Task 4. LU decomposition of square matrix with partial pivoting

e-mail: andrzej.kedziorski@fizyka.umk.pl
tel.: 56611-3274
pokój: 485B
http://www.fizyka.umk.pl/~tecumseh/EDU/MNII/

Task 4

Write a program that performs LU decomposition of a square matrix **A** using Doolittle or Crout method. The program gets the dimension of the matrix **A** and its elements from the input. Modify the LU decomposition program using the Doolittle (or Crout) method to include partial pivoting.

LU decomposition

- **A** - non-singular square real matrix $n \times n$
- $\det \mathbf{A}_k \neq 0$, where $\mathbf{A}_k$ is $k \times k$ submatrix constructed from first k rows and columns of **A** matrix
- $\mathbf{A} = \mathbf{LU}$ decomposition/factorization, where **L** is **L**ower triangular matrix of $n \times n$ size, **U** is **U**pper triangular matrix of $n \times n$ size, i.e.

$$(\mathbf{L})_{ij} = \begin{cases} 0 & i < j \\ \ell_{ij} & i \geqslant j \end{cases} \qquad (\mathbf{U})_{ij} = \begin{cases} u_{ij} & i \leqslant j \\ 0 & i > j \end{cases}$$

- We have n^2 equations for the elements of **A**

$$a_{ij} = \sum_{k=1}^{n} (\mathbf{L})_{ik} (\mathbf{U})_{kj} = \sum_{k=1}^{r} \ell_{ik} u_{kj},$$

  where $r = \min(i, j)$ and $n^2 + n$ elements of **L** and **U** matrices
- However, if $\ell_{ii} = 1$ or $u_{ii} = 1$ for $i = 1, ..., n$, then we have in total exactly n^2 elements of **L** and **U** matrices to calculate.

Doolittle method

- Assume that $\ell_{ii} = 1$ for $i = 1, \ldots, n$
- We have to perform $k = 1, \ldots, n$ steps; within k-th step
  1. Calculate k-th row of **U** matrix ($j \geqslant k$)

$$a_{kj} = \sum_{p=1}^{k} \ell_{kp} u_{pj} \quad \Rightarrow \quad u_{kj} = a_{kj} - \sum_{p=1}^{k-1} \ell_{kp} u_{pj} \quad j = k, k+1, \ldots, n$$

  2. Calculate k-th column of **L** matrix ($i > k$)

$$a_{ik} = \sum_{p=1}^{k} \ell_{ip} u_{pk} \quad \Rightarrow \quad \ell_{ik} = \left(a_{ik} - \sum_{p=1}^{k-1} \ell_{ip} u_{pk} \right) / u_{kk} \quad i = k+1, \ldots, n$$

- In first step we in fact rewrite the first row of **A** matrix to first row of **U** matrix and, subsequently, we have all required data to evaluate first column of **L** matrix
- Within k-th step we have $\ell_{kk} = 1$, and $k-1$ first rows of **U** matrix and $k-1$ first columns of **L** matrix, which allows to calculate k-th row of **U** and, subsequently, we can calculate k-th column of **L**

Crouta method

- Assume that $u_{ii} = 1$ for $i = 1, \ldots, n$
- We have to perform $k = 1, \ldots, n$ steps; within k-th step
  1. Calculate k-th column of **L** matrix ($i \geqslant k$)

$$a_{ik} = \sum_{p=1}^{k} \ell_{ip} u_{pk} \quad \Rightarrow \quad \ell_{ik} = a_{ik} - \sum_{p=1}^{k-1} \ell_{ip} u_{pk} \quad i = k, k+1, \ldots, n$$

  2. Calculate k-th row of **U** matrix ($j > k$)

$$a_{kj} = \sum_{p=1}^{k} \ell_{kp} u_{pj} \quad \Rightarrow \quad u_{kj} = \left(a_{kj} - \sum_{p=1}^{k-1} \ell_{kp} u_{pj} \right) / \ell_{kk} \quad j = k+1, \ldots, n$$

- In first step we in fact rewrite the first column of **A** matrix to first column of **L** matrix and, subsequently, we have all required data to evaluate first row of **U** matrix
- Within k-th step we have $u_{kk} = 1$, $k-1$ first columns of **L** matrix and $k-1$ first rows of **U** matrix, which allows to calculate k-th column of **L** and, subsequently, we can calculate k-th row of **U**

TO DO

1. From the input[1] read size n and the elements of $\mathbf{A}$ matrix
2. Perform LU decomposition of $\mathbf{A}$ matrix using Doolittle or Crout method
3. Print on the output the triangular matrices $\mathbf{L}$ and $\mathbf{U}$
4. Check $\mathbf{A} = \mathbf{LU}$
5. Compare the results using existing functions (e.g. "lu" in Matlab)

[1] Or from file

Partial pivoting - motivations

- Perform LU decomposition of matrix

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

- Interchange rows in $\mathbf{A}$ matrix

$$\mathbf{A}' = \begin{pmatrix} 1 & 1 & 1 \\ 3 & 3 & -3 \\ 2 & -2 & 2 \end{pmatrix}$$

  and perform LU decomposition of matrix $\mathbf{A}'$

- Is it possible to perform LU decomposition in both cases?

Partial pivoting in Doolittle method

- k-th step of Doolittle method
  1. Calculate k-th row of $\mathbf{U}$ matrix ($j \geqslant k$)

$$u_{kj} = a_{kj} - \sum_{p=1}^{k-1} \ell_{kp} u_{pj} \quad j = k, k+1, \ldots, n$$

  2. Calculate k-th column of $\mathbf{L}$ matrix ($i > k$)

$$\ell_{ik} = \left(a_{ik} - \sum_{p=1}^{k-1} \ell_{ip} u_{pk} \right) / u_{kk} \quad i = k+1, \ldots, n$$

- Problems: $u_{kk} = 0$ or $|u_{kk}| \sim 0$ (e.g. "numerical trash")
- Partial pivoting:
  1 calculate k-th row of $\mathbf{U}$ matrix
  1a before the calculation of k-th column of $\mathbf{L}$ matrix we look in k-th row of $\mathbf{U}$ matrix for the element of maximum absolute value, i.e.

$$\max_{j=k,\ldots,n} |u_{kj}| \Rightarrow u_{kj_{\max}}$$

  1b interchange columns k and $j_{\max}$ of $\mathbf{U}$ matrix (also in $\mathbf{A}$)
  2 calculate k-th column of $\mathbf{L}$ matrix

Doolittle method with partial pivoting

- We obtain $\mathbf{A}' = \mathbf{LU}$ decomposition, in which $\mathbf{A}'$ is the $\mathbf{A}$ matrix, in which we have interchanged columns
- $\mathbf{A}'$ matrix can be represented as $\mathbf{A}' = \mathbf{A}\mathbf{P}^{Tr}$, where $\mathbf{P}$ is the permutation matrix; $\mathbf{P}$ is orthogonal, i.e. $\mathbf{P}^{Tr} = \mathbf{P}^{-1}$
- Decomposition of $\mathbf{A}$ takes the following form

$$\mathbf{A}' = \mathbf{A}\mathbf{P}^{Tr} = \mathbf{LU} \quad | \cdot \mathbf{P}$$
$$\mathbf{A} = \mathbf{LUP}$$

- Single interchange of the columns i and j of $\mathbf{U}$ (as well as $\mathbf{A}$) matrix can be represented by the following matrix product $\mathbf{U}\mathbf{P}^{ij}$ (as well as $\mathbf{A}\mathbf{P}^{ij}$), where $\mathbf{P}^{ij}$ is the unit matrix $n \times n$, in which we have interchanged columns i and j
- In each step $k = 1, \ldots, n-1$ of Doolittle method we perform (up to) single interchange of the columns of $\mathbf{U}$ and $\mathbf{A}$ matrices, thus the final result may be written in the following way

$$\mathbf{LUP} = \mathbf{LUP}_{n-1}\mathbf{P}_{n-2}...\mathbf{P}_{k}...\mathbf{P}_{2}\mathbf{P}_{1},$$

where $\mathbf{P}_k$ is the matrix representing single interchange of the columns performed in k-th step of Doolittle method [2]

[2] In practice, the permutation matrix $\mathbf{P}$ can be obtained starting from unit matrix by the successive interchanges of the appropriate pairs of rows

Parial pivoting in Crout method

- k-th step of Crout method
  1. Calculate k-th column of $\mathbf{L}$ matrix ($i > k$)

$$\ell_{ik} = a_{ik} - \sum_{p=1}^{k-1} \ell_{ip} u_{pk} \quad i = k+1, \ldots, n$$

  2. Calculate k-th ro of $\mathbf{U}$ matrix ($j \geqslant k$)

$$u_{kj} = \left(a_{kj} - \sum_{p=1}^{k-1} \ell_{kp} u_{pj} \right) / \ell_{kk} \quad j = k, k+1, \ldots, n$$

- Problems: $\ell_{kk} = 0$ or $|\ell_{kk}| \sim 0$ (e.g. "numerical trash")
- Partial pivoting:

  1 calculate k-th column of $\mathbf{L}$ matrix

  1a before the calculation of k-th row of $\mathbf{U}$ matrix we look in k-th column of $\mathbf{L}$ matrix for the element of the maximum absolute value, i.e.

$$\max_{i=k,\ldots,n} |\ell_{ik}| \Rightarrow \ell_{i_{\max} k}$$

  1b interchange rows k and $i_{\max}$ in $\mathbf{L}$ matrix (also in $\mathbf{A}$)

  2 calculate k-th row of $\mathbf{U}$ matrix

Partial pivoting in Crout method

- We obtain $\mathbf{A}' = \mathbf{LU}$, where $\mathbf{A}'$ is the $\mathbf{A}$ matrix with permuted rows
- $\mathbf{A}'$ matrix can be represented as $\mathbf{A}' = \mathbf{P}^{Tr}\mathbf{A}$, where $\mathbf{P}$ is the premutation matrix; $\mathbf{P}$ is orthogonal, i.e. $\mathbf{P}^{Tr} = \mathbf{P}^{-1}$
- Decomposition of $\mathbf{A}$ matrix takes the form

$$\mathbf{P}\cdot| \quad \mathbf{P}^{Tr}\mathbf{A} = \mathbf{LU}$$

$$\mathbf{A} = \mathbf{PLU}$$

- Single interchange of the columns i and j in matrix $\mathbf{L}$ (and $\mathbf{A}$) can be represented by the matrix product $\mathbf{P}^{ij}\mathbf{L}$ (and $\mathbf{P}^{ij}\mathbf{A}$), where $\mathbf{P}^{ij}$ is the unit matrix $n \times n$ with interchanged rows i and j
- In each step $k = 1, \ldots, n - -1$ of Crout method we perform (up to) single interchange of rows in $\mathbf{L}$ (and $\mathbf{A}$) matrix, thus the final result may be written in the following way

$$\mathbf{PLU} = \mathbf{P}_1\mathbf{P}_2 \ldots \mathbf{P}_k \ldots \mathbf{P}_{n-2}\mathbf{P}_{n-1}\mathbf{LU},$$

  where $\mathbf{P}_k$ is the matrix representing single interchange of rows in k-th step of Crout method [3]

[3] In practice, the permutation matrix $\mathbf{P}$ can be obtained starting from unit matrix by the successive interchanges of the appropriate pairs of columns

TO DO - inclusion of partial pivoting into the program performing LU decomposition

1. From the input[4] read size n and the elements of $\mathbf{A}$ matrix
2. Perform LU decomposition of $\mathbf{A}$ matrix using Doolittle or Crout method with partial pivoting
3. Print on the output the triangular matrices $\mathbf{L}$, $\mathbf{U}$ and permutaion matrix $\mathbf{P}$
4. Check $\mathbf{A} = \mathbf{LUP}$ (or $\mathbf{A} = \mathbf{PLU}$)
5. Compare the results using existing functions (e.g. "lu" in Matlab)

[4] Or from file