Numerical Methods – Info for lab*

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*Note: The pseudocode algorithms are taken in most part from the book "Metode Numerice în Pseudocod. Aplicaţii", M. Popa, R. Militaru, ed. SITECH, Craiova 2012.

1 Introductive notions

Let the matrix with m rows and n columns

$$A = (a_{ij})_{\substack{1 \le i \le m \\ 1 \le j \le n}}.$$

Reading of a matrix in C:

```
// Declaration of variables
int n,m,i,j;
float a[10][10];
printf("give the number of the rows m=");
scanf("%d",&m);
printf("give the number of the columns n=");
scanf("%d",&n);
// we read the elemnts of matrix A
 for(i=1;i<=m;i++)
   for(j=1;j<=n;j++)
       {
      printf("\n a[%d][%d]=",i,j);
      scanf("%f",&a[i][j]);
         }
```

Printing of a matrix in C:

```
for(i=1;i<=m;i++)
    {
      for(j=1;j<=n;j++)
        printf("%f", a[i][j]);
        printf("\n");
    }
```

Sum and differences of two matrices

Exercise 1. Let

$$A = \begin{pmatrix} 3 & 0 \\ 1 & 3 \\ -2 & -2 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} -1 & 2 \\ 0 & 7 \\ 0 & 5 \end{pmatrix}$$

Compute $A+B$, $A-B$ and $B-A$.

Pseudocode Algorithm to compute A+B

// Read $m, n-$the numbers of rows and columns corresponding to A and B, and the elements of A and B

1. read m, n, a_{ij}, b_{ij}, $1 \le i \le m$, $1 \le j \le n$
2. for $i = 1, 2, ..., m$
   2.1. for $j = 1, 2, ..., n$
   // Compute the elements of matrix C=A+B

2.1.1 $c_{ij} \leftarrow a_{ij} + b_{ij}$
3. we print the matrix $C = (c_{ij})_{\substack{1\le i\le m\\1\le j\le n}}$.

The algorithm to multiply two matrices

Let
$$A = (a_{ij})_{\substack{1\le i\le m\\1\le j\le n}} \in \mathcal{M}_{mn}(\mathbb{R}) \quad \text{and} \quad B = (b_{ij})_{\substack{1\le i\le n\\1\le j\le p}} \in \mathcal{M}_{np}(\mathbb{R}).$$
Then $A \cdot B = (c_{ij})_{\substack{1\le i\le m\\1\le j\le p}} \in \mathcal{M}_{mp}(\mathbb{R})$, where

$$c_{ij} = \sum_{k=1}^{n} a_{ik} \cdot b_{kj}, \quad \forall 1 \le i \le m, \forall 1 \le j \le p. \tag{1}$$

Exercise 2. Compute $A \cdot B$, where
$$A = \begin{pmatrix} 3 & 0 \\ 1 & 3 \\ -2 & -2 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 2 & 2 \\ 1 & 3 & -1 \end{pmatrix}.$$

Pseudocode Algorithm to compute AB
1. read m, n, p, a_{ij}, $1 \le i \le m$, $1 \le j \le n$, b_{ij}, $1 \le i \le n$, $1 \le j \le p$
2. for $i = 1, 2, ..., m$
   2.1. for $j = 1, 2, ..., p$
      2.1.1 $c_{ij} \leftarrow 0$
      2.1.2 for $k = 1, 2, ..., n$
         2.1.2.1 $c_{ij} \leftarrow c_{ij} + a_{ik} \cdot b_{kj}$
3. we print the matrix $C = (c_{ij})_{\substack{1\le i\le m\\1\le j\le p}}$.

The algorithm to interchange two rows into a matrix

Exercise 3. Let
$$A = \begin{pmatrix} 0 & 2 & 2 & 2 \\ 1 & 3 & -1 & 2 \\ 4 & 3 & 0.5 & 2 \end{pmatrix}.$$
Interchange the row 2 with row 3 in above matrix and print the matrix.

Pseudocode Algorithm
1. read m, n, a_{ij}, $1 \le i \le m$, $1 \le j \le n$
2. for $j = 1, 2, ..., n$
   2.1. $aux \leftarrow a_{2j}$
   2.2. $a_{2j} \leftarrow a_{3j}$
   2.3. $a_{3j} \leftarrow aux$
3. we print the matrix $(a_{ij})_{\substack{1\le i\le m\\1\le j\le n}}$.

Exercise 4. Let

$$A = \begin{pmatrix} 0 & 2 & 1 \\ 1 & 0 & -1 \\ 4 & 1 & 2 \end{pmatrix} \quad \text{şi} \quad B = \begin{pmatrix} 2 & 0 & 1 \\ 3 & -1 & -1 \\ 0 & 1 & -1 \end{pmatrix}.$$

a) Compute $A - 2B$, A^2, BA, AB, $B + 2I_3$;
b) Interchange the row 3 with row 1 in matrix B and print the matrix;
c) Compute the sum of the elements on the principal diagonal of matrix $A \cdot B$ (i.e. the trace of $A \cdot B \overset{not}{=} Tr(A \cdot B)$).

The maximum and minimum of elements in a vector

Exercise 5. Let

$$v = \left(2,\, -2,\, 3,\, \frac{1}{3},\, -0.5\right).$$

Find the maximum and minimum of elements of vector v.

Pseudocode Algorithm

1. read n, v_i, $1 \le i \le n$
2. $max \leftarrow v[1]$
3. for $i = 1, 2, ..., n$
    3.1. if $max < v[i]$ then
        3.1.1 $max \leftarrow v[i]$
4. print max

2 Gauss elimination method – the basic version

Describing the problem: We consider the linear system

$$A \cdot x = b, \tag{2}$$

where $A \in \mathcal{M}_n(\mathbb{R})$ is the matrix associated to system (2) and $b \in \mathbb{R}^n$ is the vector containing the free terms of system (2).
Our goal is to determine, if possible, $x \in \mathbb{R}^n$, where x represents the unique solution of system (2).

The method:
We consider the augmented matrix $(A \,|\, b) = (a_{ij})_{\substack{1 \le i \le n \\ 1 \le j \le n+1}}$, where $a_{i,n+1} = b_i$, $1 \le i \le n$.
The Gauss method consists of processing the augmented matrix $(A \,|\, b)$ such that, in $n-1$ steps the matrix A becomes upper-triangular:

$$\left(\begin{array}{ccccc|c} a_{11}^{(n)} & a_{12}^{(n)} & \dots & a_{1,n-1}^{(n)} & a_{1,n}^{(n)} & a_{1,n+1}^{(n)} \\ 0 & a_{22}^{(n)} & \dots & a_{2,n-1}^{(n)} & a_{2,n}^{(n)} & a_{2,n+1}^{(n)} \\ \vdots & \vdots & \dots & \vdots & & \vdots \\ 0 & 0 & \dots & a_{n-1,n-1}^{(n)} & a_{n-1,n}^{(n)} & a_{n-1,n+1}^{(n)} \\ 0 & 0 & \dots & 0 & a_{n,n}^{(n)} & a_{n,n+1}^{(n)} \end{array}\right) = A^{(n)}, \quad \text{where} \quad A^{(1)} = (A \,|\, b). \tag{3}$$

If $a_{kk}^{(k)} \neq 0, 1 \leq k \leq n-1$, where the element $a_{kk}^{(k)}$ is called **pivot**, in order to arrive at matrix (3) we apply the following algorithm. For $k = 1, 2, \ldots, n-1$,,

- we copy the first k rows (lines);
- on column "k", under pivot, the elements will be null (zero);
- the remaining elements, situated below the row "k" and at the right hand side of the column "k", will be determined using the so-called "rectangle rule", described below:

$$\begin{array}{cccccc} & \vdots & & \vdots & \\ \text{row } k \quad \cdots & a_{kk}^{(k)} & \cdots\cdots\cdots & a_{kj}^{(k)} & \cdots \\ & \vdots & & \vdots & \\ \text{row } i \quad \cdots & a_{ik}^{(k)} & \cdots\cdots\cdots & a_{ij}^{(k)} & \cdots \\ & \vdots & & \vdots & \\ & \text{column } k & & \text{column } j & \end{array} \Rightarrow a_{ij}^{(k+1)} = \frac{a_{kk}^{(k)} a_{ij}^{(k)} - a_{ik}^{(k)} a_{kj}^{(k)}}{a_{kk}^{(k)}}.$$

Therefore, for $1 \leq k \leq n-1$, we will use the following formulae:

$$(4) \qquad a_{ij}^{(k+1)} = \begin{cases} a_{ij}^{(k)} & 1 \leq i \leq k, \ i \leq j \leq n+1 \\ 0 & 1 \leq j \leq k, \ j+1 \leq i \leq n \\ a_{ij}^{(k)} - \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \cdot a_{kj}^{(k)} & k+1 \leq i \leq n, \ k+1 \leq j \leq n+1. \end{cases}$$

After arriving at the upper-triangular matrix described by (3), we realize that we have actually arrived at an upper-triangular system equivalent to (2):

$$(5) \qquad \begin{cases} a_{11}^{(n)} x_1 + a_{12}^{(n)} x_2 + \ldots + a_{1n}^{(n)} x_n = a_{1,n+1}^{(n)} \\ \qquad a_{22}^{(n)} x_1 + \ldots + a_{2n}^{(n)} x_n = a_{2,n+1}^{(n)} \\ \qquad \qquad \ldots\ldots\ldots\ldots \\ \qquad \quad a_{ii}^{(n)} x_1 + \ldots + a_{in}^{(n)} x_n = a_{i,n+1}^{(n)} \\ \qquad \qquad \ldots\ldots\ldots\ldots \\ \qquad \qquad \qquad a_{nn}^{(n)} x_n = a_{n,n+1}^{(n)}. \end{cases}$$

This system is solvable by using the back substitution method, that is, by applying the following formulae:

$$(6) \qquad x_n = a_{n,n+1}^{(n)} / a_{nn}^{(n)}, \qquad \text{if } a_{nn}^{(n)} \neq 0,$$

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

$$(7) \qquad x_i = \left(a_{i,n+1}^{(n)} - \sum_{j=i+1}^{n} a_{ij}^{(n)} \cdot x_j \right) / a_{ii}^{(n)}.$$

Pseudocode Algorithm

// Read n, the dimension of matrix A and the augmented matrix $(A \,|\, b)$

1. read n, a_{ij}, $1 \leq i \leq n$, $1 \leq j \leq n+1$
2. for $k = 1, 2, ..., n-1$
   2.1. if $a_{kk} \neq 0$ then
      //Apply the formulae from Gauss method (the rectangle rule), see (11).
      2.1.1. for $i = k+1, k+2, ..., n$
         2.1.1.1. for $j = k+1, k+2, ..., n+1$
            2.1.1.1.1. $a_{ij} \leftarrow a_{ij} - a_{ik} \cdot a_{kj} / a_{kk}$
3. if $a_{nn} = 0$ then
   3.1. write *'The system does not have unique solution'*
   3.2. *exit*
//Determine x_n by applying formula (6)
4. $a_{n,n+1} \leftarrow a_{n,n+1} / a_{nn}$
//Determine $x_i, n-1 \geq i \geq 1$, by applying formulae (7)
5. for $i = n-1, n-2, ..., 1$
   5.1. $S \leftarrow 0$
   5.2. for $j = i+1, i+2, ..., n$
      5.2.1. $S \leftarrow S + a_{ij} \cdot a_{j,n+1}$
   5.3. $a_{i,n+1} \leftarrow (a_{i,n+1} - S) / a_{ii}$
6. write $'x_i =', a_{i,n+1}$, $1 \leq i \leq n$.

Exercises:

I. Include additional instructions at the second step of the algorithm to take into account the case when $a_{kk} = 0$:

a) announce that $a_{kk} = 0$;

b) instead of announcing that $a_{kk} = 0$, find $a_{lin,k} \neq 0$ with $lin = k+1, k+2, ..., n$ and switch the lines lin and k.

II. Mathematically (=by hand) solve the following systems using the Gauss method

$$a)\begin{cases} x_1 + 2x_2 + 3x_3 + x_4 = 7 \\ 2x_1 + x_2 + 2x_3 + 3x_4 = 8 \\ 2x_1 - x_2 - 4x_3 + 4x_4 = 1 \\ 2x_1 + x_3 - 3x_4 = 0 \end{cases} \qquad b)\begin{cases} x_1 + 3x_2 - 2x_3 - 4x_4 = -2 \\ 2x_1 + 6x_2 - 7x_3 - 10x_4 = -6 \\ -x_1 - x_2 + 5x_3 + 9x_4 = 9 \\ -3x_1 - 5x_2 + 15x_4 = 13 \end{cases} \qquad c)\begin{cases} x - y - 3z = 8 \\ 3x - y + z = 4 \\ 2x + 3y + 19z = 10. \end{cases}$$

3 Gauss method with partial/total pivoting at every step

The problem: We consider the linear system

$$A \cdot x = b, \tag{8}$$

where $A \in \mathcal{M}_n(\mathbb{R})$ is the matrix associated to system (8) and $b \in \mathbb{R}^n$ is the vector containing the free terms of system (8).
Our goal is to determine, if possible, $x \in \mathbb{R}^n$, where x represents the unique solution of system (8).

Recalling the basic Gauss method:

We consider the augmented matrix $(A\,|\,b) = (a_{ij})_{\substack{1\le i\le n\\ 1\le j\le n+1}}$, where $a_{i,n+1} = b_i$, $1 \le i \le n$.

The Gauss method consists of processing the augmented matrix $(A\,|\,b)$ such that, in $n-1$ steps the matrix A becomes upper-triangular:

$$(9)\qquad \left(\begin{array}{ccccc|c} a_{11}^{(n)} & a_{12}^{(n)} & \dots & a_{1,n-1}^{(n)} & a_{1,n}^{(n)} & a_{1,n+1}^{(n)} \\ 0 & a_{22}^{(n)} & \dots & a_{2,n-1}^{(n)} & a_{2,n}^{(n)} & a_{2,n+1}^{(n)} \\ \vdots & \vdots & \dots & \vdots & & \vdots \\ 0 & 0 & \dots & a_{n-1,n-1}^{(n)} & a_{n-1,n}^{(n)} & a_{n-1,n+1}^{(n)} \\ 0 & 0 & \dots & 0 & a_{n,n}^{(n)} & a_{n,n+1}^{(n)} \end{array}\right) = A^{(n)}, \quad \text{where } A^{(1)} = (A\,|\,b).$$

(10) **At every step k we test if $a_{kk}^{(k)} \neq 0, 1 \le k \le n-1$.**

If $a_{kk}^{(k)} \neq 0, 1 \le k \le n-1$, (where the element $a_{kk}^{(k)}$ is called **pivot**), in order to arrive at matrix (9), we apply the following algorithm. For $k = 1, 2, \dots, n-1$,,

- we copy the first k rows (lines);
- on column "k", under the pivot, the elements will be null (zero);
- the remaining elements, situated below the row "k" and at the right hand side of the column "k", will be determined using the so-called "rectangle rule", described below:

$$\begin{array}{lccccc} & & \vdots & & \vdots & \\ \text{row } k & \cdots & a_{kk}^{(k)} & \cdots\cdots\cdots & a_{kj}^{(k)} & \dots \\ & & \vdots & & \vdots & \\ \text{row } i & \cdots & a_{ik}^{(k)} & \cdots\cdots\cdots & a_{ij}^{(k)} & \dots \\ & & \vdots & & \vdots & \\ & & \text{column } k & & \text{column } j & \end{array} \Rightarrow a_{ij}^{(k+1)} = \frac{a_{kk}^{(k)} a_{ij}^{(k)} - a_{ik}^{(k)} a_{kj}^{(k)}}{a_{kk}^{(k)}}.$$

Therefore, for $1 \le k \le n-1$, we will use the following formulae:

$$(11)\qquad a_{ij}^{(k+1)} = \begin{cases} a_{ij}^{(k)} & 1 \le i \le k,\ i \le j \le n+1 \\ 0 & 1 \le j \le k,\ j+1 \le i \le n \\ a_{ij}^{(k)} - \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \cdot a_{kj}^{(k)} & k+1 \le i \le n,\ k+1 \le j \le n+1. \end{cases}$$

After arriving at the upper-triangular matrix described by (9), we realize that we have actually arrived at an upper-triangular system equivalent to (8):

$$(12) \qquad \begin{cases} a_{11}^{(n)}x_1 + a_{12}^{(n)}x_2 + ... + a_{1n}^{(n)}x_n = a_{1,n+1}^{(n)} \\ \qquad a_{22}^{(n)}x_1 + ... + a_{2n}^{(n)}x_n = a_{2,n+1}^{(n)} \\ \qquad \ldots\ldots\ldots \\ \qquad a_{ii}^{(n)}x_1 + ... + a_{in}^{(n)}x_n = a_{i,n+1}^{(n)} \\ \qquad \ldots\ldots\ldots \\ \qquad\qquad a_{nn}^{(n)}x_n = a_{n,n+1}^{(n)}. \end{cases}$$

This system is solvable by using the back substitution method, that is, by applying the following formulae:

$$(13) \qquad x_n = a_{n,n+1}^{(n)}/a_{nn}^{(n)}, \quad \text{if } a_{nn}^{(n)} \neq 0,$$

and, for $i = n-1, n-2, ..., 1,$

$$(14) \qquad x_i = \left(a_{i,n+1}^{(n)} - \sum_{j=i+1}^{n} a_{ij}^{(n)} \cdot x_j \right) / a_{ii}^{(n)}.$$

The Gauss method with partial or total pivoting at every step makes a numerical improvement of the above described method by choosing a better pivot at every step. The modality of choosing the pivot makes the difference between partial pivoting and total pivoting. For the Gauss method with partial pivoting at every step, instead of (10) we will proceed as follows:

★At every step "k" we search, on column k, the element $a_{i_k,k}^{(k)}$, $k \leq i_k \leq n$, with the property

$$\left|a_{i_k k}^{(k)}\right| = \max_{k \leq i \leq n} \left|a_{ik}^{(k)}\right|.$$

Then:
1) if $a_{i_k,k}^{(k)} = 0$, system (8) does not have a unique solution.
2) if $a_{i_k,k}^{(k)} \neq 0$, the role of the pivot will be played by $a_{i_k,k}^{(k)}$. If, in addition, $i_k \neq k$, then we have to place $a_{i_k,k}^{(k)}$ on the position of $a_{k,k}^{(k)}$, and, to this end, we interchange row k with row i_k in the matrix $A^{(k)}$.

A mathematical example: Solve the following system by using the Gauss method with partial pivoting at every step

$$\begin{cases} 2x_1 + 2x_2 + 3x_3 + x_4 = 6 \\ 3x_1 + 3x_2 + 2x_3 + x_4 = 2 \\ x_1 + x_4 = 0 \\ x_1 + x_2 + x_3 = 2 \end{cases}$$

Solution: The extended matrix corresponding to the system is

$$A^{(1)} = (A|b) = \left(\begin{array}{cccc|c} 2 & 2 & 3 & 1 & 6 \\ 3 & 3 & 2 & 1 & 2 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 2 \end{array} \right).$$

We search the pivot to be put in the position of a_{11} on the first column. More precisely, we search the element with the largest absolute value from the first column of the matrix $A^{(1)}$, i.e

$$\max_{1\le i\le 4}\left|a_{i1}^{(1)}\right| = \max\left\{\left|a_{11}^{(1)}\right|, \left|a_{21}^{(1)}\right|, \left|a_{31}^{(1)}\right|, \left|a_{41}^{(1)}\right|\right\} = \left|a_{21}^{(1)}\right| = 3.$$

We interchange row 1 with row 2 in $A^{(1)}$ and we obtain

$$A^{(1)} \overset{L_1\leftrightarrow L_2}{=} \left(\begin{array}{cccc|c} \boxed{3} & 3 & 2 & 1 & 2 \\ 2 & 2 & 3 & 1 & 6 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 2 \end{array}\right).$$

We now proceed with the Gaussian elimination method as usual. We choose $a_{11}^{(1)} = 3 \neq 0$ to be the pivot and we keep row 1 from $A^{(1)}$ as it was. In the first column, under the pivot the elements will be zero and the other elements are calculated using the "rectangle rule":

$$a_{22}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{22}^{(1)} - a_{21}^{(1)}\cdot a_{12}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 2 - 2\cdot 3}{3} = 0, \qquad a_{23}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{23}^{(1)} - a_{21}^{(1)}\cdot a_{13}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 3 - 2\cdot 2}{3} = \frac{5}{3},$$

$$a_{24}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{24}^{(1)} - a_{21}^{(1)}\cdot a_{14}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 1 - 2\cdot 1}{3} = \frac{1}{3}, \qquad a_{25}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{25}^{(1)} - a_{21}^{(1)}\cdot a_{15}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 6 - 2\cdot 2}{3} = \frac{14}{3},$$

$$a_{32}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{32}^{(1)} - a_{31}^{(1)}\cdot a_{12}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 0 - 1\cdot 3}{3} = -1, \qquad a_{33}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{33}^{(1)} - a_{31}^{(1)}\cdot a_{13}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 0 - 1\cdot 2}{3} = -\frac{2}{3},$$

$$a_{34}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{34}^{(1)} - a_{31}^{(1)}\cdot a_{14}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 1 - 1\cdot 1}{3} = \frac{2}{3}, \qquad a_{35}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{35}^{(1)} - a_{31}^{(1)}\cdot a_{15}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 0 - 1\cdot 2}{3} = -\frac{2}{3},$$

$$a_{42}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{42}^{(1)} - a_{41}^{(1)}\cdot a_{12}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 1 - 1\cdot 3}{3} = 0, \qquad a_{43}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{43}^{(1)} - a_{41}^{(1)}\cdot a_{13}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 1 - 1\cdot 2}{3} = \frac{1}{3},$$

$$a_{44}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{44}^{(1)} - a_{41}^{(1)}\cdot a_{14}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 0 - 1\cdot 1}{1} = \frac{1}{3}, \qquad a_{45}^{(2)} = \frac{a_{11}^{(1)}\cdot a_{45}^{(1)} - a_{41}^{(1)}\cdot a_{15}^{(1)}}{a_{11}^{(1)}} = \frac{3\cdot 2 - 1\cdot 2}{3} = \frac{4}{3}.$$

Therefore, we obtain the matrix

$$A^{(2)} = \left(\begin{array}{cccc|c} 3 & 3 & 2 & 1 & 2 \\ 0 & 0 & \frac{5}{3} & \frac{1}{3} & \frac{14}{3} \\ 0 & -1 & -\frac{2}{3} & \frac{2}{3} & -\frac{2}{3} \\ 0 & 0 & \frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{array}\right).$$

We search

$$\max_{2\le i\le 4}\left|a_{i2}^{(2)}\right| = \max\left\{\left|a_{22}^{(2)}\right|, \left|a_{32}^{(2)}\right|, \left|a_{42}^{(2)}\right|\right\} = \left|a_{32}^{(2)}\right| = |-1|.$$

We interchange row 2 with row 3 in in $A^{(2)}$ and we get

$$A^{(2)} \overset{L_2\leftrightarrow L_3}{=} \left(\begin{array}{cccc|c} 3 & 3 & 2 & 1 & 2 \\ 0 & -1 & -\frac{2}{3} & \frac{2}{3} & -\frac{2}{3} \\ 0 & 0 & \frac{5}{3} & \frac{1}{3} & \frac{14}{3} \\ 0 & 0 & \frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{array}\right).$$

We remark that on column 2 under the pivot $a_{22}^{(2)} = -1$ all the elements are null and we get

$$A^{(3)} = A^{(2)}.$$

We search

$$\max_{3\leq i\leq 4}\left|a_{i3}^{(3)}\right| = \max\left\{\left|a_{33}^{(3)}\right|, \left|a_{43}^{(3)}\right|\right\} = \left|a_{33}^{(3)}\right| = \left|\frac{5}{3}\right|.$$

We choose $a_{33}^{(3)} = \frac{5}{3}$ to be the pivot and we keep rows 1, 2 and 3 from $A^{(3)}$ as they were. In column 3, under the pivot the elements will be zero and the other elements are calculated using the "rectangle rule":

$$a_{44}^{(4)} = \frac{a_{33}^{(3)}\cdot a_{44}^{(3)} - a_{43}^{(3)}\cdot a_{34}^{(3)}}{a_{33}^{(3)}} = \frac{\frac{5}{3}\cdot\left(-\frac{1}{3}\right) - \frac{1}{3}\cdot\frac{1}{3}}{\frac{5}{3}} = -\frac{2}{5},$$

$$a_{45}^{(4)} = \frac{a_{33}^{(3)}\cdot a_{45}^{(3)} - a_{43}^{(3)}\cdot a_{35}^{(3)}}{a_{33}^{(3)}} = \frac{\frac{5}{3}\cdot\frac{4}{3} - \frac{1}{3}\cdot\frac{14}{3}}{\frac{5}{3}} = \frac{2}{5}.$$

We obtain

$$A^{(4)} = \left(\begin{array}{cccc|c} 3 & 3 & 2 & 1 & 2\\ 0 & -1 & -\frac{2}{3} & \frac{2}{3} & -\frac{2}{3}\\ 0 & 0 & \frac{5}{3} & \frac{1}{3} & \frac{14}{3}\\ 0 & 0 & 0 & -\frac{2}{5} & \frac{2}{5}\end{array}\right).$$

The corresponding system of $A^{(4)}$ is

$$\begin{cases} 3x_1 + 3x_2 + 2x_3 + x_4 = 1\\ -x_2 - \frac{2}{3}x_3 + \frac{2}{3}x_4 = -\frac{2}{3}\\ \frac{5}{3}x_3 + \frac{1}{3}x_4 = \frac{14}{3}\\ -\frac{2}{5}x_4 = \frac{2}{5}.\end{cases}$$

The solution is

$$\begin{cases} x_4 = \frac{2}{5}/\left(-\frac{2}{5}\right) = -1\\ x_3 = \left(\frac{14}{3} - \frac{1}{3}x_4\right)/\frac{5}{3} = \left(\frac{14}{3} - \frac{1}{3}\cdot(-1)\right)/\frac{5}{3} = 3\\ x_2 = (-\frac{2}{3} - \frac{2}{3}x_4 + \frac{2}{3}x_3)/(-1) = (-\frac{2}{3} - \frac{2}{3}\cdot(-1) + \frac{2}{3}\cdot 3)/(-1) = -2\\ x_1 = (2 - x_4 - 2x_3 - 3x_2)/3 = (2 - (-1) - 2\cdot 3 - 3\cdot(-2))/3 = 1,\end{cases}$$

and, therefore

$$\begin{pmatrix} x_1\\ x_2\\ x_3\\ x_4\end{pmatrix} = \begin{pmatrix} 1\\ -2\\ 3\\ -1\end{pmatrix}.$$

Let us now provide the pseudocode algorithm for this method.

Pseudocode Algorithm for the Gauss method with partial pivoting

1. read n, a_{ij}, $1 \leq i \leq n$, $1 \leq j \leq n+1$
2. for $k = 1, 2, ..., n-1$
    2.1. $piv \leftarrow |a_{kk}|$
    2.2. $lin \leftarrow k$
    2.3. for $i = k+1, k+2, ..., n$
        2.3.1. if $piv < |a_{ik}|$ then
            2.3.1.1. $piv \leftarrow |a_{ik}|$
            2.3.1.2. $lin \leftarrow i$

2.4. if $piv = 0$ then
  2.4.1. write *'The system does not have unique a solution'*
  2.4.2. *exit*
2.5. if $lin \neq k$ then
  2.5.1. for $j = k, k+1, ..., n+1$
    2.5.1.1. swap a_{kj} with $a_{lin,j}$
2.6. for $i = k+1, k+2, ..., n$
  2.6.1. for $j = k+1, k+2, ..., n+1$
    2.6.1.1. $a_{ij} \leftarrow a_{ij} - a_{ik} \cdot a_{kj}/a_{kk}$
3. dacă $a_{nn} = 0$ then
  3.1. write *'The system does not have a unique solution'*
  3.2. *exit*
4. $a_{n,n+1} \leftarrow a_{n,n+1}/a_{nn}$
5. for $i = n-1, n-2, ..., 1$
  5.1. $S \leftarrow 0$
  5.2. for $j = i+1, i+2, ..., n$
    5.2.1. $S \leftarrow S + a_{ij} \cdot a_{j,n+1}$
  5.3. $a_{i,n+1} \leftarrow (a_{i,n+1} - S)/a_{ii}$
6. write $'x_i ='$, $a_{i,n+1}$, $1 \leq i \leq n$.

Exercises:

1. Complete the above algorithm such that, at each stage, the following things to be displayed:
   - the value of the pivot;
   - the position where we find the element that will play the role of the pivot (the row and the column);
   - the indices of the lines that have been permuted;
   - the total number of permutations of lines effectuated.
2. On the above mathematical example we noticed that every time we have 0 under the pivot, the corresponding line does not change. Can you improve the algorithm based on this remark? (the idea is to reduce the cost of the algorithm).
3. When solving the following linear systems using the Gauss method with partial pivoting at every step one notices that it does not have a unique solution:

$$\begin{cases} 12x_1 + 6x_2 + 4x_3 + x_4 = -22 \\ 24x_1 + 10x_2 + 4x_3 + x_4 = -54 \\ -2x_1 + x_4 = 6 \\ 8x_1 + 4x_2 + 2x_3 + x_4 = -16 \end{cases}$$

   But what happens when you solve the system using the above algorithm on a computer? Find an explanation and improve the algorithm.

Let us pass now to the Gauss method with total pivoting at every step. Then, instead of (10) we will proceed as follows:

★At every step "k" we search the element $a^{(k)}_{i_k,j_k}$, $k \le i_k \le n$, $k \le j_k \le n$, with the property

$$\left|a^{(k)}_{i_k j_k}\right| = \max_{\substack{k\le i\le n\\ k\le j\le n}} \left|a^{(k)}_{ij}\right|.$$

Then:
1) if $a^{(k)}_{i_k,j_k} = 0$, $\forall k \le i_k, j_k \le n$, the system (2) does not have unique solution.
2) if $a^{(k)}_{i_k,j_k} \ne 0$, the role of the pivot will be played by $a^{(k)}_{i_k,j_k}$. If, in addition, $i_k \ne k$ or $j_k \ne k$, we have to place $a^{(k)}_{i_k,j_k}$ on the position of $a^{(k)}_{k,k}$, and, to this end, we interchange row k with row i_k (if $i_k \ne k$) and/or we interchange the column k with column j_k (if $j_k \ne k$) in the matrix $A^{(k)}$.

A mathematical example. a) Solve the following system by using the Gauss method with total pivoting at every step

$$\begin{cases} -2x_1 + x_3 = 1 \\ x_1 + 4x_2 + x_4 = -3 \\ 2x_1 - 3x_4 = -3 \\ -2x_1 + x_3 + x_4 = 2. \end{cases}$$

b) Find the value of the determinant of the matrix A, corresponding to the above system.
Sol: a) The extended matrix corresponding to the system is

$$\overline{A} = \left(\begin{array}{cccc|c} -2 & 0 & 1 & 0 & 1 \\ 1 & 4 & 0 & 1 & -3 \\ 2 & 0 & 0 & -3 & -3 \\ -2 & 0 & 1 & 1 & 2 \end{array}\right).$$

We search the element with the property

$$\left|piv^{(1)}\right| = \max_{1\le i,j\le 4} \left|a^{(1)}_{ij}\right| = \left|a^{(1)}_{22}\right| = 4.$$

The pivot $piv^{(1)}$ should be $a^{(1)}_{22} = 4$.

First we interchange row 1 with row 2 (and we have seen that this does not have any impact on the solution of the system), and secondly, we interchange column 1 with column 2 in $A^{(1)}$, but this means that we also interchange x_1 with x_2, so this should be remembered at the end! We obtain the matrix

$$A^{(1)} \overset{L_1 \leftrightarrow L_2}{=} \left(\begin{array}{cccc|c} 1 & 4 & 0 & 1 & -3 \\ -2 & 0 & 1 & 0 & 1 \\ 2 & 0 & 0 & -3 & -3 \\ -2 & 0 & 1 & 1 & 2 \end{array}\right) \underset{\sim}{\boxed{C_1 \leftrightarrow C_2}} \left(\begin{array}{cccc|c} \boxed{4} & 1 & 0 & 1 & -3 \\ 0 & -2 & 1 & 0 & 1 \\ 0 & 2 & 0 & -3 & -3 \\ 0 & -2 & 1 & 1 & 2 \end{array}\right).$$

We choose $a^{(1)}_{11} = 4 \ne 0$ as a pivot and we remark that

$$A^{(2)} = A^{(1)}.$$

We search the element with the property

$$\left|piv^{(2)}\right| = \max_{2\leq i,j\leq 4}\left|a_{ij}^{(2)}\right| = \left|a_{34}^{(2)}\right| = |-3|.$$

We interchange row 2 with row 3, and then we interchange column 2 with column 4 in $A^{(2)}$, meaning that we also interchange x_2 with x_4. We obtain

$$A^{(2)} \overset{L_2\leftrightarrow L_3}{\sim} \left(\begin{array}{cccc|c} 4 & 1 & 0 & 1 & -3 \\ 0 & 2 & 0 & -3 & -3 \\ 0 & -2 & 1 & 0 & 1 \\ 0 & -2 & 1 & 1 & 2 \end{array}\right) \underset{\sim}{\boxed{C_2\leftrightarrow C_4}} \left(\begin{array}{cccc|c} 4 & 1 & 0 & 1 & -3 \\ 0 & \boxed{-3} & 0 & 2 & -3 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 1 & 1 & -2 & 2 \end{array}\right).$$

We choose $a_{22}^{(2)} = -3 \neq 0$ as a pivot and we keep rows 1 and 2 from $A^{(2)}$ as they were. In the second column, under the pivot the elements will be zero and the other elements are calculated using the "rectangle rule", and we obtain

$$A^{(3)} = \left(\begin{array}{cccc|c} 4 & 1 & 0 & 1 & -3 \\ 0 & -3 & 0 & 2 & -3 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -\frac{4}{3} & 1 \end{array}\right).$$

We search the element with the property

$$\left|piv^{(3)}\right| = \max_{3\leq i,j\leq 4}\left|a_{ij}^{(3)}\right| = \left|a_{34}^{(3)}\right| = |-2|.$$

We interchange column 3 with column 4 in $A^{(3)}$, meaning that we also interchange x_3 with x_4. We obtain

$$A^{(3)} \underset{\sim}{\boxed{C_2\leftrightarrow C_4}} \left(\begin{array}{cccc|c} 4 & 1 & 1 & 0 & -3 \\ 0 & -3 & 2 & 0 & -3 \\ 0 & 0 & \boxed{-2} & 1 & 1 \\ 0 & 0 & -\frac{4}{3} & 1 & 1 \end{array}\right).$$

We choose $a_{33}^{(3)} = -2 \neq 0$ pivot and we get

$$A^{(4)} = \left(\begin{array}{cccc|c} 4 & 1 & 1 & 0 & -3 \\ 0 & -3 & 2 & 0 & -3 \\ 0 & 0 & -2 & 1 & 1 \\ 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} \end{array}\right).$$

We deduce, by back substitution method, the intermediate solution

$$\begin{cases} x_4 = 1 \\ x_3 = 0 \\ x_2 = 1 \\ x_1 = -1, \end{cases}$$

and we interchange in the following order

$$\begin{cases} \text{component } 3 \leftrightarrow \text{component } 4 \text{ (since } C_3 \leftrightarrow C_4) \\ \text{component } 2 \leftrightarrow \text{component } 4 \text{ (since } C_2 \leftrightarrow C_4) \\ \text{component } 1 \leftrightarrow \text{component } 2 \text{ (since } C_1 \leftrightarrow C_2). \end{cases}$$

More precisely, we have

$$\begin{cases} x_1 = -1 \\ x_2 = 1 \\ x_3 = 0 \\ x_4 = 1 \end{cases} \overset{x_3 \leftrightarrow x_4}{\Rightarrow} \begin{cases} x_1 = -1 \\ x_2 = 1 \\ x_3 = 1 \\ x_4 = 0 \end{cases} \overset{x_2 \leftrightarrow x_4}{\Rightarrow} \begin{cases} x_1 = -1 \\ x_2 = 0 \\ x_3 = 1 \\ x_4 = 1 \end{cases} \overset{x_1 \leftrightarrow x_2}{\Rightarrow} \begin{cases} x_1 = 0 \\ x_2 = -1 \\ x_3 = 1 \\ x_4 = 1. \end{cases}$$

So the solution of the system is

$$\begin{cases} x_1 = 0 \\ x_2 = -1 \\ x_3 = 1 \\ x_4 = 1. \end{cases}$$

b) $det(A) = (-1)^{2+3} a_{11}^{(4)} \cdot a_{22}^{(4)} \cdot a_{33}^{(4)} \cdot a_{44}^{(4)} = -4 \cdot (-3) \cdot (-2) \cdot \frac{1}{3} = -8$

Let us provide the pseudocode algorithm for this method as well.

Pseudocode Algorithm for the Gauss method with total pivoting

1. read n, a_{ij}, $1 \le i \le n$, $1 \le j \le n+1$, ε
2. $npc \leftarrow 0$
3. for $k = 1, 2, ..., n-1$
    3.1. $piv \leftarrow |a_{kk}|$
    3.2. $lin \leftarrow k$
    3.3. $col \leftarrow k$
    3.4. for $j = k, k+1, ..., n$
        3.4.1. for $i = k, k+1, ..., n$
            3.4.1.1. if $piv < |a_{ij}|$ then
                3.4.1.1.1. $piv \leftarrow |a_{ij}|$
                3.4.1.1.2. $lin \leftarrow i$
                3.4.1.1.3. $col \leftarrow j$
    3.5. if $piv \le \varepsilon$ then
        3.5.1. write *'The system does not have a unique solution'*
        3.5.2. *exit*
    3.6. if $lin \ne k$ then
        3.6.1. for $j = k, k+1, ..., n+1$
            3.6.1.1. swap a_{kj} with $a_{lin,j}$
    3.7. if $col \ne k$ then
        3.7.1. $npc \leftarrow npc + 1$
        3.7.2. $c(npc, 1) \leftarrow k$
        3.7.3. $c(npc, 2) \leftarrow col$
        3.7.4. for $i = 1, 2, ..., n$
            3.7.4.1. swap a_{ik} with $a_{i,col}$
    3.8. for $i = k+1, k+2, ..., n$
        3.8.1. if $a_{ik} \ne 0$
            3.8.1.2. for $j = k+1, k+2, ..., n+1$
                3.8.1.2.1. if $a_{kj} \ne 0$
                    3.8.1.2.1.1. $a_{ij} \leftarrow a_{ij} - a_{ik} \cdot a_{kj} / a_{kk}$
4. if $|a_{nn}| \le \varepsilon$ then

4.1. write *'The system does not have a unique solution'*
4.2. *exit*
5. $a_{n,n+1} \leftarrow a_{n,n+1}/a_{nn}$
6. for $i = n-1, n-2, ..., 1$
 6.1. $S \leftarrow 0$
 6.2. for $j = i+1, i+2, ..., n$
  6.2.1. $S \leftarrow S + a_{ij} \cdot a_{j,n+1}$
 6.3. $a_{i,n+1} \leftarrow (a_{i,n+1} - S)/a_{ii}$
7. if $npc \neq 0$ then
 7.1. for $i = npc, npc-1, ..., 1$
  7.1.1. swap $a_{c(i,1),n+1}$ with $a_{c(i,2),n+1}$
8. write $'x_i ='$, $a_{i,n+1}$, $1 \leq i \leq n$.

Exercises:

1. Complete the above algorithm such that it will calculate in addition the value of the determinant of the matrix associated to the system.

4 The LR Doolitle factorization method for solving linear systems

The problem: We consider the linear system

$$A \cdot x = b, \tag{15}$$

where $A \in \mathcal{M}_n(\mathbb{R})$ is the matrix associated to system (15) and $b \in \mathbb{R}^n$ is the vector containing the free terms of system (15).
Our goal is to determine, if possible, $x \in \mathbb{R}^n$, where x represents the unique solution of system (15).

Describing the method:
The LR Doolitle factorization method consists in the decomposition of the matrix A in the following form

$$A = L \cdot R, \text{where}$$

$$L = \begin{pmatrix} 1 & 0 & ... & 0 \\ l_{21} & 1 & ... & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & ... & 1 \end{pmatrix} = \text{lower-triangular matrix}; \quad R = \begin{pmatrix} r_{11} & r_{12} & ... & r_{1n} \\ 0 & r_{22} & ... & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & ... & r_{nn} \end{pmatrix} = \text{upper-triangular matrix}.$$

The elements of matrices L and R are determined by the following formulae

$$(16) \qquad \begin{cases} r_{1j} = a_{1j}, & 1 \leq j \leq n \\ l_{i1} = a_{i1}/r_{11}, & 2 \leq i \leq n \\ r_{kj} = a_{kj} - \sum_{h=1}^{k-1} l_{kh} \cdot r_{hj}, & 2 \leq k \leq n, \quad k \leq j \leq n. \\ l_{ik} = \left(a_{ik} - \sum_{h=1}^{k-1} l_{ih} \cdot r_{hk} \right) / r_{kk}, & 2 \leq k \leq n, \quad k+1 \leq i \leq n. \end{cases}$$

Remarks:

1) Any non-singular (invertible) matrix A admits an LR factorization (if necessary, we permute some rows).

2) In calculus, the order of determining the elements of matrices L and R using formulae (16) is the following: first row from R, first column from L, second row from R, second column from L, etc. After determing L and R we replace A by $L \cdot R$ in system (15):

$$A \cdot x = b \Longleftrightarrow L \cdot \underbrace{R \cdot x}_{=y} = b.$$

By denoting $Rx = y$, we get to solve the following systems:

$$\begin{cases} L \cdot y = b \\ R \cdot x = y. \end{cases}$$

The advantage of solving two systems instead of one comes from the fact that both L and R are triangular matrices.

We solve $L \cdot y = b$ by direct substitution:

$$(17) \qquad \begin{cases} y_1 = b_1, \\ y_i = b_i - \sum_{k=1}^{i-1} l_{ik} \cdot y_k, \quad i = 2, 3, ..., n. \end{cases}$$

We solve $R \cdot x = y$ by back substitution:

$$(18) \qquad \begin{cases} x_n = y_n / r_{nn}, \\ x_i = \left(y_i - \sum_{k=i+1}^{n} r_{ik} \cdot x_k \right) / r_{ii}, \quad i = n-1, n-2, ..., 1. \end{cases}$$

A mathematical example: Solve the following system using the LR Doolitlle factorization method:

$$\begin{cases} -x_1 + 2x_2 + 3x_3 = -8 \\ x_1 - 2x_2 - x_3 = 4 \\ -2x_1 + 6x_2 + 6x_3 = -14. \end{cases}$$

Proof. The extended matrix is

$$\overline{A} = \left(\begin{array}{ccc|c} -1 & 2 & 3 & -8 \\ 1 & -2 & -1 & 4 \\ -2 & 6 & 6 & -14 \end{array} \right).$$

We check if the principal minors of matrix A are nonzero.
$\Delta_1 = -1 \neq 0$,
$\Delta_2 = \begin{vmatrix} -1 & 2 \\ 1 & -2 \end{vmatrix} = 0.$
Since the determinant $\Delta_2 = 0$, we interchange the row 2 with row 3 in the extended matrix $\overline{A}$, and we obtain

$$\overline{A} \overset{L_2 \leftrightarrow L_3}{=} \left(\begin{array}{ccc|c} -1 & 2 & 3 & -8 \\ -2 & 6 & 6 & -14 \\ 1 & -2 & -1 & 4 \end{array} \right).$$

We have
$\Delta_1 = -1 \neq 0$,
$\Delta_2 = \begin{vmatrix} -1 & 2 \\ -2 & 6 \end{vmatrix} = -2 \neq 0$,
$\Delta_3 = \det(A) = \begin{vmatrix} -1 & 2 & 3 \\ -2 & 6 & 6 \\ 1 & -2 & -1 \end{vmatrix} = -4 \neq 0.$

Since $\Delta_1, \Delta_2, \Delta_3 \neq 0$, the matrix $A = \begin{pmatrix} -1 & 2 & 3 \\ -2 & 6 & 6 \\ 1 & -2 & -1 \end{pmatrix}$ admits a LR factorization. More precisely, we search two matrixes

$$L = \begin{pmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} \quad \text{and} \quad R = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{pmatrix},$$

such that $L \cdot R = A$.

We determine the elements of first line of the matrix R:
$r_{11} = a_{11} = -1.$
$r_{12} = a_{12} = 2.$
$r_{13} = a_{13} = 3.$

We determine the elements of the first column of the matrix L:
$l_{21} = \frac{a_{21}}{r_{11}} = \frac{-2}{-1} = 2.$
$l_{31} = \frac{a_{31}}{r_{11}} = \frac{1}{-1} = -1.$

We determine the elements of the second line of the matrix R:
$r_{22} = a_{22} - l_{21}r_{12} = 6 - 2 \cdot 2 = 2.$
$r_{23} = a_{23} - l_{21}r_{13} = 6 - 2 \cdot 3 = 0.$

We determine the elements of the second column of the matrix L:
$l_{32} = (a_{32} - l_{31}r_{12})/r_{22} = (-2 - (-1) \cdot 2)/2 = 0.$

We determine the elements of the third line of the matrix R:
$r_{33} = a_{33} - l_{31}r_{13} - l_{32}r_{23} = -1 - (-1) \cdot 3 - 0 \cdot 0 = 2.$

So, we get

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad R = \begin{pmatrix} -1 & 2 & 3 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Then our system $Ax = b$ is equivalent to

$$L \cdot (R \cdot x) = b.$$

If we denote $R \cdot x = y$, we need solve the following two triangular systems:
$(S1) : \ L \cdot y = b,$
$(S2) : \ R \cdot x = y.$

The lower-triangular system $(S1)$ is equivalent to

$$\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} -8 \\ -14 \\ 4 \end{pmatrix}$$

We remark that the free terms column b is chosen from the matrix $\overline{A}$ in which we already interchanged the lines. The solution y is obtain by direct substitution

$$\begin{cases} y_1 = -8 \\ y_2 = -14 - 2y_1 = 2 \\ y_3 = 4 + y_1 - 0y_2 = -4. \end{cases}$$

The upper-triangular system $(S2)$ is equivalent to

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

The solution x is obtain by back substitution

$$\begin{cases} x_3 = -4/2 = -2 \\ x_2 = (2 - 0x_3)/2 = 1 \\ x_1 = (-8 - 3x_3 - 2x_2)/(-1) = 4. \end{cases}$$

So, the solution of system is
$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \\ -2 \end{pmatrix}$$
□

Pseudocode Algorithm

1. read n, a_{ij}, $1 \leq i \leq n$, $1 \leq j \leq n+1$

2. if $a_{11} = 0$ then
   2.1. $i \leftarrow 1$
   2.2. repeat
      2.2.1. $i \leftarrow i + 1$
      until $a_{i1} \neq 0$ or $i > n$
   2.3. if $i > n$ then
      2.3.1. write *'The system does not have a unique solution'*
      2.3.2. exit
   2.4. for $j = 1, 2, ..., n + 1$
      2.4.1. swap a_{1j} with a_{ij}
3. for $i = 2, 3, ..., n$
   3.1. $a_{i1} \leftarrow a_{i1}/a_{11}$
4. for $k = 2, 3, ..., n$
   4.1. $i \leftarrow k$
   4.2. repeat
      4.2.1. $S \leftarrow 0$; $piv \leftarrow 0$;
      4.2.2. for $h = 1, 2, ..., k - 1$
         4.2.2.1. $S \leftarrow S + a_{ih} \cdot a_{hk}$
      4.2.3. $piv \leftarrow a_{ik} - S$
      4.2.4. $i \leftarrow i + 1$
      until $piv \neq 0$ or $i > n$
   4.3. if $piv = 0$ then
      4.3.1. write *'The system does not have a unique solution'*
      4.3.2. *exit*
   4.4. if $i \neq k + 1$ then
      4.4.1. for $j = 1, 2, ...n + 1$
         4.4.1.1. swap a_{kj} with $a_{i-1,j}$
   4.5. for $j = k, k + 1, ..., n$
      4.5.1. $S \leftarrow 0$
      4.5.2. for $h = 1, 2, ..., k - 1$
         4.5.2.1. $S \leftarrow S + a_{kh} \cdot a_{hj}$
      4.5.3. $a_{kj} \leftarrow a_{kj} - S$
   4.6. for $i = k + 1, k + 2, ..., n$
      4.6.1. $S \leftarrow 0$
      4.6.2. for $h = 1, 2, ..., k - 1$
         4.6.2.1. $S \leftarrow S + a_{ih} \cdot a_{hk}$
      4.6.3. $a_{ik} \leftarrow (a_{ik} - S)/a_{kk}$
5. for $i = 2, 3, ..., n$
   5.1. $S \leftarrow 0$
   5.2. for $k = 1, 2, ..., i - 1$
      5.2.1. $S \leftarrow S + a_{ik} \cdot a_{k,n+1}$
   5.3. $a_{i,n+1} \leftarrow a_{i,n+1} - S$
6. $a_{n,n+1} \leftarrow a_{n,n+1}/a_{nn}$
7. for $i = n - 1, n - 2, ..., 1$
   7.1. $S \leftarrow 0$
   7.2. for $j = i + 1, i + 2, ..., n$
      7.2.1. $S \leftarrow S + a_{ij} \cdot a_{j,n+1}$

7.3. $a_{i,n+1} \leftarrow (a_{i,n+1} - S)/a_{ii}$

8. write $'x_i =', a_{i,n+1}, 1 \le i \le n$.

Exercises:

1. Display the matrices L and R.
2. Calculate the determinant of matrix A using the LR factorization method and complete this into the algorithm.

5 LR factorization for tridiagonal matrix with application to solving linear systems

The problem: We consider the linear system

$$A \cdot x = t, \tag{19}$$

where $A = \begin{pmatrix} a_1 & b_1 & 0 & 0 & ... & 0 & 0 \\ c_1 & a_2 & b_2 & 0 & ... & 0 & 0 \\ 0 & c_2 & a_3 & b_3 & ... & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & ... & a_{n-1} & b_{n-1} \\ 0 & 0 & 0 & 0 & ... & c_{n-1} & a_n \end{pmatrix}$ is a tridiagonal matrix and $t \in \mathbb{R}^n$ is the free term of system (19).

Our goal is to determine, if possible, $x \in \mathbb{R}^n$, where x represents the unique solution of system (19).

Describing the method: We search

$L = \begin{pmatrix} 1 & 0 & 0 & ... & 0 & 0 \\ l_1 & 1 & 0 & ... & 0 & 0 \\ 0 & l_2 & 1 & ... & 0 & 0 \\ \vdots & \vdots & \vdots & ... & \vdots & \vdots \\ 0 & 0 & 0 & ... & l_{n-1} & 1 \end{pmatrix}$ -lower-triangular matrix; $R = \begin{pmatrix} r_1 & s_1 & 0 & 0 & ... & 0 \\ 0 & r_2 & s_2 & 0 & ... & 0 \\ 0 & 0 & r_3 & s_3 & ... & 0 \\ \vdots & \vdots & \vdots & \vdots & ... & \vdots \\ 0 & 0 & 0 & 0 & ... & s_{n-1} \\ 0 & 0 & 0 & 0 & ... & r_n \end{pmatrix}$ -upper-triangular matrix;

with property $A = L \cdot R$. To determine the elements of matrices L and R we apply the following formulae

$$\begin{cases} r_1 = a_1, & \\ s_i = b_i, & 1 \le i \le n-1 \\ l_i = c_i / r_i, & 1 \le i \le n-1 \\ r_{i+1} = a_{i+1} - l_i \cdot s_i, & 1 \le i \le n-1. \end{cases} \tag{20}$$

The system (19) it is equivalent with

$$L \cdot \underbrace{R \cdot x}_{=y} = t.$$

To find the solution x, we solve successive the systems

$$\begin{cases} L \cdot y = t \\ R \cdot x = y. \end{cases}$$

We have the following formulae

(21) $$\begin{cases} y_1 = t_1, \\ y_i = t_i - l_{i-1} \cdot y_{i-1}, \quad i = 2, 3, ..., n. \end{cases}$$

respectively,

(22) $$\begin{cases} x_n = y_n / r_n, \\ x_i = (y_i - s_i \cdot x_{i+1}) / r_i, \quad i = n-1, n-2, ..., 1. \end{cases}$$

Example: Solve the following system:

$$a) \begin{cases} -2x_1 + 3x_2 = 1 \\ 5x_1 + 3x_2 - x_3 = 7 \\ -x_2 + x_3 = 0. \end{cases} .$$

Solution: The matrix associated to this system is

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

We notice that A is a tridiagonal matrix.

We check if the diagonal minors of matrix A are non-zero.
$\Delta_1 = -2 \neq 0$,
$\Delta_2 = \begin{vmatrix} -2 & 3 \\ 5 & 3 \end{vmatrix} = -21 \neq 0$,
$\Delta_3 = \det(A) = \begin{vmatrix} -2 & 3 & 0 \\ 5 & 3 & -1 \\ 0 & -1 & 1 \end{vmatrix} = -19 \neq 0.$

Since $\Delta_1, \Delta_2, \Delta_3 \neq 0$, the matrix A admits a LR factorization. More precisely, we search

$$L = \begin{pmatrix} 1 & 0 & 0 \\ l_1 & 1 & 0 \\ 0 & l_2 & 1 \end{pmatrix} \quad \text{şi} \quad R = \begin{pmatrix} r_1 & s_1 & 0 \\ 0 & r_2 & s_2 \\ 0 & 0 & r_3 \end{pmatrix},$$

such that $L \cdot R = A$.

We keep the three diagonals with non-zero elements from A into three vectors:

$$a = (a_1, a_2, a_3) = (-2, 3, 1), \quad b = (b_1, b_2) = (3, -1), \quad c = (c_1, c_2) = (5, -1),$$

where a is for the main diagonal, b is for the diagonal above a, and c is for the diagonal below a. We apply formulae (20) for $n = 3$ in order to determine the vectors

$$l = (l_1, l_2), \quad r = (r_1, r_2, r_3), \quad s = (s_1, s_2),$$

and to find this way matrices L and R. We have

$$r_1 = -2,$$

and by $s_i = b_i$, for $1 \leq i \leq 2$ we deduce

$$s = (3, -1).$$

Then,

$$l_1 = \frac{c_1}{r_1} = \frac{5}{-2} = -\frac{5}{2}, \quad r_2 = a_2 - l_1 s_1 = 3 - \left(-\frac{5}{2}\right) \cdot 3 = \frac{21}{2},$$

$$l_2 = \frac{c_2}{r_2} = -\frac{2}{21}, \quad r_3 = a_3 - l_2 s_2 = 1 - \left(-\frac{2}{21}\right) \cdot (-1) = \frac{19}{21}.$$

We have obtained

$$l = \left(-\frac{5}{2}, -\frac{2}{21}\right), \quad r = \left(-2, \frac{21}{2}, \frac{19}{21}\right),$$

so

$$L = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{5}{2} & 1 & 0 \\ 0 & -\frac{2}{21} & 1 \end{pmatrix}, \qquad R = \begin{pmatrix} -2 & 3 & 0 \\ 0 & \frac{21}{2} & -1 \\ 0 & 0 & \frac{19}{21} \end{pmatrix}.$$

Since $A = LR$, solving the system written in its matrix form, $Ax = t$, where $t = \begin{pmatrix} 1 \\ 7 \\ 0 \end{pmatrix}$, is equivalent to solving $L(Rx) = t$. We denote $Rx = y$ and we notice that we actually have to solve

$$\begin{cases} Ly = t, \\ Rx = y. \end{cases}$$

The matrix equation $Ly = t$, that is,

$$\begin{pmatrix} 1 & 0 & 0 \\ -\frac{5}{2} & 1 & 0 \\ 0 & -\frac{2}{21} & 1 \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 7 \\ 0 \end{pmatrix},$$

is equivalent to solving the system

$$\begin{cases} y_1 & = 1, \\ -\frac{5}{2}y_1 + y_2 & = 7 \\ -\frac{2}{21}y_2 + y_3 & = 0, \end{cases}$$

We introduce $y_1 = 1$ in the second equation of the system and we obtain $y_2 = \frac{19}{2}$. We introduce $y_2 = \frac{19}{2}$ in the third equation of the system and we obtain $y_3 = \frac{19}{21}$. We have found

$$y = \begin{pmatrix} 1 \\ \frac{19}{2} \\ \frac{19}{21} \end{pmatrix}.$$

We solve now $Rx = y$, that is,

$$\begin{pmatrix} -2 & 3 & 0 \\ 0 & \frac{21}{2} & -1 \\ 0 & 0 & \frac{19}{21} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{19}{2} \\ \frac{19}{21} \end{pmatrix}.$$

In fact, we solve

$$\begin{cases} -2x_1 + 3x_2 & = 1, \\ \frac{21}{2}x_2 - x_3 & = \frac{19}{2} \\ \qquad \frac{19}{21}x_3 & = \frac{19}{21}, \end{cases}$$

From the last equation of the system, $x_3 = 1$. We introduce this in the above equation and we obtain $x_2 = 1$. We introduce this in the above equation and we obtain $x_1 = 1$. Therefore the solution of the initial system is

$$x = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Pseudocode Algorithm

1. read n, a_i, $1 \le i \le n$, b_i, $1 \le i \le n-1$, c_i, $1 \le i \le n-1$, t_i, $1 \le i \le n$
2. for $i = 1, 2, ..., n-1$
   2.1. if $a_i = 0$ then
      2.1.1. write *'The system does not have a unique solution because the diagonal element from line ', i, 'is null.'*
      2.1.2. *exit*
   2.2. $c_i \leftarrow c_i / a_i$
   2.3. $a_{i+1} \leftarrow a_{i+1} - b_i \cdot c_i$
3. for $i = 2, 3, ..., n$
   3.1. $t_i \leftarrow t_i - c_{i-1} \cdot t_{i-1}$
4. if $a_n = 0$ then
   4.1. write *'The system does not have a unique solution because the diagonal element from line ', n, 'is null.'*
   4.2. *exit*
5. $t_n \leftarrow t_n / a_n$
6. for $i = n-1, n-2, ..., 1$
   6.1. $t_i \leftarrow (t_i - b_i \cdot t_{i+1}) / a_i$
7. write $'x_i =', t_i, 1 \le i \le n.$

6 Chio pivotal condensation method for solving determinants

The problem: We consider the matrix $A = (a_{ij})_{1 \le i,j \le n} \in \mathbb{R}^{n \times n}$ and the target is to compute $\det(A)$.

Describing the method: We apply the formula

$$\det(A) = \frac{1}{a_{11}^{n-2}} \begin{vmatrix} \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{13} \\ a_{21} & a_{23} \end{vmatrix} & \dots & \begin{vmatrix} a_{11} & a_{1n} \\ a_{21} & a_{2n} \end{vmatrix} \\ \begin{vmatrix} a_{11} & a_{12} \\ a_{31} & a_{32} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix} & \dots & \begin{vmatrix} a_{11} & a_{1n} \\ a_{31} & a_{3n} \end{vmatrix} \\ \vdots & \vdots & \dots & \vdots \\ \begin{vmatrix} a_{11} & a_{12} \\ a_{n1} & a_{n2} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{13} \\ a_{n1} & a_{n3} \end{vmatrix} & \dots & \begin{vmatrix} a_{11} & a_{1n} \\ a_{n1} & a_{nn} \end{vmatrix} \end{vmatrix}, \tag{23}$$

where $a_{11} \neq 0$, and we apply again the above formula for $n-1, n-2, ...$ until we obtain a determinant of order 2.

Remarks:

1. If $a_{11} = 0$ and there exists $2 \leq i \leq n$ for which $a_{i1} \neq 0$, then we switch the rows 1 and i in A, and we change the sign of $\det(A)$.

2. If $a_{11} = 0$, $\forall 2 \leq i \leq n$, we have $a_{i1} = 0$, then $\det(A) = 0$.

Example: Compute the determinant of the following matrices using Chio's Method:

$$A = \begin{pmatrix} 2 & 1 & 0 & 1 \\ 6 & 3 & 2 & -1 \\ 1 & 2 & 1 & 0 \\ 1 & 1 & -2 & 3 \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & -2 & 1 & 0 \\ 5 & 1 & -1 & 3 \\ 4 & 2 & 2 & 5 \\ 6 & 1 & -3 & -1 \end{pmatrix}.$$

Solution: a) We first make the calculus for $\det(A)$. We apply formula (23) for the determinant of the square matrix A of order n.

$$\det(A) = \begin{vmatrix} 2 & 1 & 0 & 1 \\ 6 & 3 & 2 & -1 \\ 1 & 2 & 1 & 0 \\ 1 & 1 & -2 & 3 \end{vmatrix} = \frac{1}{2^{4-2}} \begin{vmatrix} \begin{vmatrix} 2 & 1 \\ 6 & 3 \end{vmatrix} & \begin{vmatrix} 2 & 0 \\ 6 & 2 \end{vmatrix} & \begin{vmatrix} 2 & 1 \\ 6 & -1 \end{vmatrix} \\ \begin{vmatrix} 2 & 1 \\ 1 & 2 \end{vmatrix} & \begin{vmatrix} 2 & 0 \\ 1 & 1 \end{vmatrix} & \begin{vmatrix} 2 & 1 \\ 1 & 0 \end{vmatrix} \\ \begin{vmatrix} 2 & 1 \\ 1 & 1 \end{vmatrix} & \begin{vmatrix} 2 & 0 \\ 1 & -2 \end{vmatrix} & \begin{vmatrix} 2 & 1 \\ 1 & 3 \end{vmatrix} \end{vmatrix}$$

$$= \frac{1}{4} \begin{vmatrix} 0 & 4 & -8 \\ 3 & 2 & -1 \\ 1 & -4 & 5 \end{vmatrix}.$$

By applying formula (23) and by performing the calculus of several determinants of order 2, we have arrived at the calculus of a determinant of order 3 instead of the initial determinant of order 4. At this point we notice that the first element a_{11} of this determinant of order 3 is zero, so we interchange the first two rows of the determinant. Therefore,

$$\det(A) = \frac{-1}{4}\begin{vmatrix} 3 & 2 & -1 \\ 0 & 4 & -8 \\ 1 & -4 & 5 \end{vmatrix}.$$

Now we apply again formula (23):

$$\det(A) = \frac{-1}{4 \cdot 3^{3-2}}\begin{vmatrix} \begin{vmatrix} 3 & 2 \\ 0 & 4 \end{vmatrix} & \begin{vmatrix} 3 & -1 \\ 0 & -8 \end{vmatrix} \\ \\ \begin{vmatrix} 3 & 2 \\ 1 & -4 \end{vmatrix} & \begin{vmatrix} 3 & -1 \\ 1 & 5 \end{vmatrix} \end{vmatrix} = \frac{-1}{12}\begin{vmatrix} 12 & -24 \\ -14 & 16 \end{vmatrix} = 12.$$

b) We now pass to the calculus of $\det(B)$. We notice that the first element of the square matrix B is $b_{11} = 0$, thus we interchange the first two rows of the determinant without forgetting to change the sign of the determinant and then we use again formula (23) for $n = 4$:

$$\det(B) = -\begin{vmatrix} 5 & 1 & -1 & 3 \\ 0 & -2 & 1 & 0 \\ 4 & 2 & 2 & 5 \\ 6 & 1 & -3 & -1 \end{vmatrix} = \frac{-1}{5^{4-2}}\begin{vmatrix} \begin{vmatrix} 5 & 1 \\ 0 & -2 \end{vmatrix} & \begin{vmatrix} 5 & -1 \\ 0 & 1 \end{vmatrix} & \begin{vmatrix} 5 & 3 \\ 0 & 0 \end{vmatrix} \\ \\ \begin{vmatrix} 5 & 1 \\ 4 & 2 \end{vmatrix} & \begin{vmatrix} 5 & -1 \\ 4 & 2 \end{vmatrix} & \begin{vmatrix} 5 & 3 \\ 4 & 5 \end{vmatrix} \\ \\ \begin{vmatrix} 5 & 1 \\ 6 & 1 \end{vmatrix} & \begin{vmatrix} 5 & -1 \\ 6 & -3 \end{vmatrix} & \begin{vmatrix} 5 & 3 \\ 6 & -1 \end{vmatrix} \end{vmatrix}$$

$$= \frac{-1}{25}\begin{vmatrix} -10 & 5 & 0 \\ 6 & 14 & 13 \\ -1 & -9 & -23 \end{vmatrix}.$$

We have seen once more that, from a determinant of order 4 we have arrived at the calculus of a determinant of order 3. We apply again (23) for this last determinant and we get

$$\det(B) = \frac{-1}{25} \cdot \frac{1}{(-10)^{3-2}}\begin{vmatrix} \begin{vmatrix} -10 & 5 \\ 6 & 14 \end{vmatrix} & \begin{vmatrix} -10 & 0 \\ 6 & 13 \end{vmatrix} \\ \\ \begin{vmatrix} -10 & 5 \\ -1 & -9 \end{vmatrix} & \begin{vmatrix} -10 & 0 \\ -1 & -23 \end{vmatrix} \end{vmatrix} =$$

$$= \frac{1}{250}\begin{vmatrix} -170 & -130 \\ 95 & 230 \end{vmatrix} = \frac{-39100 + 12350}{250} = -107.$$

Pseudocode Algorithm

1. read n, a_{ij}, $1 \le i, j \le n$
2. $det \leftarrow 1$
3. repeat
   3.1. if $a_{11} = 0$ then
      3.1.1. $i \leftarrow 2$
      3.1.2. while $(i \le n)$ and $(a_{i1} = 0)$
         3.1.2.1. $i \leftarrow i + 1$
      3.1.3. if $i > n$ then
         3.1.3.1. write $'det(A) = 0'$
         3.1.3.2. *exit*
      3.1.4. for $j = 1, 2, ..., n$
         3.1.4.1. swap a_{1j} with a_{ij}
      3.1.5. $det \leftarrow -det$
   3.2. for $i = 1, 2, ..., n - 2$
      3.2.1. $det \leftarrow det \cdot a_{11}$
   3.3. for $i = 2, 3, ..., n$
      3.3.1. for $j = 2, 3, ..., n$
         3.3.1.1. $a_{ij} \leftarrow a_{ij} \cdot a_{11} - a_{i1} \cdot a_{1j}$
   3.4. $n \leftarrow n - 1$
   3.5. for $i = 1, 2, ..., n$
      3.5.1. for $j = 1, 2, ..., n$
         3.5.1.1. $a_{ij} \leftarrow a_{i+1,j+1}$

until $(n = 1)$

4. $det \leftarrow a_{11}/det$
5. write $'det(A) ='$, det.

7 Jacobi's Method

The problem: We consider the linear system

$$A \cdot x = b, \tag{24}$$

where $A \in \mathcal{M}_n(\mathbb{R})$ is the matrix associated to system (24) and $b \in \mathbb{R}^n$ is the vector containing the free terms of system (24).
Our goal is to determine, if possible, $x \in \mathbb{R}^n$, where x represents the unique solution of system (24).

Describing the method: We take $x^{(0)} \in \mathbb{R}^n$ to be the initial approximation of the solution of the system (24), arbitrarily chosen (for example the null vector). Based on $x^{(0)}$ we obtain $x^{(1)}$, based on $x^{(1)}$ we obtain $x^{(2)}$, based on $x^{(2)}$ we obtain $x^{(3)}$ etc. We do that by applying the following formulae:

$$x_i^{(k+1)} = \left(b_i - \sum_{\substack{j=1 \\ j \ne i}}^{n} a_{ij} x_j^{(k)} \right) \Big/ a_{ii}, 1 \le i \le n,\ k \ge 0,$$

until

$$\text{dist}\left(x^{(k+1)} - x^{(k)}\right) = \max_{1 \le i \le n} \left| x_i^{(k+1)} - x_i^{(k)} \right| \le \varepsilon,$$

where ε is the error that we consider acceptable when we try to approximate the exact solution of the system (24). Then $x \backsimeq x^{(k+1)}$.

Remark: A sufficient condition to obtain the solution of system (24) within the error ε is the following: the matrix A should be strictly diagonally dominant on rows or on columns.

Example: Using Jacobi's method, solve the following system within the error 10^{-2}.

$$\begin{cases} 5x_1 - 3x_2 - x_3 = 5 \\ -2x_1 + 4x_2 + x_3 = 0 \\ 2x_1 - 2x_2 - 5x_3 = -3. \end{cases}$$

Proof. We have that

$$A = \begin{pmatrix} 5 & -3 & -1 \\ -2 & 4 & 1 \\ 2 & -2 & -5 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 5 \\ 0 \\ -3 \end{pmatrix}.$$

We check if the matrix A is strictly diagonal dominant on rows :

$$\left.\begin{array}{l} |a_{11}| = 5 \\ |a_{12}| + |a_{13}| = |-3| + |-1| = 4 \end{array}\right\} \Rightarrow |a_{11}| > |a_{12}| + |a_{13}|$$

$$\left.\begin{array}{l} |a_{22}| = 4 \\ |a_{21}| + |a_{23}| = |-2| + |1| = 3 \end{array}\right\} \Rightarrow |a_{22}| > |a_{21}| + |a_{23}|$$

$$\left.\begin{array}{l} |a_{33}| = 5 \\ |a_{31}| + |a_{33}| = |2| + |-2| = 4 \end{array}\right\} \Rightarrow |a_{33}| > |a_{31}| + |a_{32}|.$$

So, the matrix A is strictly diagonal dominant on rows, and we can be sure that the Jacobi's method enables us to obtain an approximation of the solution with the desired precision. As a simple observation, we remark that A is not strictly diagonal dominant on columns.

We write the initial system in an equivalent form

$$\begin{cases} x_1 = (5 + 3x_2 + x_3)/5 \\ x_2 = (2x_1 - x_3)/4 \\ x_3 = (-3 - 2x_1 + 2x_2)/(-5). \end{cases}$$

We choose arbitrarily the initial approximation $x^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \\ x_3^{(0)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$, and we consider the recurrence

$$\begin{cases} x_1^{(k+1)} = \left(5 + 3x_2^{(k)} + x_3^{(k)}\right)/5 \\ x_2^{(k+1)} = \left(2x_1^{(k)} - x_3^{(k)}\right)/4 \\ x_3^{(k+1)} = \left(-3 - 2x_1^{(k)} + 2x_2^{(k)}\right)/(-5). \end{cases}$$

For $k=0$ we obtain

$$\begin{cases} x_1^{(1)} = \left(5+3x_2^{(0)}+x_3^{(0)}\right)/5 = (5+3\cdot 0+0)/5 = 1 \\ x_2^{(1)} = \left(2x_1^{(0)}-x_3^{(0)}\right)/4 = (2\cdot 0-0)/4 = 0 \\ x_3^{(1)} = \left(-3-2x_1^{(0)}+2x_2^{(0)}\right)/(-5) = (-3-2\cdot 0+2\cdot 0)/(-5) = 0.6. \end{cases}$$

We check the stop condition

$$d\left(x^{(1)}-x^{(0)}\right) = \max_{1\le i\le 3}\left|x_i^{(1)}-x_i^{(0)}\right| = \max\left\{\left|x_1^{(1)}-x_1^{(0)}\right|, \left|x_2^{(1)}-x_2^{(0)}\right|, \left|x_3^{(1)}-x_3^{(0)}\right|\right\} =$$

$$= \max\{|1-0|, |0-0|, |0.6-0|\} = 1 > \varepsilon = 0.01.$$

For $k=1$ we get

$$\begin{cases} x_1^{(2)} = \left(5+3x_2^{(1)}+x_3^{(1)}\right)/5 = (5+3\cdot 0+0.6)/5 = 1.12 \\ x_2^{(2)} = \left(2x_1^{(1)}-x_3^{(1)}\right)/4 = (2\cdot 1-0.6)/4 = 0.35 \\ x_3^{(2)} = \left(-3-2x_1^{(1)}+2x_2^{(1)}\right)/(-5) = (-3-2\cdot 1+2\cdot 0)/(-5) = 1. \end{cases}$$

We check the stop condition

$$d\left(x^{(2)}-x^{(1)}\right) = \max_{1\le i\le 3}\left|x_i^{(2)}-x_i^{(1)}\right| = \max\left\{\left|x_1^{(2)}-x_1^{(1)}\right|, \left|x_2^{(2)}-x_2^{(1)}\right|, \left|x_3^{(2)}-x_3^{(1)}\right|\right\} =$$

$$= \max\{|1.12-1|, |0.35-0|, |1-0.6|\} = 0.4 > \varepsilon = 0.01.$$

For $k=2$ we obtain

$$\begin{cases} x_1^{(3)} = \left(5+3x_2^{(2)}+x_3^{(2)}\right)/5 = (5+3\cdot 0.35+1)/5 = 1.41 \\ x_2^{(3)} = \left(2x_1^{(2)}-x_3^{(2)}\right)/4 = (2\cdot 1.12-1)/4 = 0.31 \\ x_3^{(3)} = \left(-3-2x_1^{(2)}+2x_2^{(2)}\right)/(-5) = (-3-2\cdot 1.12+2\cdot 0.35)/(-5) = 0.908. \end{cases}$$

We check the stop condition

$$d\left(x^{(3)}-x^{(2)}\right) = \max_{1\le i\le 3}\left|x_i^{(3)}-x_i^{(2)}\right| = \max\left\{\left|x_1^{(3)}-x_1^{(2)}\right|, \left|x_2^{(3)}-x_2^{(2)}\right|, \left|x_3^{(3)}-x_3^{(2)}\right|\right\} =$$

$$= \max\{|1.41-1.12|, |0.31-0.35|, |0.908-1|\} = 0.19 > \varepsilon = 0.01.$$

$$\vdots$$

Using the above reasoning we obtain the solution with precision given by $\varepsilon = 0.01$ at the step 14

$$\begin{cases} x_1^{(14)} = 1.495639 \\ x_2^{(14)} = 0.503865 \\ x_3^{(14)} = 1.004191. \end{cases}$$

The exact solution of the system is $\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1.5 \\ 0.5 \\ 1 \end{pmatrix}$. □

Pseudocode Algorithm

1. read n, a_{ij}, $1 \leq i, j \leq n$, b_i, $1 \leq i \leq n$, ε, $itmax$, x_i, $1 \leq i \leq n$
2. $it \leftarrow 0$
3. repeat
   3.1. $max \leftarrow 0$
   3.2. for $i = 1, 2, ..., n$
      3.2.1. $S \leftarrow 0$
      3.2.2. for $j = 1, 2, ..., n$
         3.2.2.1. if $j \neq i$ then
            3.2.2.1.1. $S \leftarrow S + a_{ij} \cdot x_j$
      3.2.3. $y_i \leftarrow (b_i - S)/a_{ii}$
      3.2.4. if $max < |y_i - x_i|$ then
         3.2.4.1. $max \leftarrow |y_i - x_i|$
   3.3. for $i = 1, 2, ..., n$
      3.3.1. $x_i \leftarrow y_i$
   3.4. $it \leftarrow it + 1$

until ($max \leq \varepsilon$) or ($it > itmax$)

4. if $it > itmax$ then
   4.1. write *'We cannot obtain the solution in',* itmax*, 'iterations, with precision',* ε
   4.2. *exit*
5. write (*'The approximation of the solution found in '*,it, *'iterations within error'*,ε, 'is', x_i, $1 \leq i \leq n$)

Exercise: Complete the above algorithm such that one can check whether the matrix of the system is strictly diagonal dominant on rows or columns.

8 Solving linear systems – Seidel-Gauss Method

The problem: We consider the linear system

$$A \cdot x = b, \qquad (25)$$

where $A \in \mathcal{M}_n(\mathbb{R})$ is the matrix associated to system (25) and $b \in \mathbb{R}^n$ is the vector containing the free terms of system (25).
Our goal is to determine, if possible, $x \in \mathbb{R}^n$, where x represents the unique solution of system (25).

Describing the method: We take $x^{(0)} \in \mathbb{R}^n$ to be the initial approximation of the solution of the system (25), arbitrarily chosen (for example the null vector). Based on $x^{(0)}$ we obtain $x^{(1)}$, based on $x^{(1)}$ we obtain $x^{(2)}$, based on $x^{(2)}$ we obtain $x^{(3)}$ etc. We do that by applying the following formulae:

$$x_i^{(k+1)} = \left(t_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)} \right) \Bigg/ a_{ii}, 1 \leq i \leq n,\ k \geq 0,$$

until

$$\max_{1 \leq i \leq n} \left| x_i^{(k+1)} - x_i^{(k)} \right| \leq \varepsilon,$$

where ε is the error that we consider acceptable when we try to approximate the exact solution of the system (25). Then $x \simeq x^{(k+1)}$.

Remarks:

1. A sufficient condition to obtain the solution of system (25) within the error ε is the following: the matrix A should be strictly diagonally dominant on rows or on columns.

2. Another sufficient condition to obtain the solution of system (25) within the error ε is that the matrix A associated to the system is symmetric and positive-definite.

Example: Using the Seidel-Gauss method, solve the following system with precision given by $\varepsilon = 10^{-2}$:

$$\begin{cases} 5x_1 - 3x_2 - x_3 = 5 \\ -2x_1 + 4x_2 + x_3 = 0 \\ 2x_1 - 2x_2 - 5x_3 = -3. \end{cases}$$

Proof. We have

$$A = \begin{pmatrix} 5 & -3 & -1 \\ -2 & 4 & 1 \\ 2 & -2 & -5 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 5 \\ 0 \\ -3 \end{pmatrix}.$$

We remark that matrix A is strictly diagonally dominant, hence the Seidel-Gauss method works.

We write the initial system into the following form:

$$\begin{cases} x_1 = (5 + 3x_2 + x_3)/5 \\ x_2 = (2x_1 - x_3)/4 \\ x_3 = (-3 - 2x_1 + 2x_2)/(-5). \end{cases}$$

We choose an arbitrary $x^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \\ x_3^{(0)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ as an initial approximation of the solution and we consider the recurrence

$$\begin{cases} x_1^{(k+1)} = \left(5 + 3x_2^{(k)} + x_3^{(k)}\right)/5 \\ x_2^{(k+1)} = \left(2x_1^{(k+1)} - x_3^{(k)}\right)/4 \\ x_3^{(k+1)} = \left(-3 - 2x_1^{(k+1)} + 2x_2^{(k+1)}\right)/(-5). \end{cases}$$

For $k = 0$ we obtain

$$\begin{cases} x_1^{(1)} = \left(5 + 3x_2^{(0)} + x_3^{(0)}\right)/5 = (5 + 3 \cdot 0 + 0)/5 = 1 \\ x_2^{(1)} = \left(2x_1^{(1)} - x_3^{(0)}\right)/4 = (2 \cdot 1 - 0)/4 = 0.5 \\ x_3^{(1)} = \left(-3 - 2x_1^{(1)} + 2x_2^{(1)}\right)/(-5) = (-3 - 2 \cdot 1 + 2 \cdot 0.5)/(-5) = 0.8. \end{cases}$$

We check the stop condition

$$d\left(x^{(1)} - x^{(0)}\right) = \max_{1 \le i \le 3} \left|x_i^{(1)} - x_i^{(0)}\right| = \max\left\{\left|x_1^{(1)} - x_1^{(0)}\right|, \left|x_2^{(1)} - x_2^{(0)}\right|, \left|x_3^{(1)} - x_3^{(0)}\right|\right\} =$$

$$= \max\{|1 - 0|, |0.5 - 0|, |0.8 - 0|\} = 1 > \varepsilon = 0.01.$$

For $k=1$ we obtain

$$\begin{cases} x_1^{(2)} = \left(5+3x_2^{(1)}+x_3^{(1)}\right)/5 = (5+3\cdot 0.5+0.8)/5 = 1.46 \\ x_2^{(2)} = \left(2x_1^{(2)}-x_3^{(1)}\right)/4 = (2\cdot 1.46-0.8)/4 = 0.53 \\ x_3^{(2)} = \left(-3-2x_1^{(2)}+2x_2^{(2)}\right)/(-5) = (-3-2\cdot 1.46+2\cdot 0.53)/(-5) = 0.972. \end{cases}$$

We check the stop condition

$$d\left(x^{(2)}-x^{(1)}\right) = \max_{1\le i\le 3}\left|x_i^{(2)}-x_i^{(1)}\right| = \max\left\{\left|x_1^{(2)}-x_1^{(1)}\right|, \left|x_2^{(2)}-x_2^{(1)}\right|, \left|x_3^{(2)}-x_3^{(1)}\right|\right\} =$$

$$= \max\{|1.46-1|, |0.53-0.5|, |0.972-0.8|\} = 0.46 > \varepsilon = 0.01.$$

For $k=2$ we obtain

$$\begin{cases} x_1^{(3)} = \left(5+3x_2^{(2)}+x_3^{(2)}\right)/5 = (5+3\cdot 0.53+0.972)/5 = 1.5124 \\ x_2^{(3)} = \left(2x_1^{(3)}-x_3^{(2)}\right)/4 = (2\cdot 1.5124-0.972)/4 = 0.5132 \\ x_3^{(3)} = \left(-3-2x_1^{(3)}+2x_2^{(3)}\right)/(-5) = (-3-2\cdot 1.5124+2\cdot 0.5132)/(-5) = 0.99968. \end{cases}$$

We check the stop condition

$$d\left(x^{(3)}-x^{(2)}\right) = \max_{1\le i\le 3}\left|x_i^{(3)}-x_i^{(2)}\right| = \max\left\{\left|x_1^{(3)}-x_1^{(2)}\right|, \left|x_2^{(3)}-x_2^{(2)}\right|, \left|x_3^{(3)}-x_3^{(2)}\right|\right\} =$$

$$= \max\{|1.5124-1.46|, |0.5132-0.53|, |0.99968-0.972|\} = 0.0524 > \varepsilon = 0.01.$$

For $k=3$ we obtain

$$\begin{cases} x_1^{(4)} = \left(5+3x_2^{(3)}+x_3^{(3)}\right)/5 = (5+3\cdot 0.5124+0.99968)/5 = 1.507856 \\ x_2^{(4)} = \left(2x_1^{(4)}-x_3^{(3)}\right)/4 = (2\cdot 1.507856-0.99968)/4 = 0.504008 \\ x_3^{(4)} = \left(-3-2x_1^{(4)}+2x_2^{(4)}\right)/(-5) = (-3-2\cdot 1.507856+2\cdot 0.504008)/(-5) = 1.001539. \end{cases}$$

We check the stop condition

$$d\left(x^{(4)}-x^{(3)}\right) = \max_{1\le i\le 3}\left|x_i^{(4)}-x_i^{(3)}\right| = \max\left\{\left|x_1^{(4)}-x_1^{(3)}\right|, \left|x_2^{(4)}-x_2^{(3)}\right|, \left|x_3^{(4)}-x_3^{(3}\right|\right\} =$$

$$= \max\{|1.507856-1.5124|, |0.504008-0.5132|, |1.001539-0.99968|\} = 0.009192 < \varepsilon = 0.01.$$

Thus an approximation of the solution of the system of precision given by $\varepsilon = 10^{-2}$ is the following

$$\begin{cases} x_1^{(4)} = 1.507856 \\ x_2^{(4)} = 0.504008 \\ x_3^{(4)} = 1.001539. \end{cases}$$

Notice that, by using Seidel-Gauss method, we have obtain the solution of this system within the error 10^{-2} at step 4, as opposed to Jacobi's method, when we needed 14 steps.

□

Exercise. Based on what you understood from the above solved example and from the description of the Seidel-Gauss method, modify the algorithm used for Jacobi method in order to obtain the algorithm for Seidel-Gauss method.

9 Solving nonlinear equations – The method of successive approximations

The problem: We consider the equation

(26) $$f(x) = 0,$$

where $f : [a, b] \to \mathbb{R}$, $f \in C^2([a, b])$. Our goal is to approximate the solution $x^* \in [a, b]$ of the equation (26).

Describing the method: The method of successive approximations consists in the transformation of the equation (26) in an equivalent form

$$x = g(x).$$

We construct the sequence $(x_n)_{n\geq 0}$, given by

(27) $$x_{n+1} = g(x_n), \quad n \geq 0,$$

where x_0 is the initial approximation of the solution x^*.

Remarks

1. To ensure the convergence of the sequence (27) a sufficient condition is to take g to be contraction on the interval $[a, b]$.

2. If g is differentiable on $[a, b]$, then g is a contraction if and only if

$$|g'(x)| \leq q < 1, \quad \forall x \in [a, b].$$

3. As a stop criterion we will use

$$|x_{n+1} - x_n| \leq \varepsilon \Rightarrow x_{n+1} \simeq x^*,$$

where ε is the error that we consider acceptable.

Example 1. Use the method of the successive approximations to determine the root of the equation

$$x = \sqrt[4]{x + 2},$$

with precision $\varepsilon = 10^{-2}$.

Solution: We consider the function

$$f(x) = x - \sqrt[4]{x + 2}, \quad x \geq 0.$$

We search a, b such that $f(a)f(b) < 0$.

$$f(0) = -\sqrt[4]{2} < 0,$$

$$f(1) = 1 - \sqrt[4]{3} < 0,$$
$$f(2) = 2 - \sqrt[4]{4} = 2 - \sqrt{2} > 0.$$

So, the root of our equation is in the interval $x^* \in [1, 2]$.

We write the equation in an equivalent form

$$x = g(x),$$

where $g(x) = \sqrt[4]{x + 2}, \quad x \in [1, 2]$.

We prove that g is a contraction on the interval $[1, 2]$, i.e. $|g'(x)| < 1$, for every $x \in [1, 2]$. We have that

$$\left|g'(x)\right| = \left|\frac{1}{4}(x+2)^{-\frac{3}{4}}\right| = \frac{1}{4\sqrt[4]{x+2}^{\,3}} \leq \frac{1}{4\sqrt[4]{1+2}^{\,3}} < 1, \text{ for every } x \in [1, 2],$$

therefore, g is a contraction on$[1, 2]$.

We can take $x_0 \in [1, 2]$ arbitrarily. We choose $x_0 = 2$ and we use the recurrence

$$x_{n+1} = g(x_n) \Leftrightarrow x_{n+1} = \sqrt[4]{x_n + 2}, \qquad n \geq 0.$$

For $n = 0$, we get

$$x_1 = g(x_0) = \sqrt[4]{x_0 + 2} = \sqrt[4]{4} = \sqrt{2}$$

We check the stop condition:

$$|x_1 - x_0| > \varepsilon = 0.01,$$

since $|x_1 - x_0| \simeq 0.585786$. For $n = 1$, we have

$$x_2 = g(x_1) = \sqrt[4]{x_1 + 2} = \sqrt[4]{\sqrt{2} + 2}.$$

We check the stop condition:

$$|x_2 - x_1| > \varepsilon = 0.01$$

since $|x_2 - x_1| \simeq 0.054891$. For $n = 2$, we have

$$x_3 = g(x_2) = \sqrt[4]{\sqrt[4]{\sqrt{2} + 2} + 2}.$$

We check the stop condition:

$$|x_3 - x_2| < \varepsilon = 0.01$$

since $|x_3 - x_2| \simeq 0.005497$. So,

$$x_3 = \sqrt[4]{\sqrt[4]{\sqrt{2} + 2} + 2} \simeq 1.353826,$$

aproximates the solution of our equation within error $\varepsilon = 10^{-2}$ (that is, with one exact decimal).

Pseudocode Algorithm

1. read x_0, ε, $itmax$; declare g
2. $it \leftarrow 0$
3. repeat
   3.1. $x_1 \leftarrow g(x_0)$
   3.2. $dif \leftarrow |x_1 - x_0|$
   3.3. $x_0 \leftarrow x_1$
   3.4. $it \leftarrow it + 1$

until $(dif \leq \varepsilon)$ or $(it > itmax)$

4. if $it > itmax$ then
   4.1. write *'Cannot obtain the solution in'*, itmax, *'iterations, within error'*, ε
   4.2. *exit*
5. write (*'The approximation of the solution found in '*,it, *'iterations within error'*,ε, 'is', x_1).

Remark: In C, C++, the function $g(x) = \frac{4}{\sqrt{x+3}}$ may be declared as:

```
float f(float x)
  {
return   4./sqrt(x+3);
  }
```

Function	In C or C++
$\sqrt{x}$	sqrt(x)
$\sqrt[3]{x}$	cbrt(x)
$\sqrt[7]{x}$	pow(x, 1./7)
e^x	exp(x)
a^x	pow(a,x)
$\ln x$	log(x)
$\log_a x = \frac{\ln x}{\ln a}$	log(x)/log(a)

10 Krylov's method for finding the coefficients of the characteristic polynomial

Describing the problem: We consider the matrix $A \in \mathcal{M}_n$. Our goal is to determine the coefficients of the characteristic polynomial associated to this matrix

$$p_A(\lambda) = \lambda^n + c_1\lambda^{n-1} + ... + c_{n-1}\lambda + c_n.$$

The method:

1)We choose $y^{(0)} \neq 0 \in \mathbb{R}^n$ arbitrarily;
2) We compute

$$y^{(k)} = Ay^{(k-1)}, \quad 1 \leq k \leq n$$

3) We solve the linear system

$$\left(y^{(n-1)}y^{(n-2)}...y^{(1)}y^{(0)}\right)\cdot\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = -y^{(n)}. \tag{28}$$

Remarks: i) If the system (28) does not have a unique solution, then we choose another $y^{(0)} \neq 0 \in \mathbb{R}^n$ and we restart the algorithm.
ii) If the system (28) has unique solution, then the components of the solution, $c_1, c_2, ...c_n$, are the coefficients of characteristic polynomial. However, one must not forget the coefficient of λ^n which is $c_0 = 1$.

Example: Using Krylov's method, determine the eigenvalues and eigenvectors corresponding to the matrix

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

Is the matrix A invertible? If so, determine the inverse of A, using Krylov's method.

Proof. **Step 1.** We choose arbitrarily $y^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$, and we consider the vectorial recurrence

$$y^{(k+1)} = A \cdot y^{(k)}, \qquad 0 \leq k \leq 2.$$

Step 2. We compute $y^{(1)}$ and $y^{(2)}$

$$y^{(1)} = A \cdot y^{(0)} = \begin{pmatrix} 3 & 3 & -1 \\ 1 & 3 & -1 \\ 2 & 3 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix},$$

$$y^{(2)} = A \cdot y^{(1)} = \begin{pmatrix} 3 & 3 & -1 \\ 1 & 3 & -1 \\ 2 & 3 & 0 \end{pmatrix}\begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 10 \\ 4 \\ 9 \end{pmatrix}.$$

Step 3. We test if $\det(B) \neq 0$, where $B = \left(y^{(2)}y^{(1)}y^{(0)}\right) = \begin{pmatrix} 10 & 3 & 1 \\ 4 & 1 & 0 \\ 9 & 2 & 0 \end{pmatrix}$. We notice that $\det(B) = -1 \neq 0$ and we move further.
Step 4. We compute $y^{(3)}$

$$y^{(3)} = A \cdot y^{(2)} = \begin{pmatrix} 3 & 3 & -1 \\ 1 & 3 & -1 \\ 2 & 3 & 0 \end{pmatrix}\begin{pmatrix} 10 \\ 4 \\ 9 \end{pmatrix} = \begin{pmatrix} 33 \\ 13 \\ 32 \end{pmatrix}.$$

We solve the linear system

$$B \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = -y^{(3)},$$

which is equivalent to

$$\begin{pmatrix} 10 & 3 & 1 \\ 4 & 1 & 0 \\ 9 & 2 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = - \begin{pmatrix} 33 \\ 13 \\ 32 \end{pmatrix}. \tag{29}$$

We note that $\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$ is the vector which contains the coefficients of the characteristic polynomial.

We write the system (29) in an equivalent form

$$\begin{cases} 10c_1 + 3c_2 + c_3 = -33 \\ 4c_1 + c_2 = -13 \\ 9c_1 + 2c_2 = -32 \end{cases} \Rightarrow \begin{cases} c_1 = -6 \\ c_2 = 11 \\ c_3 = -6. \end{cases}$$

Step 5. The characteristic polynomial corresponding to the matrix A is

$$p_A(\lambda) = \lambda^3 + c_1\lambda^2 + c_2\lambda + c_3 = \lambda^3 - 6\lambda^2 + 11\lambda - 6.$$

To determine the eigenvalues, we solve the following equation

$$p_A(\lambda) = 0 \Leftrightarrow \lambda^3 - 6\lambda^2 + 11\lambda - 6 = 0.$$

We notice that this is a polynomial of integer coefficients. Thus, if p_A admits rational roots, these must be in the set $\mathcal{D}_6 = \{\pm 1, \pm 2, \pm 3, \pm 6\}$. We test these values to see if any of them is a root of p_A. Since

$$p_A(1) = 1 - 6 + 11 - 6 = 0,$$

we deduce that $\lambda_1 = 1$. Next we could test the other values to see if any of them is an eigenvalue as well, or we could divide $p_A(\lambda)$ by $(\lambda - 1)$, or we could apply Horner's rule for polynomials etc. For generality, we usually apply Horner's rule or we divide the polynomial by $(\lambda - \lambda_1)$. We get

$$p_A(\lambda) = (\lambda - 1)(\lambda^2 - 5\lambda + 6).$$

Solving $\lambda^2 - 5\lambda + 6 = 0$ we obtain $\lambda_2 = 2$ and $\lambda_3 = 3$.

Step 6. Since the eigenvalues are distinct real number, Krylov's method allows us to compute the eigenvectors.

For the eigenvalue $\lambda_1 = 1$, we compute

$$q_1(\lambda) = \frac{p_A(\lambda)}{\lambda - \lambda_1} = (\lambda - 2)(\lambda - 3) = \lambda^2 - 5\lambda + 6.$$

An eigenvector corresponding to eigenvalue $\lambda_1 = 1$ is

$$y^{(2)} - 5y^{(1)} + 6y^{(0)} = \begin{pmatrix} 10 \\ 4 \\ 9 \end{pmatrix} - 5 \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix} + 6 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}.$$

For the eigenvalue $\lambda_2 = 2$, we compute

$$q_2(\lambda) = \frac{p_A(\lambda)}{\lambda - \lambda_2} = (\lambda - 1)(\lambda - 3) = \lambda^2 - 4\lambda + 3.$$

An eigenvector corresponding to the eigenvalue $\lambda_2 = 2$ is

$$y^{(2)} - 4y^{(1)} + 3y^{(0)} = \begin{pmatrix} 10 \\ 4 \\ 9 \end{pmatrix} - 4 \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix} + 3 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

For the eigenvalue $\lambda_3 = 3$, we compute

$$q_3(\lambda) = \frac{p_A(\lambda)}{\lambda - \lambda_3} = (\lambda - 1)(\lambda - 2) = \lambda^2 - 3\lambda + 2.$$

An eigenvector corresponding to the eigenvalue $\lambda_3 = 3$ is

$$y^{(2)} - 3y^{(1)} + 2y^{(0)} = \begin{pmatrix} 10 \\ 4 \\ 9 \end{pmatrix} - 3 \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix} + 2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 3 \end{pmatrix}.$$

Step 7. Moreover, since the free term of the characteristic polynomial $c_3 = -10$ is nonzero, then the matrix A is invertible and its inverse is given by the formula

$$A^{-1} = -\frac{1}{c_3}(A^2 + c_1 A + c_2 I_3) = \frac{1}{6}(A^2 - 6A + 11I_3) =$$

$$= \frac{1}{6}\left[\begin{pmatrix} 10 & 15 & -6 \\ 4 & 9 & -4 \\ 9 & 15 & -5 \end{pmatrix} - 6 \begin{pmatrix} 3 & 3 & -1 \\ 1 & 3 & -1 \\ 2 & 3 & 0 \end{pmatrix} + 11 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right] = \frac{1}{6}\begin{pmatrix} 3 & -3 & 0 \\ -2 & 2 & 2 \\ -3 & -3 & 6 \end{pmatrix}.$$

□

Remark. We will provide the pseudocode algorithm only for finding the coefficients of the characteristic polynomial. For the rest of the calculus we should combine this algorithm with other methods, such is Bairstow method for finding the roots of a polynomial etc.

Pseudocode Algorithm

1. read n, a_{ij}, $1 \le i, j \le n$
2. pasul2: read $b_{i,n}$, $1 \le i \le n$ {represents $y^{(0)} \ne 0_n$}

// *we compute* $y^{(1)}, y^{(2)}, ..., y^{(n-1)}$, *using the formula* $y^{(k)} = A \cdot y^{(k-1)}$, $1 \le k \le n$

3. for $j = n-1, n-2, ..., 1$
    3.1. for $i = 1, 2, ..., n$
        3.1.1. $b_{ij} \leftarrow 0$
        3.1.2. for $k = 1, 2, ..., n$
            3.1.2.1. $b_{ij} \leftarrow b_{ij} + a_{ik} \cdot b_{k,j+1}$

// *compute* $y^{(n)}$, *using* $y^{(n)} = A \cdot y^{(n-1)}$, *and we put* $-y^{(n)}$

4. for $i = 1, 2, ..., n$
    4.1. $b_{i,n+1} \leftarrow 0$
    4.2. for $k = 1, 2, ..., n$
        4.2.1. $b_{i,n+1} \leftarrow b_{i,n+1} + a_{ik} \cdot b_{k1}$
    4.1. $b_{i,n+1} \leftarrow -b_{i,n+1}$

// *we solve the system with augmented matrix* $(b_{ij})_{\substack{1 \le i \le n \\ 1 \le j \le n+1}}$, *using one of the methods previously studied:*

- *Gauss method whit partial pivoting at every step*
- *LR Factorization (Doolitlle)*

and then we write the coefficients of the characteristic polynomial (without forgetting $c_0 = 1$).

Remark. When solving the linear system from above, if we find out that the solution is not unique, instead of exiting the program we could put

goto pasul2;

which will allow us to go back and choose another $y^{(0)} \neq 0_n$. In fact, one can check whether the determinant of B is zero (that is, $fabs(det) < 0.00001$) by using Chio's Method. In case det B=0, we put goto pasul2; (and this means that we do not need to insert this inside Gauss or LR). Otherwise we move further.

11 Fadeev's method for finding the coefficients of the characteristic polynomial

The problem: We consider the matrix $A \in \mathcal{M}_n(\mathbb{R})$. Our goal is to determine the coefficients of the characteristic polynomial

$$p_A(\lambda) = \lambda^n + c_1\lambda^{n-1} + ... + c_{n-1}\lambda + c_n,$$

associated to the matrix A.

Describing the method: The coefficients are determined using the formulae:
1) $A_1 = A$; $c_1 = -\mathrm{Tr}(A_1)$; $B_1 = c_1 I_n + A_1$;
2) $A_2 = AB_1$; $c_2 = -\mathrm{Tr}(A_2)/2$; $B_2 = c_2 I_n + A_2$;
$\vdots$
n) $A_n = AB_{n-1}$; $c_n = -\mathrm{Tr}(A_n)/n$; $B_n = c_n I_n + A_n$.

Remarks:
1) $B_n = O_n$ (that is, the null matrix), so there is no need to be calculated.
2) If $c_n \neq 0 \Rightarrow A^{-1} = -\frac{1}{c_n} B_{n-1}$.

Example: Using the Fadeev's method, determine the characteristic polynomial corresponding to the matrix

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

Is the matrix A invertible? If so, please determine the inverse matrix A^{-1}, using Fadeev's method.

Proof. Step 1:

$$A_1 = A = \begin{pmatrix} 2 & 1 & -1 \\ 2 & 1 & 1 \\ -3 & 0 & 0 \end{pmatrix},$$

$$c_1 = -Tr(A_1)/1 = -(2+1+0)/1 = -3,$$

$$B_1 = c_1 I_3 + A_1 = -3 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 2 & 1 & -1 \\ 2 & 1 & 1 \\ -3 & 0 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 1 & -1 \\ 2 & -2 & 1 \\ -3 & 0 & -3 \end{pmatrix}.$$

Step 2:

$$A_2 = AB_1 = \begin{pmatrix} 2 & 1 & -1 \\ 2 & 1 & 1 \\ -3 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 1 & -1 \\ 2 & -2 & 1 \\ -3 & 0 & -3 \end{pmatrix} = \begin{pmatrix} 3 & 0 & 2 \\ -3 & 0 & -4 \\ 3 & -3 & 3 \end{pmatrix}$$

$$c_2 = -Tr(A_2)/2 = -(3+0+3)/2 = -3,$$

$$B_2 = c_2 I_3 + A_2 = -3 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 3 & 0 & 2 \\ -3 & 0 & -4 \\ 3 & -3 & 3 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 2 \\ -3 & -3 & -4 \\ 3 & -3 & 0 \end{pmatrix}.$$

Step 3:

$$A_3 = AB_2 = \begin{pmatrix} 2 & 1 & -1 \\ 2 & 1 & 1 \\ -3 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 2 \\ -3 & -3 & -4 \\ 3 & -3 & 0 \end{pmatrix} = \begin{pmatrix} -6 & 0 & 0 \\ 0 & -6 & 0 \\ 0 & 0 & -6 \end{pmatrix},$$

$$c_3 = -Tr(A_3)/3 = -(-6-6-6)/3 = 6,$$

$$B_3 = c_3 I_3 + A_3 = 6 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} -6 & 0 & 0 \\ 0 & -6 & 0 \\ 0 & 0 & -6 \end{pmatrix} = O_3.$$

The characteristic polynomial corresponding to the matrix A is

$$p_A(\lambda) = \lambda^3 + c_1\lambda^2 + c_2\lambda + c_3 = \lambda^3 - 3\lambda^2 - 3\lambda + 6.$$

Moreover, since the free term of the characteristic polynomial $c_3 = 6$ is nonzero, then the matrix A is invertible and the corresponding inverse matrix is given by the formula

$$A^{(-1)} = -\frac{1}{c_3} B_2 = -\frac{1}{6} \begin{pmatrix} 0 & 0 & 2 \\ -3 & -3 & -4 \\ 3 & -3 & 0 \end{pmatrix}.$$

□

Remark: In the pseudocode algorithm, the role of A_k will be played by matrix D.

Pseudocode Algorithm

1. read n, a_{ij}, $1 \le i, j \le n$

// initialize B with unit matrix I_n

2. for $i = 1, 2, ..., n$
    2.1. for $j = 1, 2, ..., n$
        2.1.1. if $i = j$ then
            2.1.1.1. $b_{ij} \leftarrow 1$
            else

2.1.1.2. $b_{ij} \leftarrow 0$
3. for $k = 1, 2, ..., n-1$
// we compute the elements of A_k, using $A_k = A \cdot B_{k-1}$, and denote $D = A_k$
3.1. for $i = 1, 2, ..., n$
3.1.1. for $j = 1, 2, ..., n$
3.1.1.1. $d_{ij} \leftarrow 0$
3.1.1.2. for $h = 1, 2, ..., n$
3.1.1.2.1. $d_{ij} \leftarrow d_{ij} + a_{ih} \cdot b_{hj}$
// we compute the coefficients c_k, using $c_k = -Tr(A_k)/k$
3.2. $c_k \leftarrow 0$
3.3. for $i = 1, 2, ..., n$
3.3.1. $c_k \leftarrow c_k + d_{ii}$
3.4. $c_k \leftarrow -c_k/k$
// we compute the elements of the matrix B_k, using $B_k = c_k \cdot I_n + A_k$
3.5. for $i = 1, 2, ..., n$
3.5.1. for $j = 1, 2, ..., n$
3.5.1.1. if $i = j$ then
3.5.1.1.1. $b_{ij} \leftarrow d_{ij} + c_k$
else
3.5.1.1.2. $b_{ij} \leftarrow d_{ij}$
// compute $A_n = D$
4. for $i = 1, 2, ..., n$
4.1. for $j = 1, 2, ..., n$
4.1.1. $d_{ij} \leftarrow 0$
4.1.2. for $h = 1, 2, ..., n$
4.1.2.1. $d_{ij} \leftarrow d_{ij} + a_{ih} \cdot b_{hj}$
// compute $c_n = -Tr(A_n)/n$
5. $c_n \leftarrow 0$
6. for $i = 1, 2, ..., n$
6.1. $c_n \leftarrow c_n + d_{ii}$
7. $c_n \leftarrow -c_n/n$
8. if $c_n = 0$ then
8.1. write *'The matrix is not invertible.'*
else
8.2. write *'The inverse matrix is'*
8.3. for $i = 1, 2, ..., n$
8.3.1. for $j = 1, 2, ..., n$
8.3.1.1. write $-b_{ij}/c_n$
9. $c_0 = 1$
10. write *' The coefficients of the characteristic polynomial are'*, c_i, $0 \leq i \leq n$

12 Lagrange interpolation polynomial

Presentation of the problem: Let:

$x_0 < x_1 < ... < x_n \in \mathbb{R}$ interpolation nodes;
$f_i = f(x_i)$, $0 \leq i \leq n$, given values of the function f in the interpolation nodes;
$z \in \mathbb{R}$, with $z \in [x_0, x_n]$.

Our goal is to approximate $f(z)$, using the Lagrange interpolation polynomial on the nodes $x_0, x_1, ..., x_n$.

Presentation of the method:

$$f(z) \cong \sum_{k=0}^{n} f_k \cdot \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{z - x_i}{x_k - x_i},$$

where

$$L(x) = \sum_{k=0}^{n} f_k \cdot \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i},$$

is the Lagrange interpolation polynomial on the nodes $x_0, x_1, ..., x_n$.

Remark: $d^o(L) \leq n$.

Pseudocode Algorithm

1. read n, x_i, $0 \leq i \leq n$, f_i, $0 \leq i \leq n$, z
2. $L \leftarrow 0$
3. for $k = 0, 1, .., n$
   3.1. $P \leftarrow 1$
   3.2. for $i = 0, 1, .., n$
      3.2.1. if $i \neq k$ then
         3.2.1.1. $P \leftarrow P \cdot (z - x_i)/(x_k - x_i)$
   3.3. $L \leftarrow L + f_k \cdot P$
4. write *'The approximative value of the function f in '*, z, *'is'*, L

The above algorithm can be completed taking into account the following remarks:
1) if $z \notin [x_0, x_n]$, we can not approximate f in z;
2) if $\exists\, i \in \{0, 1, .., n\}$, such that $z = x_i$, then we will display the corresponding value of L (without to compute the sum);
3) the evaluation of the Lagrange polynomial can be done in $z_1, z_2, ..., z_n \in [x_0, x_n]$;
4) if $\exists\, i \in \{0, 1, .., n\}$, such that $f_i = 0$, then is not taken into account, in sum, the therm which contains $f_i = 0$.

Example 1. Let be the table

x_i	-1	$-\frac{2}{3}$	0	$\frac{2}{3}$	1
f_i	0	$\frac{1}{2}$	1	$\frac{1}{2}$	0

a) Determine the Lagrange interpolation polynomial which interpolates the above dates;
b) Evaluate $f\left(-\frac{1}{2}\right)$, $f\left(\frac{1}{3}\right)$, $f\,(0)$ and $f\,(2)$.

Solution: We remark that the above dates correspond the function $f(x) = \cos\left(\frac{\pi x}{2}\right),\ x \in [-1, 1]$.
We have $n = 4$ and

$$x_0 = -1,\ x_1 = -\frac{2}{3},\ x_2 = 0,\ x_3 = \frac{2}{3},\ x_4 = 1,$$

$$f_0 = 0,\ \ f_1 = \frac{1}{2},\ \ f_2 = 1,\ \ f_3 = \frac{1}{2},\ \ f_4 = 0.$$

The Lagrange interpolation polynomial is

$$L(x) = f_0 l_0(x) + f_1 l_1(x) + f_2 l_2(x) + f_3 l_3(x) + f_4 l_4(x), \quad x \in [-1, 1],$$

(30)
$$\Leftrightarrow L(x) = 0 \cdot l_0(x) + \frac{1}{2} \cdot l_1(x) + 1 \cdot l_2(x) + \frac{1}{2} \cdot l_3(x) + 0 \cdot l_4(x), \quad x \in [-1, 1],$$

where the Lagrange fundamental polynomials $l_k(x),\ 0 \le k \le 4$, are determined using the formula

$$l_k(x) = \prod_{\substack{i=0 \\ i \ne k}}^{4} \frac{x - x_i}{x_k - x_i}, \quad 0 \le k \le 4.$$

Since $f = 0$ and $f_4 = 0$, is not necessary to compute $l_0(x)$ and $l_4(x)$. In what follows we determine the Lagrange fundamental polynomials $l_1(x)$, $l_2(x)$ and $l_3(x)$. We have

$$l_1(x) = \frac{(x - x_0)(x - x_2)(x - x_3)(x - x_4)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)} = \frac{(x+1)\,(x-0)\left(x - \frac{2}{3}\right)(x-1)}{\left(-\frac{2}{3}+1\right)\left(-\frac{2}{3}-0\right)\left(-\frac{2}{3}-\frac{2}{3}\right)\left(-\frac{2}{3}-1\right)} =$$

$$= -\frac{27}{40} x(x+1)(x-1)(3x-2),$$

$$l_2(x) = \frac{(x - x_0)(x - x_1)(x - x_3)(x - x_4)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)(x_2 - x_4)} = \frac{(x+1)\left(x + \frac{2}{3}\right)\left(x - \frac{2}{3}\right)(x-1)}{(0+1)\left(0+\frac{2}{3}\right)\left(0-\frac{2}{3}\right)(0-1)} =$$

$$= \frac{1}{4}(x+1)(3x+2)(3x-2)(x-1),$$

$$l_3(x) = \frac{(x - x_0)(x - x_1)(x - x_2)(x - x_4)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)(x_3 - x_4)} = \frac{(x+1)\left(x + \frac{2}{3}\right)(x-0)\,(x-1)}{\left(\frac{2}{3}+1\right)\left(\frac{2}{3}+\frac{2}{3}\right)\left(\frac{2}{3}-0\right)\left(\frac{2}{3}-1\right)} =$$

$$= -\frac{27}{40} x(x+1)(3x+2)(x-1).$$

From relation (30) we get

$$L(x) = \frac{1}{2} \cdot \left(-\frac{27}{40}\right) x(x+1)(x-1)(3x-2) + \frac{1}{4}(x+1)(3x+2)(3x-2)(x-1) + \frac{1}{2} \cdot \left(-\frac{27}{40}\right) x(x+1)(3x+2)(x-1) =$$

$$= (x^2 - 1)\left(\frac{9}{40}x^2 - 1\right) = \frac{9}{40}x^4 - \frac{49}{40}x^2 + 1$$

b) From a) we have
$f\left(-\frac{1}{2}\right) = L\left(-\frac{1}{2}\right) = \frac{9}{40}\left(-\frac{1}{2}\right)^4 - \frac{49}{40}\left(-\frac{1}{2}\right)^2 + 1 = 0.777380,$
$f\left(\frac{1}{3}\right) = L\left(\frac{1}{3}\right) = \frac{9}{40}\left(\frac{1}{3}\right)^4 - \frac{49}{40}\left(\frac{1}{3}\right)^2 + 1 = 0.866666,$
$f(0) = f(x_2) = f_2 = 1,$
$f(2)$ cannot be evaluated, since $2 \notin [-1, 1]$.

Example 2. Let be the table

x_i	0	$\frac{1}{6}$	$\frac{1}{2}$	1
f_i	0	$\frac{1}{2}$	1	0

Evaluate $f(z)$, using the Lagrange interpolation polynomial on the above nodes, where:
$z \in \{\frac{1}{4}; \frac{1}{3}; \frac{1}{2}; 2\}$.
Sol: $\frac{1}{6} \simeq 0.166666$; $f(\frac{1}{4}) = 0.693752$; $f(\frac{1}{3}) = 0.844444$;

Example 3. Let be the table

x_i	-1	0	2	3	4
f_i	-0.3	0.2	0	1.1	1.8

a) Evaluate $f(z)$, using the Lagrange interpolation polynomial on the above nodes, where:
$z \in \{-2; -1.05; -0.5; 0; 1; 2; 2.995; 4; 67\}$.
b) Evaluate $f(-0.5)$ and $f(1)$ using a Lagrange interpolation polynomial of degree 2.
Sol: a) $f(-0.5) = 0.225$, $f(1) = -0.24$, $f(2.995) = 1.093846$

13 Newton interpolation polynomial

Presentation of the problem: Let:
$x_0 < x_1 < ... < x_n \in \mathbb{R}$ interpolation nodes;
$f_i = f(x_i)$, $0 \leq i \leq n$, given values of the function f in the interpolation nodes;
$z \in \mathbb{R}$, with $z \in [x_0, x_n]$.

Our goal is to approximate $f(z)$, using the Newton interpolation polynomial on the nodes $x_0, x_1, ..., x_n$.

Presentation of the method:

$$f(z) \cong f[x_0] + \sum_{k=1}^{n} f[x_0; x_1; ...; x_k] \cdot \prod_{i=0}^{k-1} (z - x_i),$$

where

$$N(x) = f[x_0] + \sum_{k=1}^{n} f[x_0; x_1; ...; x_k] \cdot \prod_{i=0}^{k-1} (x - x_i),$$

is the Newton interpolation polynomial on the nodes $x_0, x_1, ..., x_n$ and

$$f[x_0] = f_0,$$

$$f[x_0; x_1; ...; x_k] = \sum_{j=0}^{k} \frac{f_j}{\prod_{\substack{i=0 \\ i \neq j}}^{k} (x_j - x_i)}, \qquad 1 \leq k \leq n.$$

Remark: $d^o(N) \leq n$.

Pseudocode Algorithm
1. read n, x_i, $0 \leq i \leq n$, f_i, $0 \leq i \leq n$, z

2. $N \leftarrow f_0$
3. for $k = 1, 2, .., n$
   3.1. $s \leftarrow 0$
   3.2. for $j = 0, 1, .., k$
      3.2.1. $p \leftarrow 1$
      3.2.2. for $i = 0, 1, .., k$
         3.2.2.1. if $i \neq j$ then
            3.2.2.1.1. $p \leftarrow p \cdot (x_j - x_i)$
      3.2.3. $s \leftarrow s + f_j / p$
   3.3. $p \leftarrow 1$
   3.4. for $i = 0, 1, .., k - 1$
      3.4.1. $p \leftarrow p \cdot (z - x_i)$
   3.5. $N \leftarrow N + s \cdot p$
4. write *'The approximative value of the function f in ', z, 'is', N*

The above algorithm can be completed taking into account the following remarks:
1) if $z \notin [x_0, x_n]$, we can not approximate f in z;
2) if $\exists\, i \in \{0, 1, .., n\}$, such that $z = x_i$, then we will display the corresponding value of L (without to compute the sum);
3) the evaluation of the Newton polynomial can be done in $z_1, z_2, ..., z_n \in [x_0, x_n]$;
4) if $\exists\, i \in \{0, 1, .., n\}$, such that $s = f[x_0; x_1; ...; x_k] = 0$, then is not taken into account, in sum, the therm which contains $s = 0$.

Example 1. Let be the table of dates

x_i	-1	$-\frac{2}{3}$	0	$\frac{2}{3}$	1
f_i	0	$\frac{1}{2}$	1	$\frac{1}{2}$	0

Determine the Newton interpolation polynomial which interpolates the above dates;
b) Evaluate $f\left(-\frac{1}{2}\right)$, $f\left(\frac{1}{3}\right)$, $f\,(0)$ and$f\,(2)$.

Soluţie: We have $n = 4$, and

$$x_0 = -1,\ x_1 = -\frac{2}{3},\ x_2 = 0,\ x_3 = \frac{2}{3},\ x_4 = 1,$$

$$f_0 = 0,\ \ f_1 = \frac{1}{2},\ \ f_2 = 1,\ \ f_3 = \frac{1}{2},\ \ f_4 = 0.$$

We construct the table

x_i	Div. diff. of order 0	Divided diff. of order 1	Divided differences of order 2	Divided differences of order 3	Divided difference of order 4
$x_0 = -1$	$f[x_0] = 0$	$f[x_0; x_1] = \frac{3}{2}$	$f[x_0; x_1; x_2] = -\frac{3}{4}$	$f[x_0; x_1; x_2; x_3] = -\frac{9}{40}$	$f[x_0; x_1; ..; x_4] = \frac{9}{40}$
$x_1 = -\frac{2}{3}$	$f[x_1] = \frac{1}{2}$	$f[x_1; x_2] = \frac{3}{4}$	$f[x_1; x_2; x_3] = -\frac{9}{8}$	$f[x_1; x_2; x_3; x_4] = \frac{9}{40}$	–
$x_2 = 0$	$f[x_2] = 1$	$f[x_2; x_3] = -\frac{3}{4}$	$f[x_2; x_3; x_4] = -\frac{3}{4}$	–	–
$x_3 = \frac{2}{3}$	$f[x_3] = \frac{1}{2}$	$f[x_3; x_4] = -\frac{3}{2}$	–	–	–
$x_4 = 1$	$f[x_4] = 0$	–	–	–	–

To obtain the values from above table, we determine the divided differences with the help of the following formulas

Divided differences of order 0:

$$f[x_0] = f_0 = 0, \quad f[x_1] = f_1 = \frac{1}{2}, \quad f[x_2] = f_2 = 1, \quad f[x_3] = f_3 = \frac{1}{2}, \quad f[x_4] = f_4 = 0.$$

Divided differences of order 1:

$$f[x_0; x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0} = \frac{\frac{1}{2} - 0}{-\frac{2}{3} - (-1)} = \frac{3}{2},$$

$$f[x_1; x_2] = \frac{f[x_2] - f[x_1]}{x_2 - x_1} = \frac{1 - \frac{1}{2}}{0 - \left(-\frac{2}{3}\right)} = \frac{3}{4},$$

$$f[x_2; x_3] = \frac{f[x_3] - f[x_2]}{x_3 - x_2} = \frac{\frac{1}{2} - 1}{\frac{2}{3} - 0} = -\frac{3}{4},$$

$$f[x_3; x_4] = \frac{f[x_4] - f[x_3]}{x_4 - x_3} = \frac{0 - \frac{1}{2}}{1 - \left(-\frac{2}{3}\right)} = -\frac{3}{2}.$$

Divided differences of order 2:

$$f[x_0; x_1; x_2] = \frac{f[x_1; x_2] - f[x_0; x_1]}{x_2 - x_0} = \frac{\frac{3}{4} - \frac{3}{2}}{0 - (-1)} = -\frac{3}{4},$$

$$f[x_1; x_2; x_3] = \frac{f[x_2; x_3] - f[x_1; x_2]}{x_3 - x_1} = \frac{-\frac{3}{4} - \frac{3}{4}}{\frac{2}{3} - \left(-\frac{2}{3}\right)} = -\frac{9}{8},$$

$$f[x_2; x_3; x_4] = \frac{f[x_3; x_4] - f[x_2; x_3]}{x_4 - x_2} = \frac{\frac{3}{2} - \left(-\frac{3}{4}\right)}{1 - 0} = -\frac{3}{4}.$$

Divided differences of order 3:

$$f[x_0; x_1; x_2; x_3] = \frac{f[x_1; x_2; x_3] - f[x_0; x_1; x_2]}{x_3 - x_0} = \frac{-\frac{9}{8} - \left(-\frac{3}{4}\right)}{\frac{2}{3} - (-1)} = -\frac{9}{40},$$

$$f[x_1;x_2;x_3;x_4] = \frac{f[x_2;x_3;x_4] - f[x_1;x_2;x_3]}{x_4 - x_1} = \frac{-\frac{3}{4} - \left(-\frac{9}{8}\right)}{1 - \left(-\frac{2}{3}\right)} = \frac{9}{40},$$

Divided difference of order 4:

$$f[x_0;x_1;x_2;x_3;x_4] = \frac{f[x_1;x_2;x_3;x_4] - f[x_0;x_1;x_2;x_3]}{x_4 - x_0} = \frac{\frac{9}{40} - \left(-\frac{9}{40}\right)}{1 - (-1)} = \frac{9}{40},$$

The Newton interpolation polynomial is

$$N(x) = f[x_0] + f[x_0;x_1](x - x_0) + f[x_0;x_1;x_2](x - x_0)(x - x_1)+$$

$$+f[x_0;x_1;x_2;x_3](x-x_0)(x-x_1)(x-x_2)+f[x_0;x_1;x_2;x_3;x_4](x-x_0)(x-x_1)(x-x_2)(x-x_3), \quad x \in [-1,1],$$

$$= 0 + \frac{3}{2}(x+1) - \frac{3}{4}(x+1)\left(x + \frac{2}{3}\right) - \frac{9}{40}(x+1)\left(x + \frac{2}{3}\right)(x-0) - \frac{9}{40}(x+1)\left(x + \frac{2}{3}\right)(x-0)\left(x - \frac{2}{3}\right)$$

$$= \frac{9}{40}x^4 - \frac{49}{40}x^2 + 1, \quad x \in [-1,1].$$

We remark that the Newton interpolation polynomial is same with the Lagrange interpolation polynomial.

b) $f\left(-\frac{1}{2}\right) = N\left(-\frac{1}{2}\right) = \frac{9}{40}\left(-\frac{1}{2}\right)^4 - \frac{49}{40}\left(-\frac{1}{2}\right)^2 + 1 = 0.777380,$
$f\left(\frac{1}{3}\right) = N\left(\frac{1}{3}\right) = \frac{9}{40}\left(\frac{1}{3}\right)^4 - \frac{49}{40}\left(\frac{1}{3}\right)^2 + 1 = 0.866666,$
$f(0) = f(x_2) = f_2 = 1,$
$f(2)$ cannot be evaluated, since $2 \notin [-1,1]$.

Example 2. Let be the table

x_i	0	$\frac{1}{6}$	$\frac{1}{2}$	1
f_i	0	$\frac{1}{2}$	1	0

Evaluate $f(z)$, using the Newton interpolation polynomial on the above nodes, where:
$z \in \{\frac{1}{4}; \frac{1}{3}; \frac{1}{2}; 2\}$.
Sol: $\frac{1}{6} \simeq 0.166666$; $f(\frac{1}{4}) = 0.693752$; $f(\frac{1}{3}) = 0.844444$;

Example 3. Let be the table

x_i	-1	0	2	3	4
f_i	-0.3	0.2	0	1.1	1.8

a) Evaluate $f(z)$, using the Newton interpolation polynomial on the above nodes, where:
$z \in \{-2; -1.05; -0.5; 0; 1; 2; 2.995; 4; 67\}$.
b) Evaluate $f(-0.5)$ and $f(1)$ using a Newton interpolation polynomial of degree 3.
Sol: a) $f(-0.5) = 0.225$, $f(1) = -0.24$, $f(2.995) = 1.093846$

Approximation of double integrals with convex polygonal region of integration

Describing the problem: Our goal is to approximate the value of the defined integral

$$I(f) = \iint_{\mathcal{D}} f(x, y) dxdy,$$

where $\mathcal{D}$ is a convex polygonal domain.

The method: If $\mathcal{D}$ is a triangular region of vertices $V_i(x_i, y_i)$, $1 \le i \le 3.$, the double integral $I(f)$ can be approximated using the formula

$$I(f) = \frac{S}{12}\left[f(x_1, y_1) + f(x_2, y_2) + f(x_3, y_3) + 9f(x_G, y_G)\right], \tag{31}$$

where S is the area of the triangle $V_1V_2V_3$ and $G(x_G, y_G) = G\left(\frac{x_1+x_2+x_3}{3}, \frac{y_1+y_2+y_3}{3}\right)$ represents the center of gravity (centroid) of the triangle.

If $\mathcal{D}$ is a convex polygonal region that has more than three vertices, than we use the previous formula and the property of additivity of the integral (we represent $\mathcal{D}$ as a reunion of disjoint triangular regions). Hence the most important part of this method is approximate the value of a double integral over a triangular region and we provide the pseudocode algorithm for it.

Pseudocode Algorithm

1. read $x_1, y_1, x_2, y_2, x_3, y_3$; declare f
2. $l_1 \leftarrow \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$
3. $l_2 \leftarrow \sqrt{(x_2 - x_3)^2 + (y_2 - y_3)^2}$
4. $l_3 \leftarrow \sqrt{(x_3 - x_1)^2 + (y_3 - y_1)^2}$
5. $p \leftarrow (l_1 + l_2 + l_3)/2$
6. $S \leftarrow \sqrt{p(p - l_1)(p - l_2)(p - l_3)}$
7. $I \leftarrow \frac{S}{12} \cdot \left(f(x_1, y_1) + f(x_2, y_2) + f(x_3, y_3) + 9f\left(\frac{x_1+x_2+x_3}{3}, \frac{y_1+y_2+y_3}{3}\right)\right)$
8. write ('The value of integral is ', I)

Remark: We have used Heron's formula to determine the area of our triangular domain, but instead we could apply the formula of area that uses the determinant formed with the coordinates of the vertices and to apply Chio's method for the determinant.

Examples:

1. Approximate $I = \iint_D \sqrt{xy - y^2}dxdy$, where D is the triangle of vertices $V_1(0, 0)$, $V_2(10, 1)$ and $V_3(1, 1)$.
Sol: $I = 5.89$.

2. Approximate $I = \iint_D \frac{\sqrt{y}}{\sqrt{x}(1+xy)}dxdy$, where $D = \{(x, y) \in \mathbb{R}^2 \,|\, 1 \le x \le 3; 0 \le y \le 1\}$.

Euler's method to solve a Cauchy problem

Describing the problem: We consider the Cauchy problem

$$\begin{cases} y' = f(x, y) \\ y(x_0) = y_0. \end{cases} \tag{32}$$

The method: Let $x_0 < x_1 < ... < x_n$, where $x_{i+1} = x_i + h$, $0 \le i \le n-1$. We aim to determine the approximative values of the solution of Cauchy problem (32), denoted by y_i, where $y_i \simeq y(x_i)$, $0 \le i \le n$.
The formulae are:

$$\begin{cases} x_{i+1} = x_i + h \\ y_{i+1} = y_i + hf(x_i, y_i),\ 0 \le i \le n-1. \end{cases}$$

Remark: In the algorithm, the values $y_1, y_2, ..., y_n$, are computed, each, within an error ε.

Pseudocode Algorithm

1. read x_i, $0 \le i \le n$, y_0, ε; declare f;
2. $i \leftarrow 0$
3. repeat
   3.1. $x \leftarrow x_i$; $xx \leftarrow x_{i+1}$; $y \leftarrow y_i$
   3.2. $h \leftarrow xx - x$;
   3.3. $yy \leftarrow y + h \cdot f(x, y)$;
   3.4. repeat
      3.4.1. $h \leftarrow \frac{h}{2}$
      3.4.2. $aux \leftarrow yy$
      3.4.3. while $x < xx$
         3.4.3.1. $y \leftarrow y + h \cdot f(x, y)$
         3.4.3.2. $x \leftarrow x + h$
      3.4.4. $yy \leftarrow y$; $x \leftarrow x_i$; $y \leftarrow y_i$
      until $|yy - aux| \le \varepsilon$
   3.5. $y_{i+1} \leftarrow yy$;
   3.6. write 'The approximative value of solution in', xx 'is', yy
   3.7. $i \leftarrow i + 1$;
until $i = n$

Example: Let

$$\begin{cases} y' = \frac{2y}{x} \\ y(1) = 1. \end{cases}$$

We consider $x_i = 1 + 0.1 \cdot i$, $0 \le i \le 5$. Find the values y_1, y_2, y_3, y_4, y_5 which approximate $y(1.1)$, $y(1.2)$, $y(1.3)$, $y(1.4)$, $y(1.5)$.
Sol: For $\varepsilon = 10^{-4}$, we obtain
$y_1 = 1.209957$
$y_2 = 1.439906$
$y_3 = 1.689847$
$y_4 = 1.959781$
$y_5 = 2.249707$.
The exact values of the solution $y = x^2$ are: 1.21; 1.44; 1.69; 1.96; 2.25.