Numerical integration using Gaussian quadrature- and Monte Carlo methods

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Abstract

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I. Introduction

Integrals play a huge role in science. Many of the integrals we encounter are possible to evaluate analytically, but a vast sample is not and numerical methods have to be used. Numerical integration is, however, prone to round off errors, especially if the functions which we are evaluating do not behave "nicely". The Newton-Cotes algorithm is a very easy algorithm to implement and understand, however it doesn't produce very reliable results. Supplementing this algorithm, there have been developed a lot of other schemes. In this project, I have implemented Gaussian quadrature with weight functions based on Legendre polynomials and Laguerre polynomials, as well as two Monte Carlo methods to solve a quantum mechanical integral, specifically the quantum mechanical expectation value of the correlation energy between two electrons which repel each other via the classical Coulomb interaction.

The integral in question can be solved in closed form and its exact value is therefore used in the discussion of the reliability of the different methods.

II. Theory/Methods

II.a The Integral

The integral we will evaluate is the six-dimensional ground state expectation value of the correlation energy between to electrons in a helium atom. To do this, we assume that each electron can be modelled via the single-particle wave function

$$\psi_{1s}(\mathbf{r}_i) = e^{-\alpha r_i} \tag{1}$$

where α is a parameter corresponding to the charge of the nucleus around which the electrons are orbiting, the position vector $\mathbf{r}_i$ for electron i is given by

$$\mathbf{r}_i = x_i\mathbf{e}_x + y_i\mathbf{e}_y + z_i\mathbf{e}_z \tag{2}$$

with magnitude

$$r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}. \tag{3}$$

The wave function for two electrons is then given by

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_2)\psi(\mathbf{r}_2) = e^{-\alpha(r_1+r_2)} \tag{4}$$

Note that this is not normalized, however this will only change the integral by a factor equal to the normalization factor, and is not of interest in this project.

The integral which we wish to solve is then

$$\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \rangle = \int_{-\infty}^{\infty} \mathrm{d} \tag{5}$$

II.b Gaussian Quadrature

III. Results

IV. Results