







# Numerical integration

Calculation of definite integrals implies to replace the function by another one (usually a polynomial form) which is a good approximation and easier to compute.  **Error estimation** depends on parameters of the method and refinement of spatial grid discretization. It is interesting to check these errors using various algorithm and mesh resolution.

- Equally spaced methods :
  -  [Numerical\\_integration](#)
  -  [Trapezoidal\\_rule](#)
  -  [Newton-Cotes\\_formulas](#)
  -  [Simpson's rule and composite Simpson's rule](#)
- If intervals between interpolation points vary :
  -  [Gaussian\\_quadrature](#)
- Chapter 4 in the book "Numerical Recipes" : Integration of Functions
  - 4.0 Introduction
  - 4.1 Classical Formulas for Equally Spaced Abscissas
  - 4.2 Elementary Algorithms
  - 4.5 Gaussian Quadratures and Orthogonal Polynomials
- Python SciPy library : [SciPy Reference](#)
  - [Integration \(scipy.integrate\)](#)

## Applications

- Perform better integration calculus compare to [Employing Spreadsheets for Applying Calculus in Upper-Level Chemistry Courses](#) Paul D. Cooper, J. Chem. Educ., 2018, 95 (10), pp 1890–1893  
DOI: 10.1021/acs.jchemed.8b00193

## Références

- 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](http://www2.units.it/ipl/students_area/imm2/files/Numerical_Recipes.pdf), p 129...
  - <http://apps.nrbook.com/empanel/index.html#>

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