Basic Gauss elimination to get the triangular form

At each stage in the basic reduction process we create zeros below the diagonal in a column and we have a vector of the **multipliers**.

$$A = \begin{pmatrix} \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \end{pmatrix} \quad \to \quad \begin{pmatrix} \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ 0 & \mathsf{X} & \mathsf{X} & \mathsf{X} \\ 0 & \mathsf{X} & \mathsf{X} & \mathsf{X} \\ 0 & \mathsf{X} & \mathsf{X} & \mathsf{X} \end{pmatrix} = A^{(1)}, \quad \underline{m}_1 = \begin{pmatrix} 0 \\ m_{21} \\ m_{31} \\ m_{41} \end{pmatrix},$$

$$\to \quad \begin{pmatrix} \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ 0 & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ 0 & 0 & \mathsf{X} & \mathsf{X} \\ 0 & 0 & \mathsf{X} & \mathsf{X} \end{pmatrix} = A^{(2)}, \quad \underline{m}_2 = \begin{pmatrix} 0 \\ 0 \\ m_{32} \\ m_{42} \end{pmatrix},$$

$$\to \quad \begin{pmatrix} \mathsf{x} & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ 0 & \mathsf{x} & \mathsf{x} & \mathsf{x} \\ 0 & 0 & \mathsf{x} & \mathsf{x} \\ 0 & 0 & 0 & \mathsf{X} \end{pmatrix} = U, \quad \underline{m}_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ m_{43} \end{pmatrix}.$$

x and X are potentially non-zero.

The $A = LU$ factorization

When the basic reduction is possible we have the factorization

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ m_{21} & 1 & 0 & 0 \\ m_{31} & m_{32} & 1 & 0 \\ m_{41} & m_{42} & m_{43} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix}.$$

$$L = M_1^{-1} M_2^{-1} M_3^{-1} = I + \underline{m}_1 \underline{e}_1^T + \underline{m}_2 \underline{e}_2^T + \underline{m}_3 \underline{e}_3^T,$$

where each $M_k = I - \underline{m}_k \underline{e}_k^T$ is a **Gauss transformation matrix**.

Later we write $l_{ij} = m_{ij}$ for the entries of the lower triangular matrix. As the diagonal entries of L are all equal to 1 the matrix is said to be **unit lower triangular**.

Factorization of the principal sub-matrices

Let A_k be the $k \times k$ principal sub-matrix of A.

$$
\begin{aligned}
a_{11} &= u_{11}. \\
\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ l_{21} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{pmatrix} \\
\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} &= \begin{pmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}. \\
\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix}
\end{aligned}
$$

In general

$$\det(A_k) = u_{11} \cdots u_{kk}.$$

This factorization is possible if all the principle sub-matrices are invertible, i.e. the entries $u_{kk} \neq 0$, $k = 1, \ldots, n-1$. We also need $u_{nn} \neq 0$ to solve a system.

The order of the computations

The Gauss elimination order of the computations involves the following.

$$A = \begin{pmatrix} 2 & 3 & 1 \\ -2 & -2 & -2 \\ -2 & -4 & 4 \end{pmatrix} \longrightarrow \begin{pmatrix} 2 & 3 & 1 \\ 0 & 1 & -1 \\ 0 & -1 & 5 \end{pmatrix} \longrightarrow \begin{pmatrix} 2 & 3 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 4 \end{pmatrix}.$$

$$\underline{m}_1 = \begin{pmatrix} 0 \\ -1 \\ -1 \end{pmatrix}, \quad \underline{m}_2 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}.$$

From this we have all the entries in the factorization.

$$\begin{pmatrix} 2 & 3 & 1 \\ -2 & -2 & -2 \\ -2 & -4 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 2 & 3 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 4 \end{pmatrix}.$$

We get row 1 of U, column 1 of L, row 2 of U, column 2 of L and finally row 3 of U.

The order of the computations continued

An $A = LU$ approach involves considering the following.

$$A = \begin{pmatrix} 2 & 3 & 1 \\ -2 & -2 & -2 \\ -2 & -4 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}.$$

We could instead consider growing sub-matrices with an intermediate state being the following.

$$\begin{pmatrix} 2 & 3 & 1 \\ -2 & -2 & -2 \\ -2 & -4 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} \begin{pmatrix} 2 & 3 & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}.$$

To complete the computations we need to get l_{31} before l_{32}. We need to get u_{13} before u_{23} and both are needed to get u_{33}.

With small problems and hand calculation there is no reduction in effort.

When the LU factorization is not possible

On the exercises there is the following matrix.

$$A = \begin{pmatrix} 0 & 3 & 1 \\ -2 & 1 & -1 \\ 1 & 10 & 3 \end{pmatrix}$$

We cannot do the basic factorization as $a_{11} = 0$. However we can do the basic factorization if we re-order the rows to

$$\begin{pmatrix} -2 & 1 & -1 \\ 0 & 3 & 1 \\ 1 & 10 & 3 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 & 10 & 3 \\ -2 & 1 & -1 \\ 0 & 3 & 1 \end{pmatrix}.$$

Similarly the basic factorization does not work with the following.

$$B = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 3 \\ 5 & 4 & 3 \end{pmatrix}$$

Here the 2×2 principal sub-matrix is not invertible. If we swap rows 1 and row 3 or we swap rows 2 and 3 then we can factorize.

Factorizations for different orders

$$A = \begin{pmatrix} 0 & 3 & 1 \\ -2 & 1 & -1 \\ 1 & 10 & 3 \end{pmatrix}$$

Just swapping rows 1 and 3 leads to the following.

$$\begin{pmatrix} 1 & 10 & 3 \\ -2 & 1 & -1 \\ 0 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 1/7 & 1 \end{pmatrix} \begin{pmatrix} 1 & 10 & 3 \\ 0 & 21 & 5 \\ 0 & 0 & 2/7 \end{pmatrix}.$$

Matlab will "re-arrange" so that all multipliers are less than or equal to 1 in magnitude. Two row swaps are needed in this case and we get the following.

$$\begin{pmatrix} -2 & 1 & -1 \\ 1 & 10 & 3 \\ 0 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -1/2 & 1 & 0 \\ 0 & 2/7 & 1 \end{pmatrix} \begin{pmatrix} -2 & 1 & -1 \\ 1 & 21/2 & -5/2 \\ 0 & 0 & 2/7 \end{pmatrix}$$

Do we only swap to avoid having a pivot equal to 0?

We have to swap in the following case.

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \end{pmatrix}.$$

In theory we do not need to swap if we change the above to the following.

$$\begin{pmatrix} 10^{-20} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \end{pmatrix}.$$

However not swapping in this case leads to the wrong answer when implemented on a computer with usual floating point arithmetic. In the elimination step the "next 2,2 entry" and a rhs entry are exactly $1 - 10^{20}$ and $3 - 10^{20}$ but rounding stores this as

$$\begin{pmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -10^{20} \end{pmatrix}$$

and the rounded system has solution $x_1 = 0$ and $x_2 = 1$.

Without rounding the solution is close to $(2, 1)^T$.

The row pivoting decision

In the case of an $n \times n$ matrix at the stage when the first $k-1$ columns have been reduced the main entries to consider are the following.

$$\begin{pmatrix} a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\ a_{k+1,k}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\ \vdots & \cdots & \vdots \\ a_{n,k}^{(k-1)} & \cdots & a_{n,n}^{(k-1)} \end{pmatrix}$$

Row pivoting (known as partial pivoting) involves considering the largest of the column k entries

$$\left| a_{kk}^{(k-1)} \right|, \left| a_{k+1,k}^{(k-1)} \right|, \ldots, \left| a_{nk}^{(k-1)} \right|.$$

Swapping is done to put the largest entry in magnitude in the top position. If all entries are 0 then the matrix does not have an inverse.

When we can continue the multipliers have magnitudes ≤ 1.

Does row pivoting work in practice?

Yes. The procedure has been used for a long time and it can be used with confidence.

Is row pivoting guaranteed to work on a computer?

No.

The worst case is illustrated by considering the matrix

$$A_4 = \begin{pmatrix} 1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & -1 & 1 & 0 \\ -1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 2^2 \\ 0 & 0 & 0 & 2^3 \end{pmatrix}.$$

If we consider a sequence of matrices with this structure then the $n \times n$ matrix A_n is not too badly conditioned but the condition number of the factors L_n and U_n grow rapidly with n. If rows were swapped then it would work better but the row pivoting decision is not to swap at each stage as it does not consider the large entries in the last column.

How is L_n badly conditioned when $\det(L_n) = 1$?

On the exercises (Qu. 10) we have

$$L_5 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 \\ -1 & -1 & -1 & 1 & 0 \\ -1 & -1 & -1 & -1 & 1 \end{pmatrix}.$$

We can get the inverse L_5^{-1} col-by-col by forward substitution.

$$L_5^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 2 & 1 & 1 & 0 & 0 \\ 2^2 & 2 & 1 & 1 & 0 \\ 2^3 & 2^2 & 2 & 1 & 1 \end{pmatrix}.$$

For the corresponding matrix L_n^{-1} we have $\|L_n^{-1}\|_\infty = 2^{n-1}$.

Although a matrix is invertible if and only if its determinant is non-zero the size of the determinant is often not a good indication as to whether the matrix is nearly singular as this example shows.

Other strategies

Suppose that we are at the start of the kth stage.

$$\begin{pmatrix} a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\ a_{k+1,k}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\ \vdots & \cdots & \vdots \\ a_{n,k}^{(k-1)} & \cdots & a_{n,n}^{(k-1)} \end{pmatrix}$$

Complete pivoting finds the largest entry in magnitude in this matrix. If this is in position s, t then rows k and s are swapped and columns k and t are swapped. The factorization is then of the form

$$PAQ = LU$$

where both P and Q are permutation matrices.

Solving $A\underline{x} = \underline{b}$ when we need to swap rows

Part 1 of Qu. 8 of the the latest exercise sheet requires row swapping.

$$\begin{pmatrix} 0 & 3 & 1 \\ -2 & 1 & -1 \\ 1 & 10 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -4 \\ -8 \\ -12 \end{pmatrix}.$$

After swapping we have

$$\begin{pmatrix} 1 & 10 & 3 \\ -2 & 1 & -1 \\ 0 & 3 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -12 \\ -8 \\ -4 \end{pmatrix}.$$

If we keep the right hand side from the start then the basic Gauss elimination involves the following steps.

$$\begin{pmatrix} 1 & 10 & 3 & -12 \\ -2 & 1 & -1 & -8 \\ 0 & 3 & 1 & -4 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 10 & 3 & -12 \\ 0 & 21 & 5 & -32 \\ 0 & 3 & 1 & -4 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 10 & 3 & -12 \\ 0 & 21 & 5 & -32 \\ 0 & 0 & 2/7 & 4/7 \end{pmatrix}.$$

Solving $A\underline{x} = \underline{b}$ or first getting $A = LU$ continued

$$\begin{pmatrix} 1 & 10 & 3 \\ -2 & 1 & -1 \\ 0 & 3 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 10 & 3 \\ 0 & 21 & 5 \\ 0 & 3 & 1 \end{pmatrix} \to \begin{pmatrix} 1 & 10 & 3 \\ 0 & 21 & 5 \\ 0 & 0 & 2/7 \end{pmatrix}.$$

If you note the multipliers used then we have the factorization

$$\begin{pmatrix} 1 & 10 & 3 \\ -2 & 1 & -1 \\ 0 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 1/7 & 1 \end{pmatrix} \begin{pmatrix} 1 & 10 & 3 \\ 0 & 21 & 5 \\ 0 & 0 & 2/7 \end{pmatrix}.$$

Solving $L\underline{y} = \underline{b}$ involves

$$\begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 1/7 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} -12 \\ -8 \\ -4 \end{pmatrix}$$

By forward substitution this gives

$$y_1 = -12, \quad y_2 = -32, \quad y_3 = -4 + 32/7 = 4/7.$$

Note that $\underline{y}$ is the same as the last column when we use the right hand side in all the elimination steps.

Summary of chapter 2: $A\underline{x} = \underline{b}$

Let A be a $n \times n$ matrix and let L be unit lower triangular and U upper triangular of the same size. Also let P denote a $n \times n$ permutation matrix.

1. Triangular systems can be solved by forward or backward substitution depending on their shape.
2. If $PA = LU$ then we our system is $PA\underline{x} = P\underline{b}$ and we have $LU\underline{x} = P\underline{b} = \underline{b}'$. Solve $L\underline{y} = \underline{b}'$ followed by solving $U\underline{x} = \underline{y}$.
3. In basic Gauss elimination $P = I$. $\mathcal{O}(2n^3/3)$ operations are involved to reduce to triangular form. Without pivoting all the principal sub-matrices need to be invertible.
4. $\underline{x} = A^{-1}\underline{b}$ describes the solution but it is not an efficient way to get the solution. We can get A^{-1} column-by-column by first factorizing and then solving linear systems such as

$$\underline{x}_j = A^{-1}\underline{e}_j \quad \text{gives } A\underline{x}_j = \underline{e}_j.$$

Other factorizations and some comments

Other similar factorizations exist in this context.

- Rook pivoting is like complete pivoting and involves possibly swapping rows and columns and gives a factorization

$$PAQ = LU$$

  where P and Q are both permutation matrices. Complete pivoting is more stable than $PA = LU$ but take about twice as long to compute. Rook pivoting is more stable than $PA = LU$ and only takes slightly longer to compute.
- The following has not been covered this year but when A is real and symmetric and positive definite there is a Cholesky factorization

$$A = R^T R$$

  where R is a general upper triangular matrix with $r_{ii} > 0$. Another common term for upper triangular is right triangular.