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 its 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 applied are widley used for numerical computations.

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 gave 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.

KILDE: woho

Gauss-Legendre and Gauss-Laguerre are two types of 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.

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

2 Theory

2.1 Wavefunction of Helium

. 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 set to 2, due to the two electrons, and the length r_i is defined by

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

For 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 to the integral (1), which will be solved nummericaly with the three different methods mentioned earlier. The value of the integral corresponds to the energy between the two electrons repelling each other due to Columb interactions.

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

The analytical result is $5\pi/16^2$.

2.2 Gaussian Quadrature

The main idea of Gaussian quadrature is to integrate over a set of points x_i not equally spaced with weights w_i, which are calculated in the program Gauleg.cpp and Gauss Legendre.cpp). The weights are found throug ortogonal polynomials(Laguerre and Legendre polynomials) in a set interval. The points x_i are chosen in a optimal sense and lie in the interval.

The intgral is approximated as

$$\int_a^b W(x)f(x) \approx \sum_{i=1}^{n} \omega_i f(x_i)$$

For a more detalied derivation and explenation?? of Gaussian qudrature see (Hjort-Jensen, 2015)

2.2.1 Gauss-Legendre

Using Gauss-Legendre quadrature with Legendre polynomials will make it possible to utilize the integral numerically. The first step is to change the integration limits from $-\infty$ and ∞ to $-\lambda$ and λ. The λ's are found by inserting it for r_i in the expression $e^{-\alpha r_i}$ because $r_i \approx \lambda$ when $e^{-\alpha r_i} \approx 0$. As we see from figure 1, $\lambda \in [-5, 5]$ is therefore a good approximation for the integration limits.

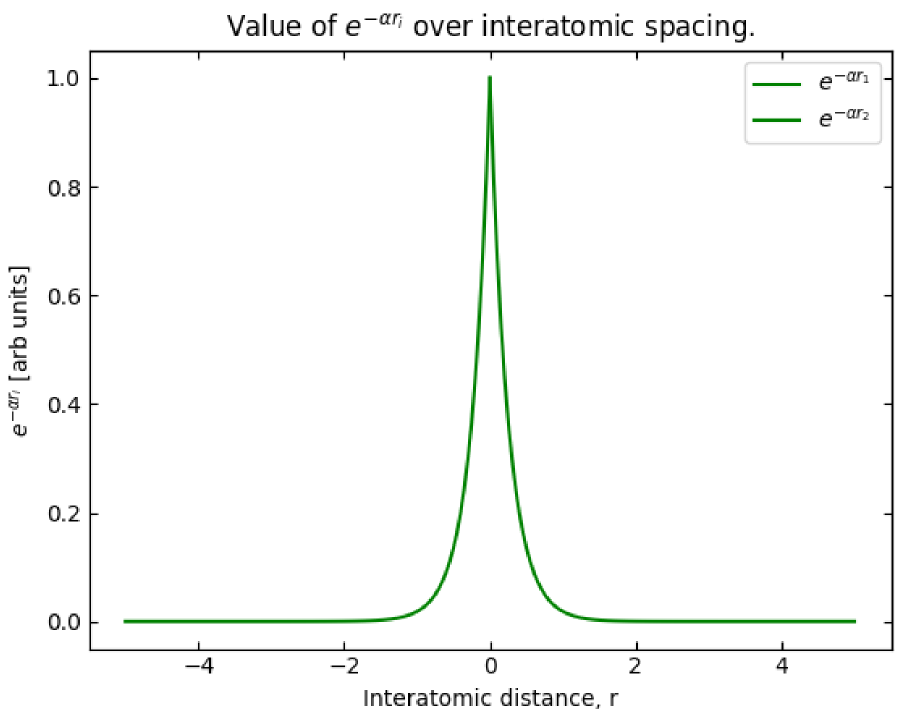

Figure 1: Plot of wavefunction in one dimension

Furthermore, the weights and mesh points are computed using "gauleg"(see program exampleprog.cpp????).

Eventually ending up with a sixdimensional integral, where all six integration limits are the same.

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

2.2.2 Improved Gauss-Quadrature- Laguerre

Gauss-Legendre quadrature gets the job done, but it is unstable and unsatisfactory. By changing to spherical coordinates and replacing Legendre- with Laguerre polynomials an improvement in accuracy is expected. The Laguerre polynomials are defined for $x \in [0, \infty)$,and in spherical coordinates:

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

with

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

and

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

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:

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

2.2.1

2.3 Monte Carlo

2.3.1 Generalized

Monte Carlo integration is based on the idea of finding the mean of a function in a domain by sampling random function values. This mean multiplied by the volume of the domain will be an approximation of the integral.

Say we have an integral I of $f(\mathbf{x})$ we want to find:

$$I = \int_D f(\mathbf{x}) d\mathbf{x}$$

where $\mathbf{x}$ is in the domain D. This integral can be approximated by using random numbers distributed on D by the probability distribution function (PDF) $p(\mathbf{x})$. Discretizing, the approximated integral now becomes

$$I \approx \langle I \rangle = \frac{1}{N} \sum_{i=0}^{N} \frac{f(\mathbf{x}_i)}{p(\mathbf{x}_i)}, \tag{2}$$

where N is the number of sampled values.

2.3.2 Naïve approach (uniform PDF)

To solve our six-dimensional integral, we first take the naïve approach and distribute our randomly chosen variables on the uniform distribution

$$\theta(x) = \begin{cases} \frac{1}{b-a}, & \text{for } x \in [a, b] \\ 0 & \text{else} \end{cases},$$

and keep our variables $\mathbf{r}_1$ and $\mathbf{r}_2$ in cartesian coordinates. Putting the uniform distribution into (2), we get the naïve approximation of an integral:

$$\langle I \rangle = \frac{V}{N} \sum_{i=0}^{N} f(\mathbf{x}_i). \tag{3}$$

Here V is the integration volume (for d dimensions in cartesian coordinates $V = (b-a)^d$, with b and a being the integration limits for each dimension).

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

Table 1: Fill me in!

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

Table 2: Fill me in!

3 Results

3.1 Laguerre/Legendre

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

3.2 Paralellization with openMP

Compile flags	-O3 -fopenMP	-O3	-fopenmp	no optimzation
Naive MC	12s	31s	71s	173s
Improved MC	15s	38s	79s	200s

Table 3: Shows the time spent on the same calculations with different compile parameters.($N = 10^8, \lambda = 5$)

4 Discussion

5 Conclusion

this is a reference to intro: 1