Project 3

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Abstract

This paper adresses different methods for solving a sixdimensional integral in a brute force way. The integral of interest is of the wave function for a helium atom in order to determine the ground energy between its two electrons. We will assume that the wave function for each elektron can be modelled like the single - particle wace function of an electron in the hydrogen atom. The function appears in several quantum mechanical applications and the methodes used to solve it are widley used when computing numericaly.

1 Introduction

Development in methods for solving integrals has been important in order to solve problems with a increasing degree of complexety. Guassian quadrature is a good example which is a method first developed by Jacobi in 1676. The first version would produce exact results for algebraic polynomials of negree n-1 or less. The "new" Guassian version has a significant increase in accuaracy with exact results for polynomials of degree 2n-1 or less due to free choise of weights.

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Gauss-Legendre and Gauss-Laguerre are two Guassian quadrature which, togheter with the well known Monte Carlo method, will be compared in accuaracy and speed for a multidimensional integral for a Helium atom.

The main idea of Gaussian quadrature is to integrate over a set of points x_i not equally spaced with weights w_i. A part of the job is to find these points and weights(Program:Gauleg and Gauss Legendre). The weights are found throug ortogonal polynomials a set interval. The points x_i are chosen in a optimal sense and lie in the interval.

Some theory is first presented with a following discussion of the three methodes mentioned above.

2 Theory

2.1 The Quantum Mechanical Problem

The problem in question is a quantum mechanical one with two electrons in a hydrogen atom.

The single-particle wave function of an electron i in the $1s$ state is given in terms of a dimensionless variable (the wave function is not normalized)

$$\vec{r}_i = x_i\vec{e}_x + y_i\vec{e}_y + z_i\vec{e}_z$$

as

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

Where α is a parameter and the length r_i is defined by

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

In this paper we will fix $\alpha = 2$, which corresponds to the helium atom, Z = 2.

Four our system with two electrons, we have the product of the two $1s$ wave functions defined as

$$\Psi(\vec{r}_1, \vec{r}_2) = e^{-\alpha(r_1+r_2)}$$

This leads us to the integral that needs solving, namely the quantum mechanical expectation value of the energy between two electrons which repel each other via the classical Coulomb interaction.

$$\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \rangle = \int_\infty^\infty d\vec{r}_1 d\vec{r}_2 e^{-2\alpha(r_1+r_2)} \frac{1}{\vec{r_1} - \vec{r_2}}$$

2.2 Gauss-Legendre Quadrature

To compute this integral we will first be utilizing the Gauss-Legendre quadrature. Step one is to change the integration limits to something a little more suitable for a computer. We will therefore change the limits $-\infty$ and ∞ to $-\lambda$ and λ. The values of λ can be found by inserting it for r_i in the formula $e^{-\alpha r_i}$ and getting it sufficiently close to zero. We will also check that this approximation is satisfactory by plotting the function.

2.3 Improved Gauss-Quadrature

While the Gauss-Legendre quadrature gets the job done, its not a pretty sight. What can be improved is to replace the Legendre polynomials with the Laguerre polynomials. These polynomials are defined for $x \in [0, \infty)$.
We will change our original integral from cartesian coordinates to spherical, thus the following relations:

$$d\vec{r}_1 d\vec{r}_2 = r_1^2 dr_1 r_2^2 dr_2 dcos(\theta_1) dcos(\theta_2) d\phi_1 d\phi_2$$

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos(\beta)}}$$

$$cos(\beta) = cos(\theta_1)cos(\theta_2) + sin(\theta_1)sin(\theta_2)cos(\phi_1 - \phi_2)$$

As previousley described, our integral is:

$$\int_{\infty}^{\infty} d\vec{r}_1 d\vec{r}_2 e^{-2\alpha(r_1+r_2)} \frac{1}{\vec{r_1} - \vec{r_2}}$$

For numerical integration, the deployment of the following relation is nessecary:

$$\int_0^{\infty} e^{-x} f(x) dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

where x_i is the i-th root of the Laguerre polynomial $L_n(x)$ and the weight w_i is given by

$$w_i = \frac{x_i}{(n+1)^2 [L_{n+1}(x_i)]^2}$$

The Laguerre polynomials are defined by Rodrigues formula:

$$L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} \left(e^{-x} x^n\right) = \frac{1}{n!} \left(\frac{d}{dx} - 1\right)^n x^n$$

or recursively relations:

$$\begin{aligned} L_0(x) &= 1 \\ L_1(x) &= 1 - x \\ L_{n+1}(x) &= \frac{(2n + 1 - x)L_n(x) - nL_{n-1}(x)}{n+1} \end{aligned}$$

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3 Results

3.1 Laguerre/Legendre

$$N \in [-5, 5]$$

Legandre		
N	Value	Error
11	0.297447	0.104681
15	0.315863	0.123098
21	0.268075	0.075310
25	0.240135	0.047370
27	0.229623	0.036858

Laguerre		
N	Value	Error
11	0.183021	0.009743
15	0.193285	0.000520
21	0.194807	0.002050
25	0.194804	0.002030
27	0.194795	0.002029

4 Discussion

5 Conclusion

this is a reference to intro: 1