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/
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