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Linear System Of Equations.
Part 2

Calcoli di Processo dell' Ingegneria Chimica

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Linear System Of Equations

In mathematics, and particularly in linear algebra, a system of linear equations, also called a linear system, is a system composed of several linear equations that must all be verified simultaneously. A solution of the system is a vector whose elements are the solutions of the equations that make up the system, that is, such that when substituted for the unknowns make the equations identities.

From the classical representation to the **matricial** form:

$$\begin{bmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & \dots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & \dots & a_{n,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$\underline{\underline{A}}\,\underline{x} = \underline{b} \quad \longrightarrow \quad \underline{x} = \underline{\underline{A}}^{-1}\,\underline{b}$$

Problem!?

What if the element on which we have to compute the coefficient for the factorization is equal to zero?

PIVOTING!

We call ***pivot*** the first non-zero element encountered in each row in a stepped matrix.

$$A = \begin{bmatrix} 0 & 5 & 7 & 4 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 22 \end{bmatrix}$$

$$a_{1,2} = 5; \quad a_{2,3} = -2; \quad a_{3,4} = 22$$

Pivoting(s)

Trivial Pivoting:

if $a_{k,k}^{(k-1)} = 0$ take the first row p under the row k for which the element $a_{p,k}^{(k-1)} \neq 0$ then we will swap the row p with the row k.

Global Pivoting:

At the $k-th$ iteration the pivot is the maximum coefficient among all the ones that are left.

$$|a_{p,q}^{(k-1)}| = \max_{k<i<n, k<j<n} \left(|a_{i,j}^{(k-1)}| \right)$$

- If $p \neq k$ the row p is swapped with the row k.
- If $q \neq k$ the column q is swapped with the column k
- If the rows are swapped, then the elements of the constant terms **b** are also swapped accordingly
- If the columns are swapped, then the elements of the unknown **x** are also swapped accordingly.

Partial Pivoting:

at the $k-th$ iteration the pivot is the maximum coefficient among the elements in the $k-th$ column:

$$|a_{p,q}^{(k-1)}| = \max_{k<i<n}\left(|a_{i,k}^{(k-1)}|\right)$$

- If $p \neq k$ the row p is swapped with the row k.
- If the rows are swapped, then the elements of the constant terms $\mathbf{b}$ are also swapped accordingly.

The **global pivot** is the most effective strategy for limiting the numerical errors, the **partial pivot** does not guarantee the same accuracy. Often, though, the difference between the two is often negligible so the partial pivot is generally preferred because of the lower computational burden.

Scaled Partial Pivoting:

At the $k-th$ iteration the index p is determined:

$$|a_{p,k}^{(k-1)}| = \max_{k<i<n} \frac{|a_{i,k}^{(k-1)}|}{\max\limits_{k<j<n} |a_{i,j}^{(k-1)}|}$$

If $p \neq k$ the row p is swapped with the row k without doing any further balancing which can introduce other rounding errors. The key step is then finding the index p which determines the optimal pivot.

Applying a further balancing potentially can introduce additional unnecessary rounding errors that could be potentially cancel out all the benefits gained by the balancing itself.

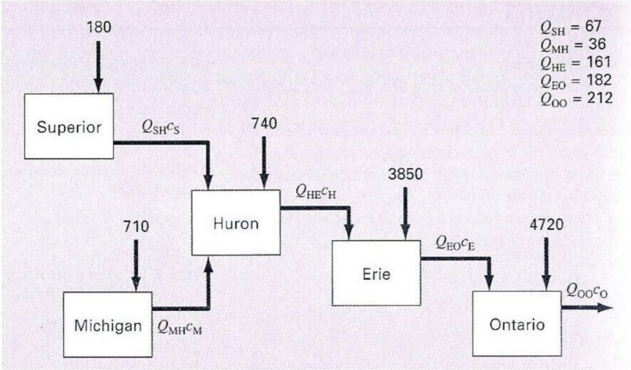
Exercises

- Write a MATLAB function to perform the Gauss Elimination with partial pivoting.
- Write a MATLAB function to perform the Gauss Elimination with balanced partial pivoting.
- Given the system of equations reported below:

$$\begin{bmatrix} 1 & 2 & 3 \\ 40 & 50 & 60 \\ 160 & 25 & 30 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

  Solve it employing the Gauss elimination method with and without partial pivoting paying attention to employ two significant figures. And compare the solution in double precision with the one obtained with MATLAB ($x_1 = 0.0036; x_2 = -1.9071; x_3 = 1.6036$)

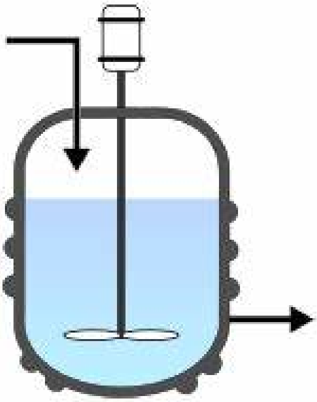
- Chloride, often used as an indicator of pollution, has increased in concentration throughout the Great Lakes during the past century. Let's write a Matlab program that estimates the concentration of chloride in the Great Lakes given the following data.



	OutFlow $[Gm^3/year]$	Chloride load $[tonn/year]$	Volume $[km^3]$
Superior	67	180	12000
Michigan	36	710	4900
Huron	161	740	3500
Erie	182	3850	480
Ontario	212	4720	1640

- A Perfectly Stirred Reactor (PSR) is a type of continuous reactor characterized by a uniform internal composition, maintained through perfect mixing. Consequently, the composition of the exiting stream is identical to that within the reactor. At steady-state operation, the species balance for component *i* can be expressed through the following equation:

$$Q_{in}C_i^0 - Q_{out}C_i = \nu_i RV$$



Here, R represents the cumulative sum of all rates of formation or destruction, adjusted by the appropriate coefficients. If the density remains constant, the equations can be formulated as follows:

$$\frac{C_i^0 - C_i}{\tau} = \nu_i R$$

We will consider the following irreversible reactions taking place:

- $R1: \; A \longrightarrow B, \; K1 = 0.2$
- $R2: \; B \longrightarrow C, \; K2 = 0.1$
- $R3: \; B \longrightarrow D, \; K3 = 0.2$
- $R4: \; A \longrightarrow D, \; K4 = 0.3$

Now the system to be solved is:

$$\begin{cases} C_{A,0} = C_A\left(1 + \tau K_1 + \tau K_4\right) \\ C_{B,0} = -C_A\left(\tau K_1\right) + C_B\left(1 + \tau K_2 + \tau K_3\right) \\ C_{C,0} = -C_B\left(\tau K_2\right) + C_C \\ C_{D,0} = -C_A\left(\tau K_4\right) - C_B\left(\tau K_3\right) + C_D C_{A,0} = C_A\left(1 + \tau K_1 + \tau K_4\right) \end{cases}$$

With $\tau = 1$s find the solution for the different inlet compositions reported below:

	1	2	3	4	5	6
$C_{A,0}$	1	0.5	0.5	0.7	0.4	0.25
$C_{B,0}$	0	0.5	0.25	0.2	0.4	0.25
$C_{C,0}$	0	0	0.25	0	0.2	0.25
$C_{D,0}$	0	0	0	0.1	0	0.25

Now modify the script for the previous excersize in order to express the kinetic constant using the arrhenius formulation in a window of temperature between (450-650 K):

- $K1 = 1e8 \times exp(-20000/1.987/T)$
- $K2 = 1e6 \times exp(-15000/1.987/T)$
- $K3 = 1e11 \times exp(-27000/1.987/T)$
- $K4 = 1e9 \times exp(-23000/1.987/T)$

Thank you for the attention!