Gaussian Elimination

The main problem to be considered here is the solution of the following matrix equation for the unknown column vector **x**

$$\mathbf{Ax} = \mathbf{b} \ .$$

Consider the scalar case

$$a_{11}x_1 = b_1 \ .$$

The solution is found by dividing by the lead coefficient, or

$$a_{11}^{-1}a_{11}x_1 = 1 \cdot x_1 = a_{11}^{-1}b_1 \ ,$$

or

$$x_1 = a_{11}^{-1}b_1 \ .$$

The same process carries over to matrices. We pre–multiply the matrix equation by an inverse of **A** which has the property that it's product with **A** gives an identity matrix. The identity matrix multiplied by a matrix leaves the original matrix unchanged, i.e.

$$\mathbf{A}^{-1}\mathbf{Ax} = \mathbf{Ix} = \mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \ ,$$

where the inverse is defined by the equation

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{I} \ .$$

The identity, **I**, has 1's on the main–diagonal and 0's elsewhere. The above procedure gives the solution

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \ .$$

The main task here is to find the inverse of **A**, which is a difficult and computationally expensive process. An alternative method is Gauss elimination. Note that Gauss elimination may also be used to find the inverse, though it is not necessary to do so.

Gauss elimination operates directly on the system of linear equations

$$\sum_{j=1}^{N} a_{ij}x_j = b_i \qquad\qquad i = 1, \ldots, N \ .$$

Consider, the simple example

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 &= b_1 \\ a_{21}x_1 + a_{22}x_2 &= b_2 \ , \end{aligned}$$

in the particular form

$$\begin{aligned} x_1 + x_2 &= 3 \\ 2x_1 + x_2 &= 1 \ . \end{aligned}$$

Multiply the first equation by 2 and subtract from second equation to get

$$\begin{aligned} x_1 + x_2 &= 3 \\ -x_2 &= -5 \ . \end{aligned}$$

Solve the second equation for $x_2 = 5$ and substitute into the first equation to obtain $x_1 = -2$. The generalization of this simple procedure to N equations in N unknowns is the Gaussian elimination method (what we will call *Naive Gauss Elimination*). The trick is to carefully keep track of all the steps in the above process. Consider the general case:

$$\begin{array}{ccccccccc} a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + \cdots + & a_{1N}x_N & = & b_1 \\ \boxed{a_{21}x_1} & + & a_{22}x_2 & + & a_{23}x_3 & + \cdots + & a_{2N}x_N & = & b_2 \\ \boxed{a_{31}x_1} & + & a_{32}x_2 & + & a_{33}x_3 & + \cdots + & a_{3N}x_N & = & b_3 \\ \vdots & & \vdots & & \vdots & & \vdots & & \vdots \\ \boxed{a_{N1}x_1} & + & a_{N2}x_2 & + & a_{N3}x_3 & + \cdots + & a_{NN}x_N & = & b_N \end{array}$$

We want to eliminate all terms in the box using the first equation. The first

step is to multiply the first equation by some number and add it to the second equation to eliminate the first term (the underlined term above). Therefore, multiply the first equation by a_{21}/a_{11} and subtract from the second equation. The second equation then becomes

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2N}x_N$$

$$- \frac{a_{21}}{a_{11}}\left[a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1N}x_N\right] = b_2 - \frac{a_{21}}{a_{11}}b_1 \ .$$

Combing terms and factoring the x's gives

$$\underline{\left[a_{21} - \frac{a_{21}}{a_{11}}a_{11}\right]}x_1 + \left[a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right]x_2 + \cdots + \left[a_{2N} - \frac{a_{21}}{a_{11}}a_{1N}\right]x_N$$

$$= b_2 - \frac{a_{21}}{a_{11}}b_1 \ .$$

Notice that the underlined term goes to zero (which is what we want), and the above equation becomes

$$\left[a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right]x_2 + \cdots + \left[a_{2N} - \frac{a_{21}}{a_{11}}a_{1N}\right]x_N = b_2 - \frac{a_{21}}{a_{11}}b_1 \ . \quad \text{(A)}$$

Notice a couple of things. First, the x_1 term has been eliminated. Second, the only things that have changed in the equations are the coefficients and every coefficient has been changed. Effectively, the second equation has become

$$a'_{21}x_1 + a'_{22}x_2 + a'_{23}x_3 + \cdots + a'_{2N}x_N = b'_2 \ ,$$

where the primed coefficients are given from (A). Now consider a general equation in the m'th "row" (where m=2,...,N), i.e.

$$
\begin{aligned}
&a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1N}x_N = b_1 \\
&a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2N}x_N = b_2 \\
&\vdots \qquad \vdots \qquad \vdots \qquad\qquad \vdots \qquad \vdots \\
&\boxed{a_{m1}x_1} + a_{m2}x_2 + a_{m3}x_3 + \cdots + a_{mN}x_N = b_m \\
&\vdots \qquad \vdots \qquad \vdots \qquad\qquad \vdots \qquad \vdots \\
&a_{N1}x_1 + a_{N2}x_2 + a_{N3}x_3 + \cdots + a_{NN}x_N = b_N
\end{aligned}
$$

To eliminate the boxed term just multiply the first equation by a_{m1}/a_{11} and subtract from the m'th equation. This gives

$$
\left[a_{m2} - \frac{a_{m1}}{a_{11}}a_{12}\right]x_2 + \cdots + \left[a_{mN} - \frac{a_{m1}}{a_{11}}a_{1N}\right]x_N = b_m - \frac{a_{m1}}{a_{11}}b_1 \ .
$$

If these coefficients give new coefficients a_{ij} and b_i (and we replace those coefficients in the manner of a Fortran program) then the new "b" on the right hand side is

$$
\text{new "b"} \nearrow \quad b_m = b_m - \frac{a_{m1}}{a_{11}}b_1 \ . \quad \nwarrow \text{old "b"}
$$

Now let's redo the above operations and look at how a general "a" coefficient is modified. Consider a general term at the n position of the first and m'th equations (where n=2,...,N)

$$
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n + \cdots + a_{1N}x_N = b_1
$$

$$
a_{m1}x_1 + a_{m2}x_2 + a_{m3}x_3 + \cdots + a_{mn}x_n + \cdots + a_{mN}x_N = b_m \ .
$$

Again, multiply the first equation by a_{m1}/a_{11} and subtract from the m'th equation to obtain

$$a_{m1}x_1 + a_{m2}x_2 + a_{m3}x_3 + \cdots + a_{mn}x_n + \cdots + a_{mN}x_N$$
$$- \frac{a_{m1}}{a_{11}}\left[a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n + \cdots + a_{1N}x_N\right]$$
$$= b_m - \frac{a_{m1}}{a_{11}}b_1 \ .$$

Grouping terms gives the following equation

$$\left[a_{m1} - \frac{a_{m1}}{a_{11}}a_{11}\right]^{0} x_1 + \left[a_{m2} - \frac{a_{m1}}{a_{11}}a_{12}\right]x_2 + \cdots$$
$$+ \underline{\left[a_{mn} - \frac{a_{m1}}{a_{11}}a_{1n}\right]}x_n + \cdots + \left[a_{mN} - \frac{a_{m1}}{a_{11}}a_{1N}\right]x_N = b_m - \frac{a_{m1}}{a_{11}}b_1$$

Again, the new ”b” coefficient is

$$b_m = b_m - \frac{a_{m1}}{a_{11}}b_1$$

and the new (m,n) ”a” coefficient (i.e. the underlined coefficient of x_n) is

$$a_{mn} = a_{mn} - \frac{a_{m1}}{a_{11}}a_{1n} \ .$$

Therefore, the new m’th equation has the form

$$0 + a_{m2}x_2 + a_{m3}x_3 + \cdots + a_{mn}x_n + \cdots + a_{mN}x_N = b_m$$

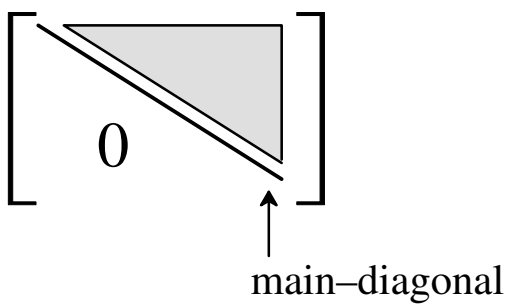
Providing that we use the new coefficients defined above. After applying this process to the full equation set, we end up with

$$
\begin{aligned}
& a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1N}x_N = b_1 \\
0 \; & + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2N}x_N = b_2 \\
0 \; & + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3N}x_N = b_3 \\
\vdots \; & \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\
0 \; & + a_{N2}x_2 + a_{N3}x_3 + \cdots + a_{NN}x_N = b_N
\end{aligned}
$$

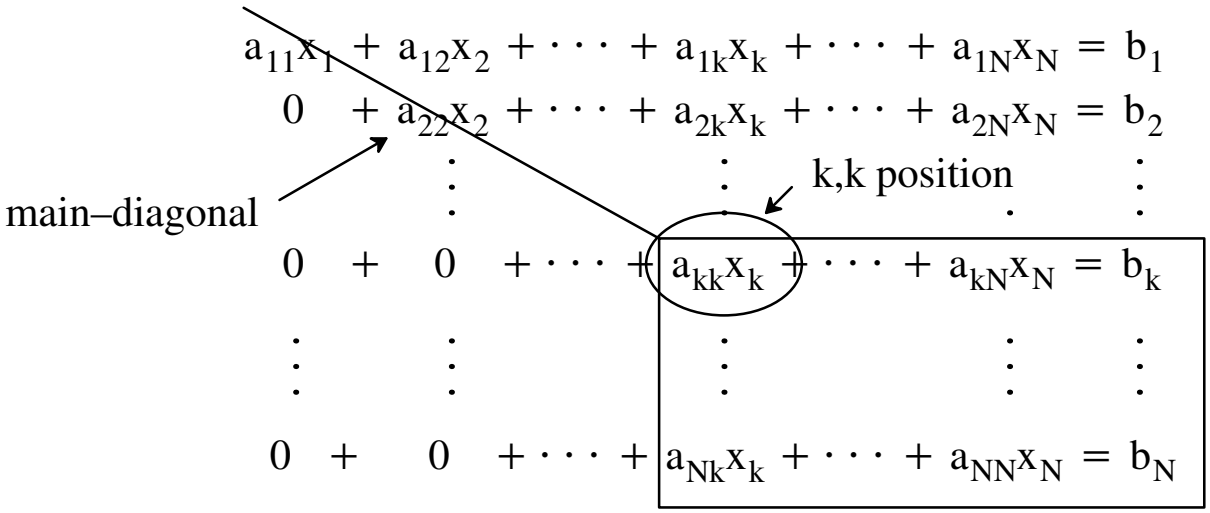
Now do the same the same thing but with the subset of the original equations which are boxed above. The (2,2) dashed underlined term is used to eliminate all the x_2 terms in the m=3,...,N equations, giving

$$
\begin{aligned}
& a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1N}x_N = b_1 \\
0 \; & + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2N}x_N = b_2 \\
0 \; & + \; 0 \; + a_{33}x_3 + \cdots + a_{3N}x_N = b_3 \\
\vdots \; & \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\
0 \; & + \; 0 \; + a_{N3}x_3 + \cdots + a_{NN}x_N = b_N
\end{aligned}
$$

This process continues. We proceed down the main diagonal, using each new main diagonal term to eliminate all terms in the column below the main diagonal. The end result is an upper triangular matrix, i.e.



In order to implement the Gaussian elimination algorithm, we need to figure out how to modify a general coefficient in the matrix. Suppose that we are dealing with the subset of equations whose upper left–hand element is at the (k,k) position along the main–diagonal (where k=1,...,N)



We can eliminate the column below the (k,k) position in the same way we eliminated the other columns (i.e. it is the same problem as we had for the first column, except now the first column is k). Therefore, consider the subset of boxed equations shown above:

$$
\begin{array}{llll}
\underline{a_{kk}x_k} & + a_{kk+1}x_{k+1} & + \cdots + a_{kN}x_N & = b_k \\
a_{k+1k}x_k & + a_{k+1k+1}x_{k+1} & + \cdots + a_{k+1N}x_N & = b_{k+1} \\
\vdots & \vdots & \vdots & \vdots \\
\boxed{a_{mk}x_k} & + a_{mk+1}x_{k+1} & + \cdots + a_{mN}x_N & = b_m \\
\vdots & \vdots & \vdots & \vdots \\
a_{Nk}x_k & + a_{Nk+1}x_{k+1} & + \cdots + a_{NN}x_N & = b_N
\end{array}
$$

As before, we want to eliminate all terms underneath the underlined term. In the general case we want to eliminate the first term in the m'th equation (i.e. the boxed term, where m=k+1,...,N) using the first term in the k'th equation (i.e. the underlined term). Consider the k'th and m'th equations:

$$a_{kk}x_k + a_{kk+1}x_{k+1} + \cdots + \underline{a_{kn}x_n} + \cdots + a_{kN}x_N = b_k$$

$$a_{mk}x_1 + a_{mk+1}x_{k+1} + \cdots + \underline{a_{mn}x_n} + \cdots + a_{mN}x_N = b_m$$

General n'th column terms have also been identified in both equations (the underlined terms). Now multiply the k'th equation by a_{mk}/a_{kk} and subtract from the m'th equation to obtain the new m'th equation

$$\left[a_{mk} - \frac{a_{mk}}{a_{kk}}a_{kk}\right]x_k + \left[a_{mk+1} - \frac{a_{mk}}{a_{kk}}a_{kk+1}\right]x_{k+1} + \cdots$$
$$+ \underline{\left[a_{mn} - \frac{a_{mk}}{a_{kk}}a_{kn}\right]}x_n + \cdots + \left[a_{mN} - \frac{a_{mk}}{a_{kk}}a_{kN}\right]x_N = \underline{b_m - \frac{a_{mk}}{a_{kk}}b_k}$$

Notice that the first term on the left hand side is zero, as desired, and the above equation becomes

$$0 + \left[a_{mk+1} - \frac{a_{mk}}{a_{kk}}a_{kk+1}\right]x_{k+1} + \cdots + \underline{\left[a_{mn} - \frac{a_{mk}}{a_{kk}}a_{kn}\right]}x_n + \cdots$$
$$+ \left[a_{mN} - \frac{a_{mk}}{a_{kk}}a_{kN}\right]x_N = \underline{b_m - \frac{a_{mk}}{a_{kk}}b_k}$$

The new "a" coefficient at a general (m,n) position in the above equation is the underlined term, which is

$$a_{mn} = a_{mn} - \frac{a_{mk}}{a_{kk}}a_{kn} \ , \qquad \begin{matrix} m = k+1, ..., N \\ n = k+1, ..., N \ , \end{matrix}$$

while the new "b" coefficient is (the dashed underlined term)

$$b_m = b_m - \frac{a_{mk}}{a_{kk}}b_k \ .$$

The first part of the Gauss–Elimination algorithm is:

1. Cycle through the elements of the main diagonal with k=1,...,N, where the *current diagonal position* is (k,k).

2. Eliminate all terms below the current diagonal position.

a. cycle an index through all terms below the current diagonal position, say m=k+1,...,N

b. modify all terms in the equation using

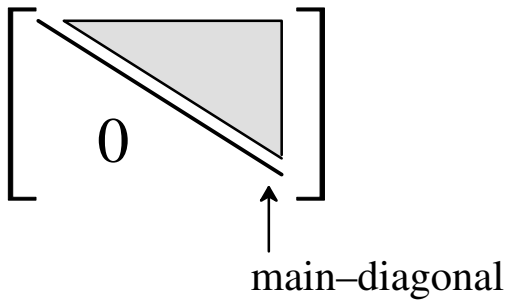
$$a_{mn} = a_{mn} - \frac{a_{mk}}{a_{kk}} a_{kn} \ , \qquad n = k, ..., N$$

Note that this automatically sets the (m,k) term to zero.

c. modify the right hand side using

$$b_m = b_m - \frac{a_{mk}}{a_{kk}} b_k \ .$$

The end result of the above algorithm is an upper triangular matrix of the form



The last equation will have zero's to the left of the main–diagonal and a non–zero main–diagonal term (i.e. (N,N)):

$$a_{NN} x_N = b_N \ .$$

Solve this equation for x_N. The second to last equation is

$$a_{N-1N-1}x_{N-1} + a_{N-1N}x_N = b_{N-1} \ .$$

Substitute the solution for x_N into this equation and solve for x_{N-1}. In general, the original system of equations, namely

$$\sum_{j=1}^{N} a_{ij}x_j = b_i \qquad i = 1, \ldots, N \ ,$$

has been changed to the following upper triangular system (note that the diagonal term is (i,i) and so all terms with j<i are zero)

$$\sum_{j=i}^{N} a_{ij}x_j = b_i \qquad i = 1, \ldots, N$$

If we solve from the bottom of the matrix to the top of the matrix, then the only unknown in any given equation is the main diagonal term. Split this term off from the above equation as follows

$$a_{ii}x_i + \sum_{j=i+1}^{N} a_{ij}x_j = b_i$$

and solve for the unknown x_i:

$$x_i = \frac{1}{a_{ii}}\left[b_i - \sum_{j=i+1}^{N} a_{ij}x_j\right] \qquad i = N-1, \ldots, 1$$

given that

$$x_N = \frac{b_N}{a_{NN}} \ .$$

This process is called *back–substitution*. This completes the Gauss Elimination algorithm. In many cases the above algorithm will work. However, it can run into problems.

Pivoting

We will call the above algorithm Naive Gauss Elimination because it does not always work. Consider the following example

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 1 \\ 2x_1 + 4x_2 + x_3 &= 3 \\ 0 + x_2 + x_3 &= 2 \end{aligned}$$

Gauss elimination starts by multiplying the first equation by 2 and subtracting the result from the second equation to give

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 1 \\ 0 + \underline{0} - x_3 &= 1 \\ 0 + x_2 + x_3 &= 2 \end{aligned} \qquad \text{(B)}$$

The problem here is that there is a zero in the diagonal position of the second equation (the underlined term). We cannot use the underlined diagonal term to eliminate the x_2 term in the third equation.

Pivoting is a strategy to get around the above problem. For example, in the above system we could interchange the second and third equations to obtain

$$\begin{aligned} x_1 + 2x_2 + x_3 &= 1 \\ 0 + x_2 + x_3 &= 2 \\ 0 + 0 - x_3 &= 1 \end{aligned}$$

Now there is a non–zero element in the (2,2) position. In fact, the problem here is upper triangular and so we can proceed with back–substitution. *Row pivoting* interchanges rows, as in the above example. Note that in matrix form equation (B), i.e.

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & 0 & -1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}, \qquad \text{(C)}$$

has been changed to

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}.$$

This means that the coefficients of both ”a” and ”b” have been changed and the program must keep track of these changes. Another strategy is to interchange the second and third ”columns” in (B):

$$\begin{aligned} x_1 + x_3 + 2x_2 &= 1 \\ 0 - x_3 + 0 &= 1 \\ 0 + \underline{x_3} + x_2 &= 2 \end{aligned}$$

Again, the underlined main–diagonal term is non–zero and we may continue with the Gauss elimination algorithm. This is called *column pivoting*. In matrix notation, the original matrix problem (C) has been changed to

$$\begin{bmatrix} 1 & 1 & 2 \\ 0 & -1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_3 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}, \qquad \text{(C)}$$

Notice that ”b” is unchanged, but the coefficients of ”a” and the order of unknowns in ”x” have been changed.

Most Gauss Elimination algorithms use both column and row pivoting. In

a true pivoting algorithm, the program searches through the columns and rows for the largest element and transfers that one to the main diagonal. Algorithms with only row or column interchanges, i.e. not both, are said to have *partial pivoting*. Obviously, pivoting involves a lot of work and the program must keep track of all the row and column interchanges. For many applications the naive Gauss elimination algorithm is adequate and faster than algorithms with pivoting.

Ill–Conditioned Matrices

It is possible that even after pivoting the algorithm produces a zero on the main diagonal. An example of this is the case when a matrix cannot be inverted (i.e. the inverse does not exist, similar to a division by zero in the scalar case). It is also possible that a main diagonal term may be non–zero, but very small. Such a matrix is said to be *ill–conditioned*. This causes problems. A matrix which has an irremovable zero on the main diagonal cannot be inverted. Also, the solution to an ill–conditioned problem with a small element on the main diagonal will have sensitive dependence to changes to the right hand side vector ”b”. There are methods known as *pre–conditioning* which may sometimes be used to correct these difficulties. Note that if the matrix does not have an inverse then you cannot fix the problem.