

System of linear equations

Numerical methods used to solve such problem allow to introduce and experiment on [Time_complexity](#), considering cubic time behavior of standard algorithms and *i.e.* quadratic time solutions using LU decomposition.

Theory

- [System_of_linear_equations](#)
- [Gaussian_elimination](#), Gauss and Gauss-Jordan eliminations (diagonalization, triangularization)
- [Pivot_element](#), pivoting
- [LU_decomposition](#)
 - [Triangular_matrix#Forward_and_back_substitution](#)
- Chapter 2 in the book "Numerical Recipes" :
 - 2.0 Introduction
 - 2.1 Gauss-Jordan Elimination
 - 2.2 Gaussian Elimination with Backsubstitution
 - 2.3 LU Decomposition and Its Application
- Python NumPy library : [NumPy Reference](#)
 - [Linear algebra \(numpy.linalg\) : numpy.linalg.solve](#)
- Time complexity analysis
 - Hint : in Python, use the timeit module

Jupyter notebooks

- Example file (to be continued) :
https://notebooks.azure.com/linusable/libraries/samples-public/html/notebooks/calculation_methods_applied_to_chemistry/Gauss-Jordan-01.ipynb


Exercices and applications

- Exercices :
 - write a python function for diagonalisation with partial pivoting
 - random numbers → linear systems
 - comparison with numpy standard library
 - measurements of execution time to check cubic complexity

1D problems with neighbours

- Thermal diffusion and chemical diffusion (transient or stationary) on a regular 1D space with equidistant steps. ODE equations can be written such a given evolution equation for node # i

only implies nodes $i+1$ and $i-1$

- Using  [tridiagonal Thomas algorithm](#) allows to save computational time thanks to n complexity
- ? Python library with Thomas algorithm

What you must have learned in this chapter

- Except ill-conditioned, linear systems can be solved “exactly” using linear algebra algorithms in a finite and known number of arithmetic operations.
- The accuracy is determined by the number of numerical figures which are encoded in floating point description
- For a general system of n equations, diagonalisation requires of the order of n^3 operations. Also for solving a system using these method.
- If the coefficient matrix is the same for different systems (only the independent coefficients are different), it is possible to solve systems with the order of n^2 operations, if the matrix of coefficients is decomposed in the product of two triangular matrix (Lower-Upper decomposition). This n^3 step is realised only once.

References :

- Numerical recipes, The Art of Scientific Computing 3rd Edition, William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, 2007, isbn: 9780521880688
 - <http://numerical.recipes/>
 - in C : <http://apps.nrbook.com/c/index.html>
 - http://www2.units.it/ipl/students_area/imm2/files/Numerical_Recipes.pdf
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