Linear systems: Direct Methods

We call **linear system of order n** (n positive integer), an expression of the form

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

where $A = (a_{ij})$ is a *given matrix* of size $n \times n$, $\mathbf{b} = (b_j)$ is a *given vector* and $\mathbf{x} = (x_j)$ is the *unknown vector* of the system. The previous relation is equivalent to the n equations

$$\sum_{j=1}^{n} a_{ij} x_j = b_i, \quad i = 1, \dots, n.$$

The matrix A is called non-singular if $\det(A) \neq 0$; the solution $\mathbf{x}$ will be unique (for any given vector $\mathbf{b}$) if and only if the matrix associated to the linear system is non-singular.

In theory, if A is non-singular, the solution is given by the Cramer's rule:

$$x_i = \frac{\det(B_i)}{\det(A)}, \quad i = 1, \dots, n,$$

where B_i is the matrix by substituting the i-th column of A by the vector $\mathbf{b}$:

$$B_i = \begin{array}{c} \begin{bmatrix} a_{11} & \dots & b_1 & \dots & a_{1n} \\ a_{21} & \dots & b_2 & \dots & a_{2n} \\ \vdots & & \vdots & & \vdots \\ 0a_{n1} & \dots & b_n & \dots & a_{nn} \end{bmatrix} \\ \uparrow \\ i \end{array}$$

Unfortunately, the application of this rule is unacceptable for the practical solution of systems because the computational cost is of the order of $(n+1)!$ floating point operations per second (flops). In fact, every determinant requires $n!$ flops.

Triangular systems

A matrix $U = (u_{ij})$ is **upper triangular** if

$$u_{ij} = 0 \; \forall i, j : 1 \leq j < i \leq n$$

and a matrix $L = (l_{ij})$ is **lower triangular** if

$$l_{ij} = 0 \; \forall i, j : 1 \leq i < j \leq n.$$

A diagonal matrix is a special triangular matrix. Respectively, the system to be solved is called **upper or lower triangular system**.

Remark: If a matrix A in non-singular and triangular, knowing that

$$\det(A) = \prod_{i=1}^{n} \lambda_i(A) = \prod_{i=1}^{n} a_{ii}$$

($\lambda_i(A)$ being the i-th eigenvalue of A), we can deduce that $a_{ii} \neq 0$, for all $i = 1, \dots, n$.

If L is lower triangular and non-singular, the linear system $L\mathbf{y} = \mathbf{b}$ corresponds to

$$\begin{cases} l_{11}y_1 & = b_1 \\ l_{21}y_1 + l_{22}y_2 & = b_2 \\ \vdots \\ l_{n1}y_1 + l_{n2}y_2 + \ldots + l_{nn}y_n & = b_n \end{cases}$$

Thus:

$$\boxed{y_1 = \frac{b_1}{l_{11}}}, \qquad [1 \text{ operation}]$$

and for $i = 2, 3, \ldots, n$

$$\boxed{y_i = \frac{1}{l_{ii}}\left(b_i - \sum_{j=1}^{i-1} l_{ij}y_j\right)}. \qquad [1 + 2(i-1) \text{ operations}]$$

This algorithm is called **forward substitutions algorithm**.

The forward substitutions algorithm requires n^2 operations, where n is the size of the system, since

$$1 + \sum_{i=2}^{n}(1 + 2(i-1)) = 1 + \sum_{i=1}^{n}(2i-1) - 1 = n^2.$$

If U is upper triangular and non-singular, the system $U\mathbf{x} = \mathbf{y}$ is:

$$\begin{cases} u_{11}x_1 + \ldots + u_{1,n-1}x_{n-1} + u_{1n}x_n & = y_1 \\ \vdots \\ u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n & = y_{n-1} \\ u_{nn}x_n & = y_n \end{cases}$$

Thus:

$$\boxed{x_n = \frac{y_n}{u_{nn}}},$$

and for $i = n-1, n-2, \ldots, 2, 1$

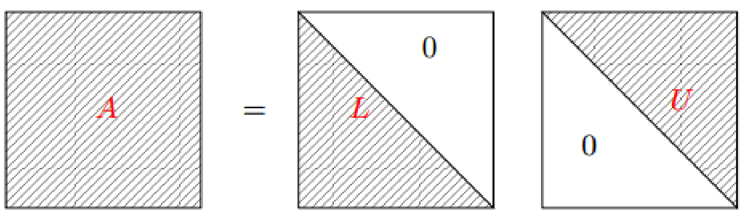
$$\boxed{x_i = \frac{1}{u_{ii}}\left(y_i - \sum_{j=i+1}^{n} u_{ij}x_j\right)}.$$

This algorithm is called **backward substitutions algorithm**. The cost is, once again, n^2 operations.

The LU factorization method

Let $A = (a_{ij})$ be a non-singular $n \times n$ matrix. Assume that there exist a matrix $U = (u_{ij})$, **upper triangular** and a matrix $L = (l_{ij})$, **lower triangular** such that

$$A = LU. \qquad (1)$$



We call (1) a **factorization / decomposition LU of A**.

If we know the factorization LU of A, solving the system $A\mathbf{x} = \mathbf{b}$ is equivalent to solving two systems defined by triangular matrices. Indeed,

$$A\mathbf{x} = \mathbf{b} \iff LU\mathbf{x} = \mathbf{b} \iff \begin{cases} L\mathbf{y} = \mathbf{b} \,, \\ U\mathbf{x} = \mathbf{y} \,. \end{cases}$$

We can easily calculate the solutions of both systems:

- first, we use the forward substitutions algorithm to solve $L\mathbf{y} = \mathbf{b}$ (order n^2 flops);
- then, we use the backward substitutions algorithm to solve $U\mathbf{x} = \mathbf{y}$ (order n^2 flops).

It is required to find first (if possible) the matrices L and U, which requires a number of operations of the order $\frac{2n^3}{3}$ flops, that is better than $(n+1)!$.

Example. Lets try to find a factorization LU in the case case where the size of the matrix A is $n = 2$. We can write the equation (1) as

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix},$$

Or equivalently:

$$\begin{array}{llll} (a) & l_{11}u_{11} = a_{11}, & (b) & l_{11}u_{12} = a_{12}, \\ (c) & l_{21}u_{11} = a_{21}, & (d) & l_{21}u_{12} + l_{22}u_{22} = a_{22}. \end{array}$$

We have then a system (non-linear) with 4 equations and 6 unknowns; in order to have the same number of equations and unknowns, we fix the diagonal of L by taking $l_{11} = l_{22} = 1$. Consequently, from (a) and (b) we have $u_{11} = a_{11}$ and $u_{12} = a_{12}$; finally, if we assume $a_{11} \neq 0$, we obtain $l_{21} = \frac{a_{21}}{a_{11}}$ and $u_{22} = a_{22} - l_{21}u_{12} = a_{22} - \frac{a_{21}a_{12}}{a_{11}}$ using the equations (c) and (d). $\blacksquare$

To determine a factorization LU of the matrix A of any size n, we apply the following method.

1. The elements of L and U satisfy the non-linear system

$$\sum_{r=1}^{\min(i,j)} l_{ir}u_{rj} = a_{ij}, \quad i, j = 1, \ldots, n; \tag{2}$$

2. The system (2) has n^2 equations and $n^2 + n$ unknowns, so it is undetermined. Consequently, the LU factorization is not unique. We can wipe out n unknowns if we set the n diagonal elements of L equal to 1:

$$l_{ii} = 1, \quad i = 1, \ldots, n.$$

   We will see that in this case there exists an algorithm (*Gauss factorization*) allowing us to efficiently compute the factors L and U.

Any $n \times n$ matrix A admits a LU factorization with partial pivoting (LUP)[1] [we will see it later]. It turns out that all square matrices can be factorized in this form, and the factorization is numerically stable in practice. Instead, if A is invertible, then it admits an LU factorization if and only if all its leading principal minors[2] are nonzero (like for the GEM).

The Gauss elimination method

The **Gauss elimination method** (GEM) transforms the system

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

with $A \in \mathbb{R}^{n \times n}$, in an equivalent system (i.e. with the same solution) of the form:

$$U\mathbf{x} = \hat{\mathbf{b}},$$

where U is an upper triangular matrix and $\hat{\mathbf{b}}$ is a properly modified second member. This system can be solved by a backward substitutions method.

In the transformation, we essentially use the property that says that we do not change the solution of the system if we add to a given equation a linear combination of other equations.

Let us consider an invertible matrix $A \in \mathbb{R}^{n\times n}$ in which the diagonal element a_{11} is assumed to be non-zero. we set $A^{(1)} = A$ and $\mathbf{b}^{(1)} = \mathbf{b}$. We introduce the **multiplier**

$$l_{i1} = \frac{a_{i1}^{(1)}}{a_{11}^{(1)}},\ i = 2, 3, \ldots, n, \qquad A^{(1)} = \begin{bmatrix} a_{11}^{(1)} & \cdots & a_{1j}^{(1)} & \cdots & a_{1n}^{(1)} \\ \vdots & & \vdots & & \vdots \\ a_{i1}^{(1)} & \cdots & a_{ij}^{(1)} & \cdots & a_{in}^{(1)} \\ \vdots & & \vdots & & \vdots \\ a_{n1}^{(1)} & \cdots & a_{nj}^{(1)} & \cdots & a_{nn}^{(1)} \end{bmatrix}$$

where the $a_{ij}^{(1)}$ represent the elements of $A^{(1)}$. This multiplier will yield 0 as coefficient for the unknown x_1 in the lines $i \geq 2$ when combined with the first line of the matrix. In this way the unknown x_1 can be removed from the rows $i = 2, \ldots, n$ by subtracting l_{i1} times the first row and doing the same at the right-hand side.

Let us define

$$\begin{aligned} a_{ij}^{(2)} &= a_{ij}^{(1)} - l_{i1}a_{1j}^{(1)}, \qquad i, j = 2, \ldots, n, \\ b_i^{(2)} &= b_i^{(1)} - l_{i1}b_1^{(1)}, \qquad\quad i = 2, \ldots, n, \end{aligned}$$

where the $b_i^{(1)}$ are the components of $\mathbf{b}^{(1)}$. The coefficients l_{i1} will set to 0 all the elements a_{ij} below the pivot, and $\mathbf{b}^{(2)}$ will be the adjusted $\mathbf{b}$ accordingly to the changes made to the matrix A. We get a new system of the form

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \cdots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & \cdots & a_{2n}^{(2)} \\ \vdots & \vdots & & \vdots \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ b_n^{(2)} \end{bmatrix},$$

which will be written as $A^{(2)}\mathbf{x} = \mathbf{b}^{(2)}$ and that is equivalent to the system we had at the beginning.

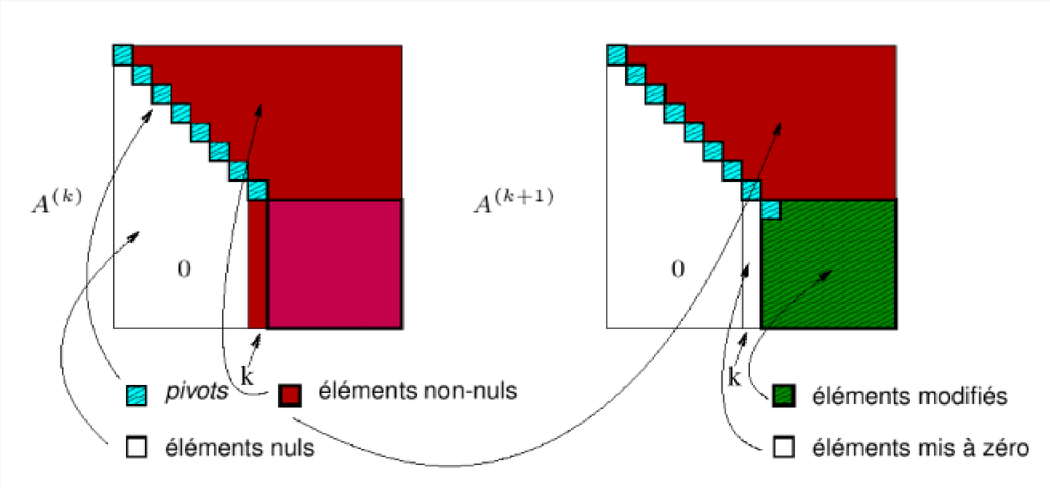
Once again we can transform this system by removing the unknown x_2 from the rows $3, \ldots, n$. By repeating this step we obtain a finite series of systems

$$A^{(k)}\mathbf{x} = \mathbf{b}^{(k)},\ 1 \leq k \leq n,$$

where, for $k \geq 2$, the matrix $A^{(k)}$ is of the form

$$A^{(k)} = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \cdots & \cdots & \cdots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & & & a_{2n}^{(2)} \\ \vdots & & \ddots & & & \vdots \\ 0 & \cdots & 0 & a_{kk}^{(k)} & \cdots & a_{kn}^{(k)} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & a_{nk}^{(k)} & \cdots & a_{nn}^{(k)} \end{bmatrix},$$

where we assume $a_{ii}^{(i)} \neq 0$ for $i = 1, \ldots, k-1$.



GEM: diagram showing how the matrix $A^{(k+1)}$ is obtained from the matrix $A^{(k)}$.

It is clear that for $k = n$ we obtain the following upper triangular system $A^{(n)}\mathbf{x} = \mathbf{b}^{(n)}$:

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \ldots & \ldots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & & a_{2n}^{(2)} \\ \vdots & & \ddots & & \vdots \\ 0 & & & \ddots & \vdots \\ 0 & & & & a_{nn}^{(n)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ \vdots \\ \vdots \\ b_n^{(n)} \end{bmatrix}.$$

To be consistent with the previous notation, we write as U the upper triangular matrix $A^{(n)}$. The elements on the main diagonals, the $a_{kk}^{(k)}$, are called **pivots** and have to be non-zero for $k = 1, \ldots, n-1$.

In order to make explicit the formula to get from the k-th system to the $(k+1)$-th, for $k = 1, \ldots, n-1$, we assume that $a_{kk}^{(k)} \neq 0$ and we define the **multiplier**

$$\boxed{l_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}}, \qquad i = k+1, \ldots, n, \qquad [(n-k) \text{ operations}] \qquad (3)$$

we set then

$$\begin{aligned} &\boxed{a_{ij}^{(k+1)} = a_{ij}^{(k)} - l_{ik}a_{kj}^{(k)}}, \quad i, j = k+1, \ldots, n, \quad [2(n-k)^2 \text{ operations}] \\ &\boxed{b_i^{(k+1)} = b_i^{(k)} - l_{ik}b_k^{(k)}}, \quad i = k+1, \ldots, n. \quad [2(n-k) \text{ operations}] \end{aligned} \qquad (38)$$

Remark. *To perform the Gauss elimination we require $2(n-k)^2$ operations to update A, $2(n-k)$ operations to update b and $(n-k)$ operations to update l, so in total*

$$\begin{aligned} 2\sum_{k=1}^{n-1}(n-k)^2 + 3\sum_{k=1}^{n-1}(n-k) &= 2\sum_{p=1}^{n-1}p^2 + 3\sum_{p=1}^{n-1}p \\ &= 2\frac{(n-1)n(2n-1)}{6} + 3\frac{n(n-1)}{2} = \frac{n(n-1)(2n+3)}{3} \end{aligned}$$

operations are required, plus n^2 operations for the resolution with the backward substitutions method of the triangular system $U\mathbf{x} = \mathbf{b}^{(n)}$. By keeping only the dominant elements (of order n^3), we can say that the Gauss elimination method has a cost of around

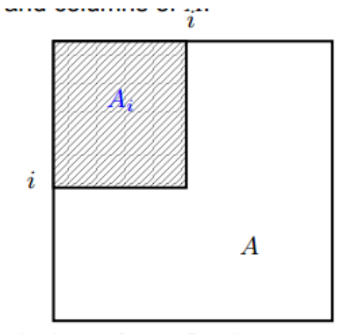
$$\frac{2}{3}n^3 \ operations.$$

The Gauss method is only properly defined if the pivots $a_{kk}^{(k)}$ are non-zero for $k = 1, \ldots, n-1$. Unfortunately, knowing that the diagonal elements of A are not zero is not enough to avoid null pivots during the elimination phase. For example, the following matrix A in (4) is invertible and its diagonal elements are non-zero

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 7 & 8 & 9 \end{bmatrix}, \quad \text{but we find} \quad A^{(2)} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & \boxed{0} & -1 \\ 0 & -6 & -12 \end{bmatrix}. \qquad (4)$$

Nevertheless, we have to stop the Gauss method at the second step, because $a_{22}^{(2)} = 0$.

Let A_i be the i-th main submatrix of A ($i = 1, \ldots, n-1$), i.e. the submatrix made of the i first rows and columns of A:



and let d_i be the principal minor of A defined as $d_i = \det(A_i)$. We have the following result.

Proposition 1. *For a given matrix $A \in \mathbb{R}^{n\times n}$, its Gauss factorization exists and is unique iff the principal submatrices A_i ($i = 1, \ldots, n-1$) are non-singular (i.e. the principal minors d_i are non-zero: $d_i \neq 0$).*

<u>Remark:</u> If $d_i \neq 0$ ($i = 1, \ldots, n-1$), then the pivots $a_{ii}^{(i)}$ are also non-zero.
The matrix of the previous example does not satisfy this condition because $d_1 = \det[1] = 1$ but $d_2 = \det \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} = 0.$

There are some categories of matrices for which the hypothesis of the Proposition 1 are fulfilled. In particular, we mention:

1. **(Strictly $>$) diagonal dominant by row matrices.** A matrix A is said diagonal dominant by row if

$$|a_{ii}| \geq \sum_{j=1,\ldots,n; j\neq i} |a_{ij}|, \quad i = 1, \ldots, n.$$

2. **(Strictly $>$) diagonal dominant by column matrices.** A matrix A is said diagonal dominant by column if

$$|a_{jj}| \geq \sum_{i=1,\ldots,n; i\neq j} |a_{ij}|, \quad j = 1, \ldots, n.$$

3. **Symmetric positive definite matrices.** A matrix A is symmetric if $A = A^T$; it is positive definite if all its eigenvalues are positive, i.e.:

$$\lambda_i(A) > 0, \quad i = 1, \ldots, n.$$

Example 3: The matrix $\begin{bmatrix} -4 & 1 & 2 \\ 2 & 5 & 0 \\ -2 & 1 & 7 \end{bmatrix}$ is diagonal dominant by row and by column, whereas $\begin{bmatrix} -3 & 1 & 2 \\ 2 & 5 & 0 \\ -2 & 1 & 7 \end{bmatrix}$ is only diagonal dominant by row (in the first column we have $|-3| < |2| + |-2|$).

Gauss ~ LU

We can show that the Gauss method is equivalent to the factorization $A = LU$ of the matrix A, with L = multiplier matrix and $U = A^{(n)}$.

More exactly:

$$\boxed{A = \underbrace{\begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ l_{21} & 1 & & & 0 \\ \vdots & l_{32} & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ l_{n1} & & & l_{n,n-1} & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \dots & \dots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & & & a_{2n}^{(2)} \\ \vdots & & \ddots & & \vdots \\ 0 & & & \ddots & \vdots \\ 0 & & & & a_{nn}^{(n)} \end{bmatrix}}_{U}.}$$

The matrices L and U only depend on A (and not on $\mathbf{b}$), so the same factorization can be reused for solving several linear systems that share the same matrix A but **different vectors $\mathbf{b}$**.

The number of operations is then considerably reduced, since most of the computational weight, around $\frac{2}{3}n^3$ flops, is due to the Gaussian elimination process. Indeed, let us consider the M linear systems:

$$A\mathbf{x}_m = \mathbf{b}_m \quad m = 1, \dots, M.$$

Therefore:

- the cost of the factorization $A = LU$ is $\frac{2}{3}n^3$ flops;
- the cost of the resolution of both triangular systems, $L\mathbf{y}_m = \mathbf{b}_m$ and $U\mathbf{x}_m = \mathbf{y}_m$ ($m = 1, \dots, M$) is $2Mn^2$ flops,

for a total of $\frac{2}{3}n^3 + 2Mn^2$ flops which is much smaller than $\frac{2}{3}Mn^3$ flops required to solve all the systems with the Gauss elimination method.

The pivoting technique

It has been already noted that the Gauss method fails if a pivot becomes zero. In that case, we can use a technique called **pivoting** that consists in exchanging the rows (or the columns) of the system in such a way that no pivot is zero.

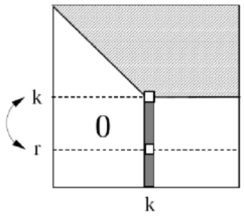
Example. Let us go back to the matrix (4) for which the Gauss method gives a null pivot at the second step. By just exchanging the second and the third rows, we get a non-zero pivot and can execute one step further. Indeed,

$$A^{(2)} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & 0 & -1 \\ 0 & -6 & -12 \end{bmatrix} \quad \Longrightarrow \quad P_2 A^{(2)} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -6 & -12 \\ 0 & 0 & -1 \end{bmatrix},$$

where $P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ is called **permutation matrix**.

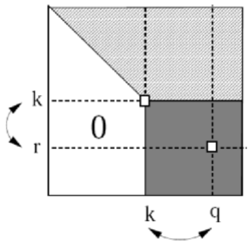
∎

The pivoting strategy used for the previous example can be generalized by finding, at every step k of the elimination, a non-zero pivot among the elements of the subcolumn $A^{(k)}(k:n,k)$. This is called a **partial pivot change** (by row).



From (3) we know that a big value of l_{ik} (coming for instance from a small $a_{kk}^{(k)}$) can amplify the rounding errors affecting the elements $a_{jk}^{(k)}$. Consequently, in order to ensure a better stability, we choose as pivot the biggest element in module of the column $A^{(k)}(k:n,k)$, and the partial pivoting is performed at every step, even if it is not strictly necessary (i.e. even if the pivot is non-zero). In this way a_{ij} and b_j are under control.

An alternative method consists looking for the pivot in the whole submatrix $A^{(k)}(k:n,k:n)$, performing what is called **complete pivoting**.



Remark that, whereas partial pivoting requires just an additional cost of n^2 tests, complete pivoting needs some $2n^3/3$, what considerably increases the cost of the Gauss method.

In general, if at the step k we have to exchange the rows k and r, we will have to multiply $A^{(k)}$ by the following **permutation matrix** P_k before continuing:

$$\begin{array}{cc}
\begin{array}{c} \\ \\ k \rightarrow \\ \\ r \rightarrow \\ \\ \\ \end{array} & \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 0 & \dots & 1 & \\ & & & \vdots & & \\ & & 1 & \dots & 0 & \\ & & & & \ddots & \\ & & & & & 1 \end{pmatrix} = P_k \\
 & \begin{array}{ccc} \uparrow & \quad & \uparrow \\ r & & k \end{array}
\end{array}$$

This means we will consider $P_k A^{(k)}$ instead of $A^{(k)}$.

Setting $\mathbf{l}_k = [0,\dots,0,l_{k+1,k},\dots,l_{n,k}]^T \in \mathbb{R}^n$, and defining

$$M_k = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & & \vdots \\ 0 & \cdots & 1 & a_{kk}^{(k)} & \cdots & a_{kn}^{(k)} \\ 0 & \cdots & -l_{k+1,k} & 1 & \cdots & 0 \\ \vdots & & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -l_{n,k} & 0 & \cdots & 1 \end{bmatrix} = I_n - \mathbf{l}_k \mathbf{e}_k^T$$

as the **k-th Gaussian transformation matrix**, one finds out that

$$(M_k)_{ip} = \delta_{ip} - (\mathbf{l}_k \mathbf{e}_k^T)_{ip} = \delta_{ip} - l_{ik}\delta_{kp}, \qquad i, p = 1, \dots, n.$$

Let us analyze how partial pivoting affects the LU factorization induced by GEM. At the first step of GEM with partial pivoting, after finding out the entry a_{r1} of maximum module in the first column, the elementary permutation matrix P_1 which exchanges the first row with the r-th row is constructed (if $r = 1$, P_1 is the identity matrix). Next, the first Gaussian transformation matrix M_1 is generated and we set $A^{(2)} = M_1 P_1 A^{(1)}$. A similar approach is now taken on $A^{(2)}$, searching for a new permutation matrix P_2 and a new matrix M_2 such that

$$A^{(3)} = M_2 P_2 A^{(2)} = M_2 P_2 M_1 P_1 A^{(1)}.$$

Executing all the elimination steps, the resulting upper triangular matrix U is now given by

$$U = A^{(n)} = M_{n-1} P_{n-1} \dots M_1 P_1 A^{(1)}. \tag{5}$$

Letting $M = M_{n-1} P_{n-1} \dots M_1 P_1$ and $P = P_{n-1} \dots P_1$, we obtain that $U = MA$ and, thus, $U = (MP^{-1})PA$. It can be checked that the matrix $L = PM^{-1}$ is unit lower triangular, so that the LU factorization reads

$$\boxed{PA = LU}, \tag{6}$$

being $P = P_{n-1} P_{n-2} \dots P_2 P_1$ the **global permutation matrix**, L the **multiplier matrix** (the new ones!) and $U = A^{(n)}$.

Once the matrices L, U and P have been calculated, the resolution of the initial system is transformed into the resolution of the triangular systems

$$A\mathbf{x} = b \quad \Longrightarrow \quad PA\mathbf{x} = P\mathbf{b} \quad \Longrightarrow \quad LU\mathbf{x} = P\mathbf{b} \quad \Longrightarrow \quad \begin{cases} L\mathbf{y} = P\mathbf{b} \,, \\ U\mathbf{x} = \mathbf{y} \,. \end{cases}$$

Remark that the coefficients of the matrix L have the same values as the multipliers calculated by a factorization LU of the matrix PA without pivoting.

If complete pivoting is performed, at the first step of the process, once the element a_{qr} of largest module in submatrix $A(1:n, 1:n)$ has been found, we must exchange the first row and column with the q-th row and the r-th column. This generates the matrix $P_1 A^{(1)} Q_1$, where P_1 and Q_1 are permutation matrices by rows and by columns, respectively. As a consequence, the action of matrix M_1 is now such that $A^{(2)} = M_1 P_1 A_{(1)} Q_1$. Repeating the process, at the last step, instead of (5) we obtain

$$U = A^{(n)} = M_{n-1} P_{n-1} \dots M_1 P_1 A^{(1)} Q_1 \dots Q_{n-1}.$$

In the case of complete pivoting the LU factorization becomes

$$\boxed{PAQ = LU} \tag{7}$$

where $P = P_{n-1} \dots P_1$ is a permutation matrix that takes into account all permutations by row, and $Q = Q_1 \dots Q_{n-1}$ is a permutation matrix that takes into account all permutations by column. By construction, the matrix L is still lower triangular, and its elements have a module lower or equal to 1. As for the partial pivoting, the elements of L are the multipliers generated by the factorization LU of the matrix PAQ with no pivoting.

Once the matrices L, U, P and Q have been calculated, for solving the linear system we notice that we can write

$$A\mathbf{x} = \mathbf{b} \quad \Longleftrightarrow \quad \underbrace{PAQ}_{LU}\underbrace{Q^{-1}\mathbf{x}}_{\mathbf{x}^*} = P\mathbf{b} \quad \Longleftrightarrow \quad LU\mathbf{x}^* = P\mathbf{b}.$$

Which brings us to the resolution of two triangular systems and an equation

$$\begin{cases} L\mathbf{y} = P\mathbf{b} \ , \\ U\mathbf{x}^* = \mathbf{y} \ , \\ \mathbf{x} = Q\mathbf{x}^* . \end{cases}$$

Remark 1. *The matrix P is a permutation matrix. In the case where the matrix P is the identity, the matrices L and U are the matrices we are looking for (such that $LU = A$). Otherwise, we have $LU = PA$.*

Remark 2. *Using the LU factorization, obtained by fixing the value 1 for the n diagonal elements of L, we can calculate the determinant of a square matrix with $O(n^3)$ operations, thanks to the Binet theorem:*

$$\det(A) = \det(L)\det(U) = \det(U) = \prod_{k=1}^{n} u_{kk}; \tag{8}$$

indeed, the determinant of a triangular matrix is is the product of the diagonal elements.

The inverse matrix

If A is a $n \times n$ *non-singular* matrix, let us call $x^{(1)}, \ldots, x^{(n)}$ the columns of its inverse matrix A^{-1}, i.e. $A^{-1} = (x^{(1)}, \ldots, x^{(n)})$. The relation $AA^{-1} = I$ can be expressed by the following n systems : for $1 \leq k \leq n$,

$$A\mathbf{x}^{(k)} = \mathbf{e}^{(k)}, \tag{9}$$

where $\mathbf{e}^{(k)} = (0, 0, \ldots, 0, 1, 0, \ldots, 0)$ is the column vector with all the elements equal to 0 except the one corresponding to the k-th row, which equals 1 (it corresponds to the k-th column of I). Once we know the matrices L and U that factorizes A, solving the n systems (9) defined by the same matrix A requires $2n \cdot n^2 = 2n^3$ operations.

The Cholesky factorization

In the case where the $n \times n$ matrix A is symmetric and positive definite, there exists a unique upper triangular matrix R with positive diagonal elements such that

$$\boxed{A = R^T R}.$$

This factorization is called **Cholesky factorization**.

The elements r_{ij} of R can be calculated using the expressions

$$r_{11} = \sqrt{a_{11}} \tag{10}$$

and for $i = 2, \ldots, n$:

$$r_{ji} = \frac{1}{r_{jj}}\left(a_{ij} - \sum_{k=1}^{j-1} r_{ki} r_{kj}\right), \quad j = 1, \ldots, i-1, \tag{11}$$

$$r_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} r_{ki}^2} \tag{12}$$

The Cholesky factorization needs around $\frac{n^3}{3}$ operations (half the operations for a LU factorization, so it uses half of the computational time!).

Memory space limitations

A square matrix of order n is called **sparse** if the number of nonzero entries is of order n (on n^2 total entries).

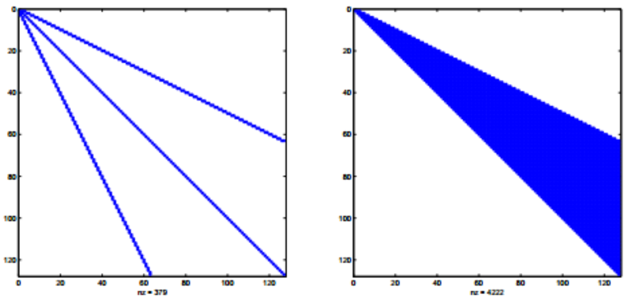
The **pattern** is the 2D representation of nonzero entries positions:

- lower band p_1: $a_{ij} = 0$ when $i > j + p_1$
- upper band p_2: $a_{ij} = 0$ when $j > i + p_2$

The maximum between p_1 and p_2 is called **matrix bandwidth**.

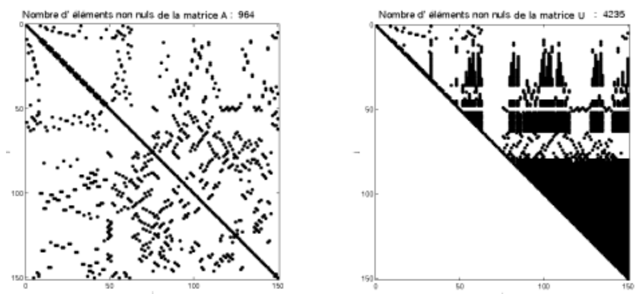
The **fill-in phenomenon** occurs when, after a LU decomposition, L and U present less sparsity then the original matrix A, leading to a bigger memory usage. To reduce the phenomenon we can apply row and column permutations to **reorder** A before performing the factorization (**pivoting**).

Example 1. Let A be a matrix of size 127×127, symmetric and positive definite. The number of non-null entries of A is 379 and thus much smaller than $(127)^2 = 16129$. It is a sparse matrix. The figure on the left shows the disposition of the non-null entries of A, whereas the one on the right shows the non-null entries of the matrix R. Even if also R is a sparse matrix, we need one order of magnitude more to allocate this matrix!



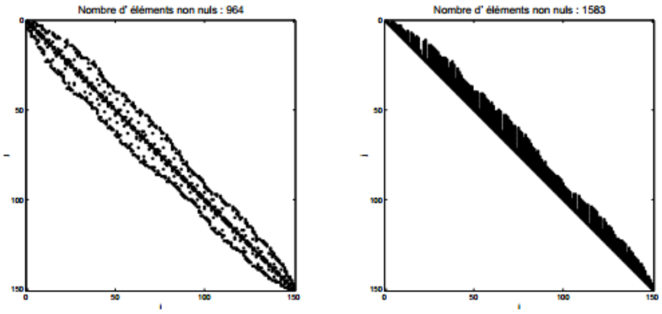
Example 2. Let us consider the problem of calculating the deformations in a structure subject to a given set of forces. The discretization using the finite elements method generates a matrix A of size 150×150. (The same matrix would have been produced by the approximation of an electric potential field.) This matrix is symmetric positive definite. The number of non-null entries of A is 964, and thus much smaller than $(150)^2 = 22500$. It is a *sparse* matrix.

The figure on the left shows the disposition of the non-null entries of A, whereas the one on the right shows the non-null entries of the matrix R.



We notice that the number of non-null entries of R is much bigger than those of A (**fill-in phenomenon**, due to the change of the structure of the matrix during the factorization). This leads to a bigger memory usage, and it's not suggested to use the sparse structure anymore. To reduce the fill-in phenomenon, we can re-order rows and columns of A in a particular fashion; this is called **re-ordering** of the matrix. There are several algorithms that allow us to do this.

For example, the following figure shows, on the left, one possibility of reordering A, while the one on the right shows the disposition of the non-null entries of the Cholesky factorization of the reordered matrix A. With the new techniques this will be much more easy and less costly.



Precision limitations

Example 3. Rounding errors can induce important differences between the calculated solution using the Gauss elimination method (GEM) and the exact solution. This happens when the *conditioning (number)* of the matrix of the system (representing how numerically stable this matrix can be) is very big.

The Hilbert matrix of size $n \times n$ is a symmetric matrix defined by:

$$A_{ij} = \frac{1}{i+j-1}, \quad i,j = 1,\dots,n$$

For example, for $n = 4$, we get:

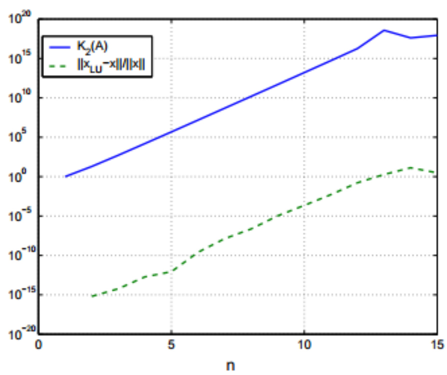
$$A = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{bmatrix}$$

This matrices are often used as benchmark to estimate the performance of the numerical method.

We consider the linear systems $A_n \mathbf{x}_n = \mathbf{b}_n$ where A_n is the Hilbert matrix of size n with $n = 4, 6, 8, 10, 12, \dots$, whereas $\mathbf{b}_n$ is chosen such that the exact solution is $\mathbf{x}_n = (1, 1, \dots, 1)^T$.

The residual are always computable so they can be used as estimation of the error when you cannot compute it.

For every n, we calculate the conditioning of the matrix, we solve the linear system by LU factorization and we get $\mathbf{x}_n^{LU}$ as the found solution. The obtained conditioning as well as the (relative) error $||\mathbf{x}_n - \mathbf{x}_n^{LU}||/||\mathbf{x}_n||$ (where $||\cdot||$ is the Euclidean norm of a vector, $||\mathbf{x}|| = \sqrt{\mathbf{x}^T \cdot \mathbf{x}}$) are shown in the figure below.



We have that the relative error is greater than 1 → 120% of error! IT'S IMPOSSIBLE!!!

Considerations on the precision

The methods we have seen until now allow us to find the solution of a linear system in a finite number of operations. That is why they are called **direct methods**. However, there are cases where these methods are not satisfactory.

Total pivoting is more stable than partial pivoting.

Definition. *We call **conditioning** of a matrix M, symmetric positive definite, the ratio between the maximum and minimum of its eigenvalues, i.e.*

$$K(M) = \frac{\lambda_{\max}(M)}{\lambda_{\min}(M)}$$

*It is also called the **spectral condition number** of M.*

It can be shown that, the bigger the conditioning of a matrix, the worse the solution obtained by a direct method.

For example, let us consider a linear system $A\mathbf{x} = \mathbf{b}$. If we solve this system with a computer, due to rounding errors, we will not find the exact solution $\mathbf{x}$ but an approximate solution $\hat{\mathbf{x}}$. The following relationship can be shown:

$$\frac{||\mathbf{x} - \hat{\mathbf{x}}||}{||\mathbf{x}||} \leq K(A)\frac{||r||}{||b||} \tag{13}$$

where $\mathbf{r}$ is the residual $\mathbf{r} = \mathbf{b} - A\hat{\mathbf{x}}$; we write as $||\mathbf{v}|| = \left(\sum_{k=1}^{n} v_k^2\right)^{1/2}$ the Euclidean norm of a vector $\mathbf{v}$.

Remark that, if the conditioning of A is big, the distance $||\mathbf{x} - \hat{\mathbf{x}}||$ between the exact solution and the numerically computed solution can be very big even if the residual is very small. So the bigger $K(A)$, the worse the solution provided by a direct method. If $K \approx 1$, the matrix is **well conditioned**. We have that $\mathbf{r}$ is an estimation of the error $||x - \hat{x}||$: if $K(A)$ is small, then the error is small when $||\mathbf{r}||$ is small; vice versa, if $K(A)$ is large we can't use $||\mathbf{r}||$ as measure for the error.

Proof for (13): Let A be a symmetric positive definite matrix, we can consider the n eigenvalues $\lambda_i > 0$ and the associated unitary eigenvectors $\{\mathbf{v}_i\}$, $i = 1, \ldots, n$: $A\mathbf{v}_i = \lambda_i \mathbf{v}_i$, $i = 1, \ldots, n$. These vectors form an orthonormal base of $\mathbb{R}^n$, which means $\mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$ for $i, j = 1, \ldots, n$. For any $\mathbf{w} \in \mathbb{R}^n$, if we write it as

$$\mathbf{w} = \sum_{i=1}^{n} w_i \mathbf{v}_i,$$

we have

$$\begin{aligned} ||A\mathbf{w}||^2 &= (A\mathbf{w})^T(A\mathbf{w}) \\ &= (\lambda_1 w_1 \mathbf{v}_1^T + \ldots + \lambda_n w_n \mathbf{v}_n^T)(\lambda_1 w_1 \mathbf{v}_1 + \ldots + \lambda_n w_n \mathbf{v}_n) \\ &= \sum_{i,j=1}^{n} \lambda_i \lambda_j w_i w_j \mathbf{v}_i^T \mathbf{v}_j = \sum_{i,j=1}^{n} \lambda_i \lambda_j w_i w_j \delta_{ij} = \sum_{i=1}^{n} \lambda_i^2 w_i^2 \end{aligned}$$

And yet, as $||\mathbf{w}||^2 = \sum_{i=1}^{n} w_i^2$, we get $||A\mathbf{w}||^2 \leq \lambda_{\max}^2 ||\mathbf{w}||^2$, i.e. $||A\mathbf{w}|| \leq \lambda_{\max} ||\mathbf{w}||$ where $\lambda_{\max}$ is the biggest eigenvalue of A.

As the eigenvalues of A^{-1} are $1/\lambda_i$, we also get $||A^{-1}\mathbf{w}|| \leq \frac{1}{\lambda_{\min}} ||\mathbf{w}|| \; \forall \mathbf{w} \in \mathbb{R}^n$, where $\lambda_{\min}$ is the smallest eigenvalue of A.

Thus, we have

$$||\mathbf{x} - \hat{\mathbf{x}}|| = ||A^{-1}\mathbf{r}|| \leq \frac{1}{\lambda_{\text{min}}}||\mathbf{r}||,$$
$$||\mathbf{b}|| = ||A\mathbf{x}|| \leq \lambda_{\text{max}}||\mathbf{x}||,$$

from where we directly find the inequality (13):

$$\frac{||\mathbf{x} - \hat{\mathbf{x}}||}{\lambda_{\text{max}}||\mathbf{x}||} \leq \frac{\lambda_{\text{min}}^{-1}||\mathbf{r}||}{||\mathbf{b}||} \iff \frac{||\mathbf{x} - \hat{\mathbf{x}}||}{||\mathbf{x}||} \leq \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}\frac{||\mathbf{r}||}{||\mathbf{b}||} \iff \frac{||\mathbf{x} - \hat{\mathbf{x}}||}{||\mathbf{x}||} \leq K(A)\frac{||\mathbf{r}||}{||\mathbf{b}||}$$

$\square$

Other direct methods

- The **Thomas algorithm** is used to perform an optimized LU factorization of a tridiagonal matrix in n operations.
- The solution of an overdetermined system $A\mathbf{x} = \mathbf{b}$ with $A \in \mathbb{R}^{m \times n},$ with $m > n$, can be computed using the QR factorization or the singular value decomposition.