$

Multiplying the first row of D by D^T we have,

$$\begin{array}{rclcrcl} d_{11}^2 & = & +1 & \therefore & d_{11} & = & +1 \quad (\text{ we could take } -1) \\ d_{11}d_{21} & = & -3 & \therefore & d_{21} & = & -3 \\ d_{11}d_{31} & = & 4 & \therefore & d_{31} & = & 4. \end{array}$$

Multiplying the 2^{nd} row of D by D^T gives,

$$\begin{aligned} d_{21}d_{11} &= -3 \ \rightarrow \text{this does not add any new information} \\ d_{21}^2 + d_{22}^2 &= 34 \ \therefore \ d_{22} = \sqrt{34-9} = +5 \quad (\text{ we could take } -5) \\ d_{21}d_{31} + d_{22}d_{32} &= -17 \ \therefore \ d_{32} = -1. \end{aligned}$$

Multiplying the 3^{rd} row of D by D^T, we see that the only new information is provided by,

$$d_{31}^2 + d_{32}^2 + d_{33}^2 = 18 \ \therefore \ d_{33} = +1 \quad (\text{ we could take } -1.)$$

Thus

$$D = \begin{bmatrix} 1 & 0 & 0 \\ -3 & 5 & 0 \\ 4 & -1 & 1 \end{bmatrix}.$$

Solving

$$D\underline{y} = \underline{b}$$

gives

$$\underline{y} = \begin{bmatrix} 9 \\ 13 \\ 2 \end{bmatrix}$$

and solving

$$D^T \underline{x} = \underline{y}$$

gives, finally,

$$\underline{x} = \begin{bmatrix} 10 \\ 3 \\ 2 \end{bmatrix}.$$

3.7 An ill-conditioned system

Consider the system of equations

$$\begin{array}{lclcl} 3x & + & 2y & = & 0 \\ 6.0001x & + & 4y & = & 1 \end{array}$$

which has solution $x = 10000$, $y = -15000$. If we use a computer working to four significant figures the matrix used would be stored as

$$\begin{bmatrix} 3.000 & 2.000 \\ 6.000 & 4.000 \end{bmatrix}$$

and would be singular. Working to five significant figures then

$$\begin{bmatrix} 3.0000 & 2.0000 \\ 6.0001 & 4.0000 \end{bmatrix}$$

but rounding errors will effect the 4^{th} decimal place and may severely affect the answer. The problem here is that the matrix is very nearly singular and small errors, perhaps the size of ever present rounding errors, could cause major changes in the solution. It is necessary to be aware of this problem and good software will detect it and give a warning.

Definition of ill-conditioned

A problem is ill-conditioned if a small relative change in the data causes a large relative change in the answer.

We note that in the above example changing A_{21} from 6.0001 to 6.0002 changes the answer by a factor of 2. That is changing one element by 0.002% changes the answer by 50%. Moreover, changing A_{21} to 6 then there are no solutions at all.