

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. [W](#)[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 :
 - [W](#)[Numerical_integration](#)
 - [W](#)[Trapezoidal_rule](#)
 - [W](#)[Newton-Cotes_formulas](#)
 - [W](#)[Simpson's rule and composite Simpson's rule](#)
- If intervals between interpolation points vary :
 - [W](#)[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, p 129...
 - <http://apps.nrbook.com/empanel/index.html#>

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