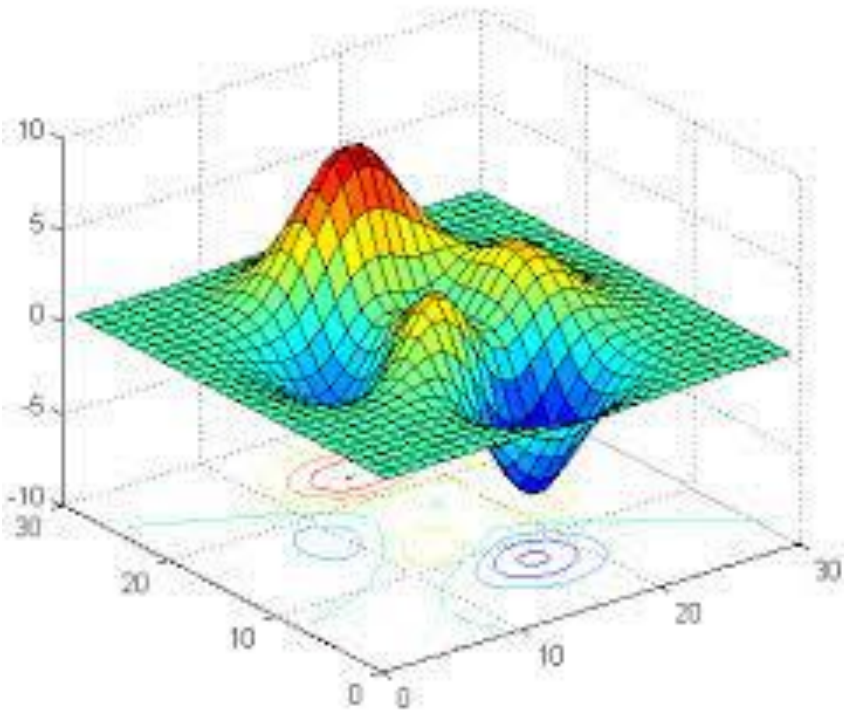
Khemis Miliana University
Faculty of Sciences of Matter and Computer Science
Department of Physics

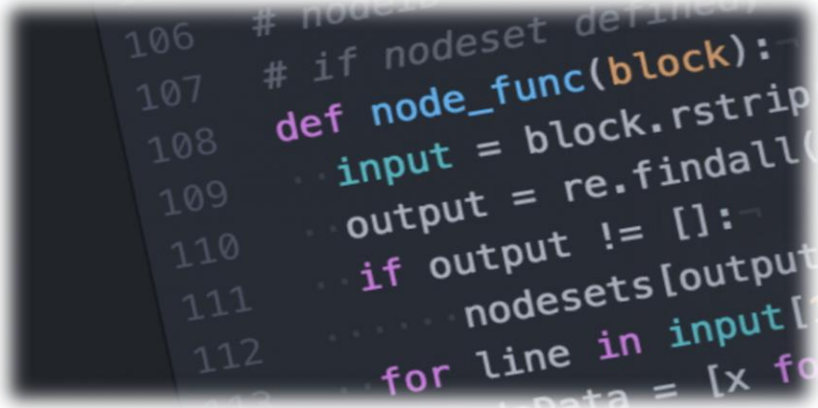


Numerical Methods & Scientific Programming

Dr. Salah-Eddine BENTRIDI
s.bentridi@univ-dbkm.dz
Univ. Khemis-Miliana

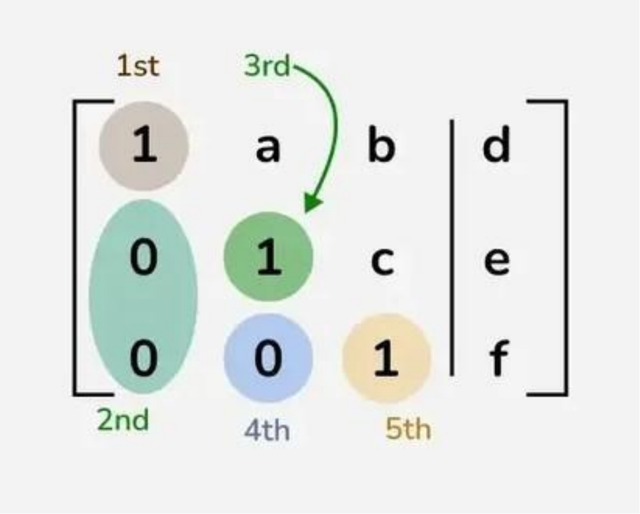
Content of the program

- Chapter 01: ***Initiation to a programming language (Python)***
  - ***Hands-on-Pythn; Basics of Python***
- Chapter 02: ***Numerical Integration***
  - ***Trapezoidal rule; Simpson's method***
- Chapter 03: ***Numerical Solution of equations – Root finding***
  - ***Bisection method; Newton's Method***
- Chapter 04: ***Numerical resolution of differential equations***
  - ***Euler's method; Runge-Kutta method***
- Chapter 05: ***Numerical resolution of linear systems***
  - ***Gauss method, Gauss-Seidel method***



Chapter 05: Numerical resolution of linear systems

Euler's method and Runge-Kutta method



Dr. Salah-Eddine BENTRIDI

s.bentridi@univ-dbkm.dz

Khemis-Miliana University

Outline

- Solutions to Systems of Linear Equations
- Gauss Elimination Method
- Gauss-Seidel Method

I. Solutions to Systems of Linear Equations

- *Consider a system of linear equations in matrix form, $\boldsymbol{Ax = y}$, where $\boldsymbol{A}$ is an $\boldsymbol{m \times n}$ matrix.*
- *Recall that this means there are $\boldsymbol{m}$ equations and $\boldsymbol{n}$ unknowns in our system.*
- *A solution to a system of linear equations is an $\boldsymbol{x}$ in $\mathbb{R}^{\boldsymbol{n}}$ that satisfies the matrix form equation.*
- *Depending on the values that populate $\boldsymbol{A}$ and $\boldsymbol{y}$, there are three distinct solution possibilities for $\boldsymbol{x}$:*
    - *Either there is no solution for $\boldsymbol{x}$,*
    - *or there is one, unique solution for $\boldsymbol{x}$,*
    - *or there are an infinite number of solutions for $\boldsymbol{x}$.*
- *Let's consider the first case*

I. Solutions to Systems of Linear Equations

The study case: There is a unique solution for x.

- *If* $\boldsymbol{rank([A,y]) = rank(A)}$*, then* $\boldsymbol{y}$ *can be written as a linear combination of the columns of* $\boldsymbol{A}$ *and there is at least one solution for the matrix equation.*
- *For there to be only one solution,* $\boldsymbol{rank(A) = n}$ *must also be true.*
- *In other words, the number of equations must be exactly equal to the number of unknowns.*

I. Solutions to Systems of Linear Equations

The study case: There is a unique solution for x.

- *To see why this property results in a unique solution, consider the following three relationships between* $\boldsymbol{m}$ *nd* $\boldsymbol{n}$: $\boldsymbol{m < n, m = n, and\ m > n}$:
  - *For the case where* $\boldsymbol{m < n}$ *,* $\boldsymbol{rank(A) = n}$ *cannot possibly be true because this means we have a "fat" matrix with fewer equations than unknowns.*
  - *Thus, we do not need to consider this subcase.*

I. Solutions to Systems of Linear Equations

The study case: There is a unique solution for x.

- *To see why this property results in a unique solution, consider the following three relationships between* $\boldsymbol{m}$ *nd* $\boldsymbol{n}$: $\boldsymbol{m < n, m = n, and\ m > n}$:
  - *When* $\boldsymbol{m = n}$ *and* $\boldsymbol{rank(A) = n}$*, then* $\boldsymbol{A}$ *is square and invertible. Since the inverse of a matrix is unique, then the matrix equation* $\boldsymbol{Ax = y}$ *can be solved by multiplying each side of the equation, on the left, by* $\boldsymbol{A^{-1}}$*.*
  - *This results in* $\boldsymbol{A^{-1}Ax = A^{-1}y \rightarrow Ix = A^{-1}y \rightarrow x = A^{-1}y}$*, which gives the unique solution to the equation.*

I. Solutions to Systems of Linear Equations

The study case: There is a unique solution for x.

- *To see why this property results in a unique solution, consider the following three relationships between* m *nd* n: $m < n, m = n, and\ m > n$:
  - *If* $m > n$ *, then there are more equations than unknowns.*
  - *However, if* $rank(A) = n$*, then it is possible to choose* n *equations (i.e., rows of* A*) such that if these equations are satisfied, then the remaining* $m - n$ *equations will be also satisfied.*
  - *In other words, they are redundant. If the* $m - n$ *redundant equations are removed from the system, then the resulting system has an* A *matrix that is* $n \times n$*, and invertible.*
  - *These facts are not proven in this text. The new system then has a unique solution, which is valid for the whole system.*

I. Solutions to Systems of Linear Equations

In what follows, we will only discuss how we solve a systems of equations when it has unique solution.

Let's say we have n equations with n variables, $\mathbf{A}\boldsymbol{x} = \boldsymbol{y}$, as shown in the following:

$$\begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n,1} & a_{n,2} & \cdots & a_{n,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{bmatrix}$$

II. Gauss Elimination Method

The Gauss Elimination method is a procedure to turn matrix A into an upper triangular form to solve the system of equations. Let's use a system of 4 equations and 4 variables to illustrate the idea. The Gauss Elimination essentially turning the system of equations to:

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\ 0 & a'_{2,2} & a'_{2,3} & a'_{2,4} \\ 0 & 0 & a'_{3,3} & a'_{3,4} \\ 0 & 0 & 0 & a'_{4,4} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y'_2 \\ y'_3 \\ y'_4 \end{bmatrix}$$

II. Gauss Elimination Method

By turning the matrix form into this, we can see the equations turn into:

$$
\begin{array}{ccccccccc}
a_{1,1}x_1 & + & a_{1,2}x_2 & + & a_{1,3}x_3 & + & a_{1,4}x_4 & = & y_1, \\
 & & a'_{2,2}x_2 & + & a'_{2,3}x_3 & + & a'_{2,4}x_4 & = & y'_2 \\
 & & & & a'_{3,3}x_3 & + & a'_{3,4}x_4 & = & y'_3, \\
 & & & & & & a'_{4,4}x_4 & = & y'_4.
\end{array}
$$

- **We can see by turning into this form, x_4 can be easily solved by dividing both sides a'_{44}, then we can back substitute it into the 3^{rd} equation to solve x_3.**
- **With x_3 and x_4, we can substitute them into the 2^{nd} equation to solve x_2 . Finally, we can get all the solution for x**
- **We solve the system of equations from bottom-up, this is called *backward substitution*. Note that, if A is a lower triangular matrix, we would solve the system from top-down by *forward substitution*.**

II. Gauss Elimination Method

Let's work on an example to illustrate how we solve the equations using Gauss Elimination.

$$\begin{aligned} 4x_1 + 3x_2 - 5x_3 &= 2 \\ -2x_1 - 4x_2 + 5x_3 &= 5 \\ 8x_1 + 8x_2 &= -3 \end{aligned}$$

- **Step 1: Turn these equations to matrix form $\boldsymbol{Ax = y}$**

$$\begin{bmatrix} 4 & 3 & -5 \\ -2 & -4 & 5 \\ 8 & 8 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 5 \\ -3 \end{bmatrix}$$

II. Gauss Elimination Method

$$\begin{aligned} 4x_1 + 3x_2 - 5x_3 &= 2 \\ -2x_1 - 4x_2 + 5x_3 &= 5 \\ 8x_1 + 8x_2 &= -3 \end{aligned}$$

- **Step 3: Now we start to eliminate the elements in the matrix, we do this by choose a pivot equation, which is used to eliminate the elements in other equations. Let's choose the first equation as the pivot equation and turn the 2^{nd} row first element to 0. To do this, we can multiply -0.5 for the 1^{st} row (pivot equation) and subtract it from the 2^{nd} row. The multiplier $is\ m_{21} = -0.5$. We will get**

$$\begin{bmatrix} 4 & 3 & -5 & 2 \\ 0 & -2.5 & 2.5 & 6 \\ 8 & 8 & 0 & -3 \end{bmatrix}$$

II. Gauss Elimination Method

$$\begin{aligned} 4x_1 + 3x_2 - 5x_3 &= 2 \\ -2x_1 - 4x_2 + 5x_3 &= 5 \\ 8x_1 + 8x_2 &= -3 \end{aligned}$$

- Step 4: Turn the 3^{rd} row first element to 0. We can do something similar, multiply 2 to the 1^{st} row and subtract it from the 3^{rd} row. The multiplier is $m_{31} = 2$. We will get:

$$\begin{bmatrix} 4 & 3 & -5 & 2 \\ 0 & -2.5 & 2.5 & 6 \\ 0 & 2 & 10 & -7 \end{bmatrix}$$

- Step 5: Turn the 3^{rd} row 2^{nd} element to 0. We can multiple by $-4/5$ for the 2^{nd} row, and subtract it from the 3^{rd} row. The multiplier is $m_{32} = -0.8$. We will get:

$$\begin{bmatrix} 4 & 3 & -5 & 2 \\ 0 & -2.5 & 2.5 & 6 \\ 0 & 0 & 12 & -2.2 \end{bmatrix}$$

II. Gauss Elimination Method

- Step 6: Therefore, we can get $x_3 = -2.2/12 = -0.183$.
- Step 7: Insert x_3 to the 2^{nd} equation, we get $x_2 = -2.583$
- Step 8: Insert x_2 and x_3 to the first equation, we have $x_1 = 2.208$.

We are using "pivoting" Gauss Elimination method here, but you should know that there is also a "naive" Gauss Elimination method with the assumption that pivot values will never be zero.

$$\begin{aligned} 4x_1 + 3x_2 - 5x_3 &= 2 \\ -2x_1 - 4x_2 + 5x_3 &= 5 \\ 8x_1 + 8x_2 &= -3 \end{aligned}$$

II. Gauss Elimination Method

- Step 6: Therefore, we can get $x_3 = -2.2/12 = -0.183$.
- Step 7: Insert x_3 to the 2^{nd} equation, we get $x_2 = -2.583$
- Step 8: Insert x_2 and x_3 to the first equation, we have $x_1 = 2.208$.

We are using "pivoting" Gauss Elimination method here, but you should know that there is also a "naive" Gauss Elimination method with the assumption that pivot values will never be zero.

$$
\begin{aligned}
4x_1 + 3x_2 - 5x_3 &= 2 \\
-2x_1 - 4x_2 + 5x_3 &= 5 \\
8x_1 + 8x_2 &= -3
\end{aligned}
$$

III. Gauss-Seidel Method

- **The above method is a direct method, in which we compute the solution with a finite number of operations. In this section, we will introduce a different class of methods, the iterative methods, or indirect methods. It starts with an initial guess of the solution and then repeatedly improve the solution until the change of the solution is below a threshold. In order to use this iterative process, we need first write the explicit form of a system of equations. If we have a system of linear equations:**

$$\begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_m \end{bmatrix}$$

III. Gauss-Seidel Method

- **The above method is a direct method, in which we compute the solution with a finite number of operations. In this section, we will introduce a different class of methods, the iterative methods, or indirect methods. It starts with an initial guess of the solution and then repeatedly improve the solution until the change of the solution is below a threshold. In order to use this iterative process, we need first write the explicit form of a system of equations. If we have a system of linear equations:**

$$\begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_m \end{bmatrix}$$

we can write its explicit form as:

$$x_i = \frac{1}{a_{i,i}} \left[y_i - \sum_{j=1, j \neq i}^{j=n} a_{i,j} x_j \right]$$

III. Gauss-Seidel Method

- The Gauss-Seidel Method is a specific iterative method, that is always using the latest estimated value for each elements in x.
- For example, we first assume the initial values for $x_2, x_3, \cdots, x_n$ (except for x_1), and then we can calculate x_1.
- Using the calculated x_1 and the rest of the x (except for x_2), we can calculate x_2.
- We can continue in the same manner and calculate all the elements in x. This will conclude the first iteration.
- We can see the unique part of Gauss-Seidel method is that we are always using the latest value for calculate the next value in x.
- We can then continue with the iterations until the value converges.