Linear Algebra: Direct Methods Computational Linear Algebra for Large Scale Problems

Stefano Berrone

stefano.berrone@polito.it

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Lower triangular matrices - Forward substitution

Let us solve the following linear system Ly = b with L lower triangular non singular matrix.

$$\begin{bmatrix} I_{11} & 0 & 0 & \dots & 0 \\ I_{21} & I_{22} & 0 & \dots & 0 \\ I_{31} & I_{32} & I_{33} & \dots & 0 \\ \vdots & & \vdots & & & \\ I_{n1} & I_{n2} & I_{n3} & \dots & I_{nn} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

Remark

If L is non-singular, all the diagonal elements do not vanish $l_{ii} \neq 0$:

$$\det(L) = \prod_{i=1}^n I_{ii}$$

Let us explicitly write the equations:

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

$$\implies y_1 = b_1/l_{11}$$

$$\implies y_2 = (b_2 - l_{21}y_1)/l_{22}$$

$$\implies y_i = (b_i - \sum_{i=1}^{i-1} l_{ij}y_j)/l_{ii}$$

The forward substitution method writes:

```
for i=1:n
    y(i)=b(i);
    for j=1:i-1
        y(i)=y(i)-L(i,j)*y(j);
    end
    y(i)=y(i)/L(i,i);
end
```

The previous expression of the method involves two for loops, we could take advantage from the fact that all the elements of a vector are stored in contiguous memory locations using BLAS functions for vectors scalar products. A Matlab/Octave formulation is:

```
y(1) =b(1)/L(1,1);
for i=2:n
y(i)=(b(i)-L(i,1:i-1)*y(1:i-1))/L(i,i);
end
```

L(i, 1: i-1) is the vector containing the elements on the matrix L in the i-th row and in the columns from 1 to i-1.

Backward substitution

Let us solve the following linear system Ux = y with U non-singular upper triangular matrix.

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & \dots & u_{1n} \\ 0 & u_{22} & u_{23} & \dots & u_{2n} \\ \vdots & & \vdots & & & \\ 0 & 0 & \dots & u_{n-1,n-1} & u_{n-1,n} \\ 0 & 0 & \dots & 0 & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}.$$

Remark

Again, from the non-singularity of U we have $u_{ii} \neq 0$, $\forall i$

$$\begin{cases} u_{11}x_1 + u_{12}x_2 + \dots + u_{1n}x_n &= y_1, \\ u_{22}x_2 + \dots + u_{2n}x_n &= y_2, \\ \vdots & & & \\ u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n &= y_{n-1}, \\ u_{nn}x_n &= y_n. \end{cases}$$

$$\Rightarrow x_n = y_n/u_{nn}.$$

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$$\Rightarrow x_{n-1} = (y_{n-1} - u_{n-1,n}x_n)/u_{n-1,n-1}.$$

$$\Rightarrow x_i = (y_i - \sum_{j=i+1}^n u_{ij}x_j)/u_{ii}.$$

Backward substitution method:

```
for i=n:-1:1
    x(i)=y(i);
    for j=i+1:n
        x(i)=x(i)-U(i,j)*x(j);
    end
    x(i)=x(i)/U(i,i);
end
```

From the optimized functions of the BLAS library:

```
x(n)=y(n)/U(n,n);
for i=n-1:-1:1
    x(i)=(y(i)-U(i,i+1:n)*x(i+1:n))/U(i,i);
end
```

Gaussian elimination

The solution of linear systems with triangular matrices is a trivial task.

Idea: Given a general (non-singular) problems is possible to transform it to an **equivalent** problem with triangular matrix?

Given a linear system Ax = b the following operations lead to equivalent linear systems (linear systems with different matrix and right hand side, but with the same solution):

- swap two equations of the system;
- multiply an equation of the system by a non zero scalar;
- exchange an equation with a new equation that is a linear combination of the former one and a different equation of the system.

Gaussian elimination:

this method consists of a repeated application of 3 such that:

- the original linear system is transformed in an equivalent one with an upper triangular matrix
- 2 and then to solve the new system with a backward substitution.

Let us write the system Ax = b explicitly:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1, \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2, \\ a_{31}x_1 + a_{32}x_2 + \dots + a_{3n}x_n = b_3, \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n = b_n. \end{cases}$$

Let $a_{11} \neq 0$

$$r_2 \leftarrow r_2 + \left(-\frac{a_{21}}{a_{11}}\right) * r_1$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2 +$$

$$-\frac{a_{21}}{a_{11}}(a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1)$$

$$0x_1 + a_{22}^{(2)}x_2 + \dots + a_{2n}^{(2)}x_n = b_2^{(2)}.$$

$$a_{22}^{(2)} = a_{22} - a_{12}a_{21}/a_{11}, \dots, a_{2n}^{(2)} = a_{2n} - a_{1n}a_{21}/a_{11}, b_2^{(2)} = b_2 - b_1a_{21}/a_{11}$$

Now in the second equation of the system we do not have the unknown x_1 anymore.

Let us apply the same approach to the remaining n-1 equations:

$$r_{i} \leftarrow r_{i} + m_{i1} * r_{1}, \quad i = 2, ..., n$$

$$m_{i1} = -\frac{a_{i1}}{a_{11}}, \quad i = 2, ..., n.$$

$$\begin{cases}
a_{11}^{(1)}x_{1} + a_{12}^{(1)}x_{2} + ... + a_{1n}^{(1)}x_{n} = b_{1}^{(1)} \\
0 + a_{22}^{(2)}x_{2} + ... + a_{2n}^{(2)}x_{n} = b_{2}^{(2)} \\
0 + a_{32}^{(2)}x_{2} + ... + a_{3n}^{(2)}x_{n} = b_{3}^{(2)} \\
\vdots \\
0 + a_{n2}^{(2)}x_{2} + ... + a_{nn}^{(2)}x_{n} = b_{n}^{(2)}
\end{cases}$$

$$a_{ij}^{(1)} = a_{ij}, b_{i}^{(1)} = b_{i}, i, j = 1, ..., n;$$

$$a_{ij}^{(2)} = a_{ij}^{(1)} + m_{i1}a_{1j}^{(1)}, b_{i}^{(2)} = b_{i}^{(1)} + m_{i1}b_{1}^{(1)}, i, j = 2, ..., n.$$

Second column:

Let $a_{22}^{(2)} \neq 0$. Let us remove x_2 from the last n-2 transformed equations:

$$r_i \leftarrow r_i + r_2 * m_{i2}, \qquad m_{i2} = -\frac{a_{i2}^{(2)}}{a_{22}^{(2)}} \qquad i = 3, ..., n$$

$$a_{ij}^{(3)} = a_{ij}^{(2)} + m_{i2}a_{2j}^{(2)}, \ b_i^{(3)} = b_i^{(2)} + m_{i2}b_2^{(2)}, \ i, j = 3, ..., n$$

After n-1 steps:

$$\begin{cases} a_{11}^{(1)}x_1 & + & a_{12}^{(1)}x_2 & + & a_{13}^{(1)}x_3 & + & \dots & + & a_{1n}^{(1)}x_n & = & b_1^{(1)} \\ 0 & + & a_{22}^{(2)}x_2 & + & a_{23}^{(2)}x_3 & + & \dots & + & a_{2n}^{(2)}x_n & = & b_2^{(2)} \\ 0 & + & 0 & + & a_{33}^{(3)}x_3 & + & \dots & + & a_{3n}^{(3)}x_n & = & b_3^{(3)} \\ & & & & \vdots & & & & & \\ 0 & + & 0 & + & 0 & + & \dots & + & a_{nn}^{(n)}x_n & = & b_n^{(n)} \end{cases}$$

Remark

The right hand side b has been subject to the same transformations of the matrix A.

Definition (pivot elements and multipliers)

The element a_{11} and the following elements $a_{ij}^{(j)}$ are called **pivot elements**. Coefficients

$$m_{ij} = -\frac{a_{ij}^{(j)}}{a_{jj}^{(j)}}$$

are called multipliers.

Gaussian Elementary Matrices

Previously, we saw that to eliminate element $a_{21}^{(1)}$ in the first step of transformation, we added the first row multiplied by the multiplier m_{21} to the second row. This is equivalent to multiplying the matrix A (and the right hand side b) by the following matrix, called the **Gaussian elementary matrix**:

$$M_{21} = egin{pmatrix} 1 & 0 & 0 & \dots & 0 \ m_{21} & 1 & 0 & \dots & 0 \ 0 & 0 & 1 & \dots & 0 \ & & dots & & & \ 0 & 0 & 0 & \dots & 1 \end{pmatrix} = I + m_{21} \mathbf{e}_2 \mathbf{e}_1^T,$$

where e_i denotes the *i*-th vector of the canonical basis of \mathbb{R}^n :

$$\mathbf{e}_i = egin{pmatrix} 0 \ dots \ 0 \ 1 \ 0 \ dots \ 0 \end{pmatrix}$$

Elementary Matrix

In general, an elementary matrix is a matrix of the form $I + \alpha u v^T$, $u, v \in \mathbb{R}^n$, $I \in \mathbb{R}^{n \times n}$. The matrix $u v^T$ is the matrix whose element at position ij is $u_i v_i$:

$$\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \begin{pmatrix} v_1 & v_2 & \dots & v_n \end{pmatrix} = \begin{pmatrix} u_1 v_1 & u_1 v_2 & \dots & u_1 v_n \\ u_2 v_1 & u_2 v_2 & \dots & u_2 v_n \\ \vdots & \vdots & \vdots & \vdots \\ u_n v_1 & u_n v_2 & \dots & u_n v_n \end{pmatrix}$$

Note that the matrix uv^T has rank 1. In particular, when $u=e_i$ and $v=e_j$, the matrix $e_ie_j^T$ is the matrix whose elements are all zero except for the element at position ij, which is 1.

Gaussian Elimination

By simple calculations, we verify that:

$$M_{21}A = egin{pmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & \dots & a_{1n}^{(1)} \ 0 & a_{22}^{(2)} & a_{23}^{(2)} & \dots & a_{2n}^{(2)} \ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} & \dots & a_{3n}^{(1)} \ & & & \vdots & & & & \\ a_{n1}^{(1)} & a_{n2}^{(1)} & a_{n3}^{(1)} & \dots & a_{nn}^{(1)} \end{pmatrix} ,$$

Similarly, to eliminate the element a_{31} , we can multiply A and b on the left by the matrix

$$M_{31} = I + m_{31}e_3e_1^T$$
.

Gaussian Elimination for General Columns

Proceeding similarly, we can zero out all the elements below the diagonal in the first column by multiplying A and b by matrices

$$M_{i1} = I + m_{i1}e_ie_1^T$$
.

Now we have:

$$M_{n1}M_{n-1,1}\dots M_{31}M_{21}Ax = M_{n1}M_{n-1,1}\dots M_{31}M_{21}b$$

which can be written as:

$$M_1Ax = M_1b$$
,

with

$$M_1 = M_{n1}M_{n-1,1}\dots M_{31}M_{21}.$$

Factorization of Matrix A

At the end of the elimination process, we have:

$$Ux = M_{n-1} \dots M_2 M_1 Ax = M_{n-1} \dots M_2 M_1 b.$$

Thus, we define:

$$M = M_{n-1} \dots M_2 M_1$$
,

and the system can be written compactly as:

$$MAx = Ux = Mb$$
.

Matrix Structure

We observe that the matrix M_k has a lower triangular structure

$$M_{k} = (I + \sum_{l=k+1}^{n} m_{lk} e_{l} e_{k}^{T}) = \begin{pmatrix} 1 & 0 & \dots & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & \dots & 0 \\ 0 & 0 & \dots & m_{k+1,k} & \dots & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & m_{n,k} & \dots & 1 \end{pmatrix}$$

We observe that the matrix M has a lower triangular structure, but

$$M = \prod_{k=1}^{n-1} M_k \neq \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ m_{21} & 1 & 0 & \dots & 0 \\ m_{31} & m_{32} & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n1} & m_{n2} & m_{n3} & \dots & 1 \end{pmatrix}$$

Calculation of the Elements of M

To compute its elements, we observe that:

$$M_{k+1}M_{k} = (I + \sum_{i=k+2}^{n} m_{i,k+1}e_{i}e_{k+1}^{T})(I + \sum_{l=k+1}^{n} m_{lk}e_{l}e_{k}^{T})$$

$$= I + \sum_{l=k+1}^{n} m_{lk}e_{l}e_{k}^{T} + \sum_{i=k+2}^{n} m_{i,k+1}e_{i}e_{k+1}^{T}$$

$$+ \sum_{i=k+2}^{n} \sum_{l=k+1}^{n} m_{i,k+1}m_{lk}e_{l}e_{k}^{T}e_{l}e_{k}^{T}$$

$$= I + \sum_{l=k+1}^{n} m_{lk}e_{l}e_{k}^{T} + \sum_{i=k+2}^{n} m_{i,k+1}e_{i}e_{k+1}^{T}$$

$$+ \sum_{i=k+2}^{n} m_{i,k+1}m_{k+1,k}e_{i}e_{k}^{T}.$$

In the last step, we consider that from the various products $e_{k+1}^T e_l$, l = k + 1, ..., n, the only non-zero is the one for l = k + 1.

Introducing L

Now we define:

$$L = M^{-1} = (M_{n-1} \dots M_2 M_1)^{-1} = M_1^{-1} M_2^{-1} \dots M_{n-1}^{-1}$$

and observe that we can write the original system Ux = MAx = Mb as

$$LUx = Ax = b.$$

The matrix L is also lower triangular. Its computation is less complicated and costly than it may appear at first sight.

Remark: Inverse of M_{ij}

We also observe that:

$$M_{ij}^{-1}=I-m_{ij}e_ie_j^T;$$

In fact:

$$M_{ij}^{-1}M_{ij} = (I - m_{ij}e_ie_j^T)(I + m_{ij}e_ie_j^T) = I + m_{ij}e_ie_j^T - m_{ij}e_ie_j^T - m_{ij}^2e_ie_j^Te_ie_j^T = I$$

since $e_i^Te_i = 0$ for $i > j$.

Inverse of M_i

Proceeding analogously to the previous case, we show that

$$M_j^{-1} = I - \sum_{i=j+1}^n m_{ij} e_i e_j^T.$$

Thus, M_j^{-1} has the same structure as M_j but with the multipliers negated. Additionally, we observe that

$$L = I - \sum_{j=1}^{n} \sum_{i=j+1}^{n} m_{ij} e_{i} e_{j}^{T},$$

so the matrix *L* has the following simple structure:

$$L = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ -m_{21} & 1 & 0 & \dots & 0 \\ -m_{31} & -m_{32} & 1 & \dots & 0 \\ & & \vdots & \ddots & \\ -m_{n1} & -m_{n2} & \dots & -m_{n,n-1} & 1 \end{pmatrix}.$$

Remark

Thus, the matrix L can be constructed during the Gaussian elimination process by simply retaining the elements m_{ii} .

Calculation of the Elements of L

To compute its elements, we observe that:

$$\begin{split} M_{k}^{-1}M_{k+1}^{-1} &= (I - \sum_{l=k+1}^{n} m_{lk}e_{l}e_{k}^{T})(I - \sum_{i=k+2}^{n} m_{i,k+1}e_{i}e_{k+1}^{T}) \\ &= I - \sum_{l=k+1}^{n} m_{lk}e_{l}e_{k}^{T} - \sum_{i=k+2}^{n} m_{i,k+1}e_{i}e_{k+1}^{T} \\ &+ \sum_{l=k+1}^{n} \sum_{i=k+2}^{n} m_{lk}m_{i,k+1}e_{l} \boxed{e_{k}^{T}e_{i}}e_{k+1}^{T} \\ &= I - \sum_{l=k+1}^{n} m_{lk}e_{l}e_{k}^{T} - \sum_{i=k+2}^{n} m_{i,k+1}e_{i}e_{k+1}^{T} \\ &+ \sum_{l=k+1}^{n} \sum_{i=k+2}^{n} m_{lk}m_{i,k+1}e_{l} \boxed{0}e_{k+1}^{T}. \end{split}$$

In the last step, we consider that from the various products $e_k^T e_i = 0$, l = k + 2, ..., n are all 0 because $i \neq k$.

LU Factorization

We have now seen that, with the same operations used in Gaussian elimination, we can factor the matrix A into the product of two matrices, L and U. It is possible to give conditions on the matrix A that guarantee the Gaussian elimination process can be successfully completed.

Definition

Let $A \in \mathbb{R}^{n \times n}$; we define A_k , with $k = 1, \ldots, n$, as the leading principal submatrix of order k, obtained by intersecting the first k rows and k columns of A.

LU Factorization Theorem

Theorem

Let A be a matrix of order n. If A_k is non-singular for k = 1, ..., n-1, then the LU factorization of A exists and is unique.

Matrices with row- or column-dominant diagonals, as well as symmetric positive-definite matrices, certainly satisfy the theorem's hypothesis.

Example

Given

$$A = \begin{pmatrix} 4 & 4 & 8 \\ 2 & 8 & 7 \\ 1 & 3 & 6 \end{pmatrix} \qquad b = \begin{pmatrix} 12 \\ 9 \\ 7 \end{pmatrix}$$

let us compute the solution of the linear system by Gaussian elimination in matrix form.

$$M_1 = egin{pmatrix} 1 & 0 & 0 \ -rac{1}{2} & 1 & 0 \ -rac{1}{4} & 0 & 1 \end{pmatrix}$$

and

$$M_1*(A|b) = \begin{pmatrix} 4 & 4 & 8 & | & 12 \\ 0 & 6 & 3 & | & 3 \\ 0 & 2 & 4 & | & 4 \end{pmatrix}.$$

Example

$$M_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{3} & 1 \end{pmatrix}$$

and

$$M_2M_1*(A|b) = \begin{pmatrix} 4 & 4 & 8 & | & 12 \\ 0 & 6 & 3 & | & 3 \\ 0 & 0 & 3 & | & 3 \end{pmatrix} = (U|b^{(3)}).$$

Applying a backward substitution we get

- $x_3 = 1$
- $x_2 = (3 3 * 1)/6 = 0$
- $x_1 = (12 4 * 0 8 * 1)/4 = 1$

LU factorization

We have build the A = LU factorization with

- L lower triangular matrix
- *U* upper triangular matrix

In order to solve the linear system we can write:

$$Ax = b$$

$$LUx = b$$

$$L\underbrace{Ux}_{y} = b$$

$$\Downarrow$$

$$Ly = b, \quad Ux = y$$

The original linear system, after the LU factorization of the matrix of coefficients can be tackled in two steps, each requiring the solution of a triangular system:

- **1** first, we compute y by solving Ly = b;
- ② then, given y, we compute x by solving Ux = y.

Remark

Solving the linear system Ly = b is equivalent to apply to b the same transformations of the Gaussian elimination. For this reason the vector y solution of Ly = b is exactly (up to numerical precision) $b^{(n)}$!

The LU factorization and the Gaussian elimination perform exactly the same operation when applied to a single linear system. The LU factorization is much more convenient when we have several linear systems with the same coefficient matrix. In this case we compute the (expensive) factorization once for all and then apply a forward and a backward substitution for each right hand side.

Computational cost

The **computational cost** of an algorithm is the order of magnitude of the number of multiplication or division performed by the algorithm computed with respect to the dimension of the problem. In this case, the characteristic dimension of the problem is the dimension n of the matrix.

 Computational cost of the LU factorization (cost of the Gaussian elimination):

$$\mathcal{O}\left(\frac{n^3}{3}\right)$$
 multiplications.

 Computational cost of the solution of a triangular system (either upper or lower):

$$\mathcal{O}\left(\frac{n^2}{2}\right)$$
 multiplications.

For the solution of a linear system the larger cost is in the LU factorization, the cost of the solution of triangular systems is negligible with respect to the cost of the factorization: the overall cost is

$$\mathcal{O}(\frac{n^3}{3}) + \mathcal{O}(n^2) \simeq \mathcal{O}(\frac{n^3}{3})$$

operations (multiplications). Larger is n smaller is $\mathcal{O}(n^2)$ with respect to $\mathcal{O}(\frac{n^3}{3})$.

Remark

Factorization approach is "mandatory" when we have to solve many linear systems with the same matrix and different right hand sides.

Example

Given

$$A = \begin{pmatrix} 4 & 4 & 8 \\ 2 & 8 & 7 \\ 1 & 3 & 6 \end{pmatrix}$$

compute its LU factorization using the computation of the previous exercise on Gaussian elimination.

The upper triangular matrix U does not change, whereas the lower triangular matrix L is simply set up by the opposite of the multipliers:

$$U = \begin{pmatrix} 4 & 4 & 8 \\ 0 & 6 & 3 \\ 0 & 0 & 2 \end{pmatrix} \qquad L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & \frac{1}{3} & 1 \end{pmatrix}$$

Remark: $det(A) = det(L) \cdot det(U) = 1 \cdot \prod_{i=1}^{n} u_{ii} = 48$.

Remark

The matrix L can be stored in the same memory locations of the lower triangular part of the matrix A when the corresponding elements are transformed in zeros.

$$\begin{pmatrix} 4 & 4 & 8 \\ 2 & 8 & 7 \\ 1 & 3 & 6 \end{pmatrix} \longrightarrow \begin{pmatrix} 4 & 4 & 8 \\ \frac{1}{2} & 6 & 3 \\ \frac{1}{4} & 2 & 4 \end{pmatrix} \longrightarrow \begin{pmatrix} 4 & 4 & 8 \\ \frac{1}{2} & 6 & 3 \\ \frac{1}{4} & \frac{1}{3} & 2 \end{pmatrix}$$

Can we always correctly finish the Gaussian elimination or the LU factorization?

Definition

Let $A \in \mathbb{R}^{n \times n}$. Let us define A_k , with k = 1, ..., n, the principal submatrix of order k of A as the matrix obtained intersecting the first k rows and the first k columns of A.

Theorem

Let A be a matrix of order n. If A_k is non singular for k = 1, ..., n-1 then the LU factorization of A exists and is unique.

Remark

The diagonal dominant matrices for rows or for columns and the symmetric positive definite matrices always satisfy this condition.

Remark

The previous theorem does not exclude the matrix A be singular. If A is singular, but $\det(A_k) \neq 0$, k = 1, ..., n-1, the LU factorization of A exists with a matrix U with at least a vanishing diagonal term U_{ii} .

Pivoting

Example

What happens if we apply the Gaussian elimination to

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
?

We need to resort to permutation matrices.

Definition

Let P_{ij} the matrix obtained by the identity matrix after a permutation of the *i*-th and the *j*-th rows:

These matrices P_{ij} are called elementary permutation matrices.

Give a matrix $A \in \mathbb{R}^{n \times n}$

- the left multiplication of A by $P_{ij} \in \mathbb{R}^{n \times n}$ ($P_{ij}A$) results in a permutation of the i-th row of the matrix A with its j-th rows;
- the right multiplication of A by P_{ij} (AP_{ij}) results in a permutation of the *i*-th column of the matrix A with its *j*-th column.

If we multiply several elementary permutation matrices we get a matrix P that we call **permutation matrix** whose product by A applies all the permutations of the single elementary permutation matrices at ones.

Theorem

Let $A \in \mathbb{R}^{n \times n}$, then exists at least a permutation matrix $P \in \mathbb{R}^{n \times n}$ for which we can get the following factorization of A:

$$PA = LU$$
.

Let us remark that for each matrix A several permutation matrices P exist such that for the matrix PA exists the LU factorization.

How can we find one of such a permutation matrices P?



Strategy of partial pivoting.

Partial Pivoting

Let us assume that at the k-th step of the Gaussian elimination/LU factorization (recall that they perform the same operations on the matrix) the pivot element $a_{kk}^{(k)}=0$. We can not compute the multiplier $m_{ik}=-a_{ik}^{(k)}/a_{kk}^{(k)}$. In order to circumvent this problem we can apply a permutation between the k-th row and a row with index i>k with the element $a_{ik}^{(k)}\neq 0$. We remark that the row index i has to be larger than k.

Example

Let us consider the following linear system:

$$\begin{cases} x_1 + x_2 + x_3 = 1 \\ x_1 + x_2 + 2x_3 = 2 \\ x_1 + 2x_2 + 2x_3 = 1 \end{cases}$$

Gaussian elimination: $m_{21} = -1$ e $m_{31} = -1 \Longrightarrow$

$$\begin{cases} x_1 + x_2 + x_3 = 1 \\ 0 + 0 + x_3 = 1 \\ 0 + x_2 + x_3 = 0 \end{cases}$$

$$a_{22}^{(2)}=0!$$

Example (follows)

The system is already in upper triangular form, so we can get the solution by a backward substitution:

$$\begin{cases} x_3 = 1 \\ x_2 = -x_3 = -1 \\ x_1 = 1 - x_2 - x_3 = 1 \end{cases}$$

In this case we have det(A) = -det(U) = -1; whereas in general, $det(A) = (-1)^s \cdot det(U)$, where s is the total number of permutations performed.

PA = LU factorization

Matrix notation of the LU factorization with pivoting

$$A^{(k+1)} = M_k P_k A^{(k)}$$

n-1 steps $(P_i^{-1} = P_i)$, permutation matrices are "involutive"):

$$A^{(n)} = M_{n-1}P_{n-1}A^{(n-1)} = \dots = M_{n-1}P_{n-1}M_{n-2}P_{n-2}\dots M_2P_2M_1P_1A$$

$$U = M_{n-1}P_{n-1}M_{n-2}P_{n-2}M_{n-3}\dots P_3M_2P_2M_1P_1A$$

$$= M_{n-1}\bar{M}_{n-2}P_{n-1}P_{n-2}M_{n-3}\dots P_3M_2P_2M_1P_1A$$

$$= M_{n-1}\bar{M}_{n-2}P_{n-1}P_{n-2}M_{n-3}\dots P_3M_2(P_2M_1P_2)P_2P_1A$$

$$= M_{n-1}\bar{M}_{n-2}P_{n-1}P_{n-2}M_{n-3}\dots P_3M_2P_3P_3\bar{M}_1P_3P_3P_2P_1A$$

$$= M_{n-1}\bar{M}_{n-2}P_{n-1}P_{n-2}M_{n-3}\dots \bar{M}_2P_3\bar{M}_1P_3P_3P_2P_1A$$

$$= M_{n-1}\bar{M}_{n-2}\dots \bar{M}_2\bar{M}_1P_{n-1}P_{n-2}\dots P_2P_1A$$

$$= M_{n-1}\bar{M}_{n-2}\dots \bar{M}_2\bar{M}_1P_{n-1}P_{n-2}\dots P_2P_1A$$

$$= MPA,$$

where

$$\bar{M}_1 = P_{n-1} \dots P_2 M_1 P_2 \dots P_{n-1}, \ \bar{M}_2 = P_{n-1} \dots P_3 M_2 P_3 \dots P_{n-1}, \bar{M}_3 = P_{n-1} \dots P_4 M_3 P_4 \dots P_{n-1}, \ \bar{M}_i = P_{n-1} \dots P_{i+1} M_i P_{i+1} \dots P_{n-1}.$$

Stefano Berrone

Note that the permutation P_i is always a permutation $P_{i,j}$ with j > i. Let us suppse that $P_2 = P_{i,2}$ and $P_3 = P_{i+1,3}$.

$$P_{2}M_{1}P_{2} = P_{2} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & \dots & 0 \\ m_{2,1} & 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ m_{i,1} & 0 & \dots & 1 & 0 & \dots & 0 \\ m_{i+1,1} & 0 & \dots & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & 0 & \dots & 1 \end{pmatrix} \\ P_{2} = P_{2} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & \dots & 0 \\ m_{2,1} & 0 & \dots & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{i,1} & 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & 0 & \dots & 1 \end{pmatrix} \\ P_{3} = P_{3} \begin{pmatrix} 1 & 0 & \dots & 0 & \dots & 0 \\ m_{i+1,1} & 0 & \dots & 0 & \dots & 0 \\ m_{3,1} & 0 & \dots & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{2,1} & 0 & \dots & 1 & 0 & \dots & 0 \\ m_{i+1,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{2,1} & 0 & \dots & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{n,1} & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$

The right product with the permutation matrices swaps the columns in the right-bottom corner of the matrix, that is an identity matrix, moving the 1s in the off-diagonal position, later the left multiplication by the same permutation matrix swaps the same lines repositioning the 1s previously moved outside the diagonal on the diagonal such that the right-bottom block of the matrix is again an identity matrix.

$$U = MPA$$

$$M^{-1}U = PA$$

Defining $L=M^{-1}$ we have found the LU factorization of the matrix PA, i.e. the factorization PA=LU.

How we can use the factorization PA = LU to solve linear systems?

In general the pivoting strategy, i.e. the permutation of rows, is applied also if the pivot elements are not zero in order to **improve stability** of the Gaussian elimination/LU factorization.

Has been proved that, in order to improve stability of the method, pivoting can prevent large multipliers that often cause an unstable amplification of errors. The strategy for preventing large multipliers is to prevent small pivot elements. Partial pivoting works in this direction performing rows permutations in order to get large values of pivot elements $a_{kk}^{(k)}$.

More precisely, at the k-th step we look for the largest absolute value among the elements $a_{rk}^{(k)}$, with $r \ge k$. When we have found it, being r the row index of this element we apply a permutation between the k-th and the r-th rows.

This strategy, trivially ensures at each step the largest possible pivot element and consequently increases the stability of the algorithm.

Remark

If the matrix A is diagonal dominant for columns, we can prove that the strategy of the partial pivoting is useless inducing no permutation of rows. Moreover, if the matrix A is symmetric positive definite the Gaussian elimination/LU factorization is stable by itself and partial pivoting is unnecessary.

We have to add that for symmetric positive definite matrices there is a more suitable factorization called Cholesky factorization.

Construction of L

$$P = P_{n-1} \dots P_1$$
$$U = A^{(n)}$$
$$I = ?$$

The matrix L can be easily obtained from the original LU factorization process of the Gaussian elimination. In fact, the key idea is that when we perform a permutation of rows, we have to permute all the row including the multipliers stored in the part of the row preceding the diagonal. This provides the same result we get if we first apply all the permutations on the matrix A and then we apply the factorization on the permuted matrix PA.

Example

$$A = \begin{pmatrix} 1 & 4 & 8 \\ 2 & 0 & 7 \\ 4 & 2 & 6 \end{pmatrix}$$

$$P_1 = P_{13}$$
:

$$P_{13}A = \begin{pmatrix} 4 & 2 & 6 \\ 2 & 0 & 7 \\ 1 & 4 & 8 \end{pmatrix}$$

$$A^{(2)} = \begin{pmatrix} 4 & 2 & 6\\ \frac{1}{2} & -1 & 4\\ \frac{1}{4} & \frac{7}{2} & \frac{13}{2} \end{pmatrix}$$

Example (follows...)

$$P_2 = P_{23}$$
:

$$P_{23}A^{(2)} = \begin{pmatrix} 4 & 2 & 6\\ \frac{1}{4} & \frac{7}{2} & \frac{13}{2}\\ \frac{1}{2} & -1 & 4 \end{pmatrix}$$

$$A^{(3)} = \begin{pmatrix} 4 & 2 & 6 \\ \frac{1}{4} & \frac{7}{2} & \frac{13}{2} \\ \frac{1}{2} & -\frac{2}{7} & \frac{41}{7} \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{2}{7} & 1 \end{pmatrix} \ U = \begin{pmatrix} 4 & 2 & 6 \\ 0 & \frac{7}{2} & \frac{13}{2} \\ 0 & 0 & \frac{41}{7} \end{pmatrix} \ P = P_{23}P_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Example

Let us consider the linear system Ax = b, with

$$A = \begin{pmatrix} \varepsilon & 1 \\ 1 & 0 \end{pmatrix}, \qquad b = \begin{pmatrix} 1 + \varepsilon \\ 1 \end{pmatrix}, \qquad \varepsilon > 0$$
The exact solution is $x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}^T$. If ε is not large, the problem is well

conditioned

$$A^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & -\varepsilon \end{pmatrix}, \qquad K_{\infty}(A) = \|A\|_{\infty} \cdot \|A^{-1}\|_{\infty} = (1+\varepsilon)^2$$
 if $\varepsilon \ll 1$, we have $K_{\infty}(A) \simeq 1$. The exact LU factorization of A is

$$L = \begin{pmatrix} 1 & 0 \\ \frac{1}{\varepsilon} & 1 \end{pmatrix}, \qquad U = \begin{pmatrix} \varepsilon & 1 \\ 0 & -\frac{1}{\varepsilon} \end{pmatrix}.$$

$$M_1 = \begin{pmatrix} 1 & 0 \\ -\frac{1}{\varepsilon} & 1 \end{pmatrix}, \qquad M_1 b = \begin{pmatrix} 1 + \varepsilon \\ -\frac{1}{\varepsilon} \end{pmatrix}.$$

And the system $Ux = M_1b$ provides the correct solution

Now, let us assume to perform these computation with $\varepsilon \simeq 0.3 \cdot 10^{-3}$ working with an arithmetic with basis $\beta=10$, t=3 digits for the mantissa and truncation or rounding (indifferent for these computations) (eps $=1.0 \cdot 10^{-2} > \varepsilon$).

The computed matrices and right hand side are:

$$\bar{b} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \bar{M}_1 = \begin{pmatrix} 1 & 0 \\ -0.333 \cdot 10^4 & 1 \end{pmatrix},$$

$$\bar{L} = \bar{M}_1^{-1} = \begin{pmatrix} 1 & 0 \\ 0.333 \cdot 10^4 & 1 \end{pmatrix}, \qquad \bar{U} = \begin{pmatrix} 0.3 \cdot 10^{-3} & 1 \\ 0 & -0.333 \cdot 10^4 \end{pmatrix}.$$

The computed right hand side vector is

$$\bar{M}_1\bar{b} = \bar{M}_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 - 0.333 \cdot 10^4 \end{pmatrix} \neq \begin{pmatrix} 1 + \varepsilon \\ -0.333 \cdot 10^4 \end{pmatrix}$$

and the new linear system to be solved is $\bar{U}x=\bar{M}_1\bar{b}$, with solution

$$ar{x}_2 = rac{-0.333 \cdot 10^4}{-0.333 \cdot 10^4} = 1, \qquad ar{x}_1 = rac{1-1}{0.3 \cdot 10^{-3}} = 0.$$

If we apply the partial pivoting:

$$\bar{\bar{A}} = \begin{pmatrix} 1 & 0 \\ 0.3 \cdot 10^{-3} & 1 \end{pmatrix}, \qquad \bar{\bar{b}} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

The computed matrices are:

$$\bar{\bar{M}}_1 = \begin{pmatrix} 1 & 0 \\ -0.3 \cdot 10^{-3} & 1 \end{pmatrix},$$

$$\bar{\bar{L}} = \bar{\bar{M}}_1^{-1} = \begin{pmatrix} 1 & 0 \\ 0.3 \cdot 10^{-3} & 1 \end{pmatrix}, \qquad \bar{\bar{U}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The computed right hand side vector is

$$\bar{\bar{M}}_1\bar{\bar{b}} = \begin{pmatrix} 1\\1 \end{pmatrix} \neq \begin{pmatrix} 1\\1-0.3 \cdot 10^{-3} \end{pmatrix}$$

and the new linear system to be solved is $\bar{U}x = \bar{M}_1\bar{b}$, with solution

$$\bar{x}_2 = \frac{1}{1} = 1, \qquad \bar{x}_1 = \frac{1}{1} = 1.$$

Example

Let us consider the following matrix

$$A = \begin{pmatrix} -2 & 4 & -10 & -1 \\ 4 & -9 & 0 & 5 \\ -4 & 5 & -5 & 5 \\ -8 & 8 & -23 & 20 \end{pmatrix}$$

First, we look for the largest value in modulus in the first column that is $a_{41}^{(1)} = -8$, then we permute the first and the fourth rows.

$$P^{(1)} = P_{14} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}; \quad P^{(1)}A = \begin{pmatrix} -8 & 8 & -23 & 20 \\ 4 & -9 & 0 & 5 \\ -4 & 5 & -5 & 5 \\ -2 & 4 & -10 & -1 \end{pmatrix}.$$

Multipliers for the first column are: $m_{21}=\frac{1}{2}$, $m_{31}=-\frac{1}{2}$, $m_{41}=-\frac{1}{4}$,

$$\label{eq:M1} \textit{M}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & 1 & 0 \\ -\frac{1}{4} & 0 & 0 & 1 \end{pmatrix}, \; \textit{A}^{(2)} = \textit{M}_1 \textit{P}^{(1)} \textit{A} = \begin{pmatrix} -8 & 8 & -23 & 20 \\ -\frac{1}{2} & -5 & -\frac{23}{2} & 15 \\ \frac{1}{2} & 1 & \frac{13}{2} & -5 \\ \frac{1}{4} & 2 & -\frac{17}{4} & -6 \end{pmatrix}.$$

We save the elements of the matrix L in the lower part of the matrix A that vanish during the process. In $A^{(2)}$ the largest element already is the pivot element, we do not need any permutation: $P_2 = I$, $P^{(2)}A^{(2)} = A^{(2)}$. New multipliers are $m_{32} = \frac{1}{5}$, $m_{42} = \frac{2}{5}$,

$$M_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & \frac{1}{5} & 1 & 0 \\ 0 & \frac{2}{5} & 0 & 1 \end{pmatrix}, \ A^{(3)} = M_2 I A^{(2)} = \begin{pmatrix} -8 & 8 & -23 & 20 \\ -\frac{1}{2} & -5 & -\frac{23}{2} & 15 \\ \frac{1}{2} & -\frac{1}{5} & \frac{42}{10} & -2 \\ \frac{1}{4} & -\frac{2}{5} & -\frac{177}{20} & 0 \end{pmatrix}.$$

Being $\frac{177}{20} > \frac{42}{10}$, we have to permute the third and the fourth rows:

$$P^{(3)} = P_{34} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}; \quad P^{(3)}A^{(3)} = \begin{pmatrix} -8 & 8 & -23 & 20 \\ -\frac{1}{2} & -5 & -\frac{23}{2} & 15 \\ \frac{1}{4} & -\frac{2}{5} & -\frac{177}{20} & 0 \\ \frac{1}{2} & -\frac{1}{5} & \frac{42}{10} & -2 \end{pmatrix}.$$

Remark We have swapped all the third and fourth rows of $A^{(3)}$, not only the upper triangular part.

The last multipliers is $m_{43} = \frac{28}{59}$.

$$M_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & \frac{28}{59} & 1 \end{pmatrix}, \ A^{(4)} = M_3 A^{(3)} = \begin{pmatrix} -8 & 8 & -23 & 20 \\ -\frac{1}{2} & -5 & -\frac{23}{2} & 15 \\ \frac{1}{4} & -\frac{2}{5} & -\frac{177}{20} & 0 \\ \frac{1}{2} & -\frac{1}{5} & -\frac{28}{59} & -2 \end{pmatrix}.$$

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 & 0 \\ \frac{1}{4} & -\frac{2}{5} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{5} & -\frac{28}{59} & 1 \end{pmatrix}, \quad U = \begin{pmatrix} -8 & 8 & -23 & 20 \\ 0 & -5 & -\frac{23}{2} & 15 \\ 0 & 0 & -\frac{177}{20} & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}.$$

The final permutation matrix P is provided by the product of all the permutation matrices $P^{(3)}$, $P^{(2)} = I$, $P^{(1)}$:

$$P = P^{(3)} \cdot I \cdot P^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot I \cdot \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

```
octave:2> A =[
      -2
                    -1;
>
              -10
      4
         -9
                0
                    5;
>
>
      -4
           5
                -5
                     5
      -8
>
           8
               -23
                    20
      ];
>
octave:2> [L U P]=lu(A)
L =
   1.00000
             0.00000
                        0.00000
                                   0.00000
  -0.50000
            1.00000
                        0.00000
                                   0.00000
   0.25000
            -0.40000
                        1.00000
                                   0.00000
   0.50000
            -0.20000
                       -0.47458
                                   1,00000
U =
   -8.00000
                8.00000
                         -23.00000
                                      20.00000
    0.00000
               -5.00000
                         -11.50000
                                      15.00000
    0.00000
                0.00000
                          -8.85000
                                       0.00000
    0.00000
                0.00000
                            0.00000
                                      -2.00000
P =
   0
       0
           0
                1
   0
       1
           0
                0
   1
       0
           0
                0
   0
       0
           1
                0
```

```
>> format rat
>> A =[ -2
          4 -10 -1; 4 -9 0 5;
   -4 5 -5 5; -8 8 -23 20];
>> [L U P]=lu(A)
L =
     1
    -1/2
                                          0
    1/4
                -2/5
                -1/5
    1/2
                           -28/59
U =
    -8
                 8
                           -23
                                         20
                 -5
                           -23/2
     0
                                         15
     0
                 0
                          -177/20
                                          0
     0
                  0
                              0
                                         -2
     0
     0
                              0
                                          0
                  0
                                          0
     0
                  0
                                          0
```

Cholesky factorization

When A is symmetric positive definite we can resort the symmetry of A and the innate stability of the LU factorization without pivoting in order to reduce the computational cost of the factorization with the **Cholesky factorization**.

Theorem (Cholesky factorization)

Let A be a symmetric positive definite matrix. There exists a unique upper triangular matrix R (or a unique lower triangular matrix $L = R^T$) with all positive diagonal elements such that

$$A = R^T R$$
 $(A = LL^T).$

The computational cost of the Cholesky factorization is

$$\mathcal{O}(\frac{n^3}{6})$$

Matlab/Octave commands

- [L,U,P]=lu(A)
- R=chol(A) Remark chol assumes that A be symmetric positive definite and considers on the upper triangular part of A.
- \

Different useful factorizations

 QR factorization (qr(A)): Q is an orthogonal matrix, R is an upper triangular matrix. This is a very stable factorization based on the application to A of a sequence of orthogonal matrices used to define Q, but it is computationally more expensive with respect to the LU factorization.

Other useful commands

- norm(x), norm(A): compute the norm of A;
- cond(A): compute the condition number of A;
- condest(A): estimates the 1-norm condition number of A.