

-Project 3 - FYS3150/FYS4150-

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1 Abstract

Determining the ground state correlation energy between two electrons in a helium atom can be done by evaluating a certain six- dimensional integral assuming that the electrons can be modelled separately, as two, single- particle wave functions of an electron in the hydrogen atom [?]. This integral is also applicable in other aspects of quantum mechanics [?]. For this reason, it's of great value to examine different approaches to solving such integrals, as well as those with higher degrees of freedom. To solve this integral, two different approaches relying on Gaussian quadrature and Monte- Carlo integration were used, as well as the implementation of parallelization to speed up the programs.

2 Introduction

The purpose of this article is to apply different versions of Gaussian quadrature and Monte- Carlo integration in solving a six- dimensional integral to examine their times expenditure and accuracy, as well as the effect of parallelizing the C++ implementations of these methods.

3 Methods

The expectation value of the correlation energy between two electrons interacting under the Coulomb interacting is given by the integral

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

where

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

and

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

$\alpha = 2$, corresponding to the charge of the nucleus of the helium atom as given by [?].

3.1 Gaussian quadrature

The method of Gaussian quadrature allows one to approximate a function $f(x)$ with a polynomial $P_{2N-1}(x)$ of degree $2n - 1$, using only N mesh points. Said polynomial is constructed using sets of orthogonal polynomials, meaning they have the property that

$$\int_a^b P_i(x) P_j(x) dx = \delta_{ij} \quad (2)$$

where $\{P_k \mid k \in \mathbb{N}\}$ is the set of polynomials orthogonal in the domain $[a, b]$, δ_{ij} is the Kronecker- delta and $P_0(x)$ is normalized to be 1. Since the polynomials $\{P_k \mid k \in \{0, \dots, N\}\}$ constitute an orthogonal set, any polynomial of degree N or less can be constructed by a linear combination them

Suppose a function $f(x)$ is approximated by the polynomial Q_{2N-1} . Then

$$\int_a^b f(x)dx \approx \int_a^b Q_{2N-1}(x)dx = \int_a^b (P_N(x)Q_{N-1}(x) + R_{N-1}(x))dx \quad (3)$$

where, due to the orthogonality of the P_k 's, Q_{2N-1} can be decomposed into P_N , R_{N-1} and

$$Q_{N-1} = \sum_{k=0}^{N-1} \beta_k P_k. \quad (4)$$

Then

$$\sum_{k=0}^{N-1} \left(\int_a^b \beta_k P_N(x) P_k(x) dx \right) + \int_a^b R_{N-1}(x) dx = \int_a^b R_{N-1}(x) dx$$

so

$$\int_a^b f(x)dx \approx \int_a^b R_{N-1}(x)dx = \sum_{k=0}^{N-1} \int_a^b \alpha_k P_k(x)dx$$

where R_{N-1} has been expressed in terms of orthogonal polynomials as was done in equation 4. Inserting $P_0(x) = 1$ this expression can be rewritten, then simplified:

$$\int_a^b R_{N-1}(x)dx = \sum_{k=0}^{N-1} \int_a^b \alpha_k P_0(x) P_k(x)dx = \int_a^b \alpha_0 = \alpha_0(b-a). \quad (5)$$

So it's only necessary to identify a single coefficient when evaluating this integral. Looking again at the polynomial $Q_{2N-1}(x)$ that serves as the approximation to the function $f(x)$. The points x_n where $n \in \{0, \dots, N-1\}$ are the zeros of P_N . Composing the polynomial as was done in equation 3

$$Q_{2N-1}(x) = P_N(x)Q_{N-1}(x) + R_{N-1}(x)$$

and assessing at the points x_n :

$$Q_{2N-1}(x_n) = P_N(x_n)Q_{N-1}(x_n) + R_{N-1}(x_n) = R_{N-1}(x_n). \quad (6)$$

So at the zeros P_N , the approximating polynomial $Q_{2N-1}(x)$ equals $R_{N-1}(x)$ which as the other polynomials, can be expressed as a linear combination of orthogonal polynomials as was done in equation 4.

$$R_{N-1}(x) = \sum_{k=0}^{N-1} \alpha_k P_k(x).$$

And at the points x_n :

$$R_{N-1}(x_n) = \sum_{k=0}^{N-1} \alpha_k P_k(x_n) \quad n \in \{0, \dots, N-1\}. \quad (7)$$

As $\{P_k \mid k \in \{0, \dots, N\}\}$ are orthogonal polynomials, no one P_k is linearly dependent on any others, thus $P_k(x_n)$ can be expressed as an invertible $N \times N$

matrix with matrix elements P_{kn} .

Multiplying both sides of equation 7 by

$$\sum_{j=0}^{N-1} P_{jk}^{-1} \quad (8)$$

yields

$$\left(\sum_{j=0}^{N-1} P_{jk}^{-1} \right) R_{N-1}(x_n) = \left(\sum_{j=0}^{N-1} P_{jk}^{-1} \right) \sum_{k=0}^{N-1} \alpha_k P_k(x_n)$$

which, due to the orthogonality of the column- vectors gives

$$\sum_{k=0}^{N-1} P_{nk}^{-1} R_{N-1}(x_k) = \alpha_n. \quad (9)$$

Returning then to equation 5, and inserting the expression 9 for $n = 0$.

$$\int_a^b R_{N-1}(x) dx = (b-a) \left(\sum_{k=0}^{N-1} P_{0k}^{-1} R_{N-1}(x_k) \right). \quad (10)$$

Remembering back to equation 6 and labelling $\omega_k = (b-a)P_{0k}^{-1}$ as the weights, the final equation is arrived at:

$$\int_a^b f(x) dx \approx \int_a^b Q_{2N-1}(x) dx = \sum_{k=0}^{N-1} \omega_k Q_{2N-1}(x_k) \quad (11)$$

where x_k are the N zeros of the orthogonal polynomial P_N of degree N , Q_{2N-1} is the polynomial approximation of the original function $f(x)$ and ω_k are the associated weights.

For the case of $-a = b = 1$, the orthogonal polynomials in question are the Legendre polynomials, orthogonal in the interval $x \in \{-1, \dots, 1\}$. Other such polynomials, orthogonal on different intervals, such as the Laguerre polynomials can be applied in the same manner, although come attached with an associated weight function $\{W(x) \mid W(x) > 0, x \in \{-1, \dots, 1\}\}$, integrable on the interval $[a, b]$ such that the integral to be evaluated is

$$\int_a^b W(x) f(x) dx$$

[?].

3.1.1 Gauss- Legendre quadrature

Expressing the integral in equation 1 in terms of x_1, y_1, z_1 and x_2, y_2, z_2 :

$$\iiint_{-\infty}^{\infty} \frac{\exp\left(-4\left(\sqrt{x_1^2 + y_1^2 + z_1^2} + \sqrt{x_2^2 + y_2^2 + z_2^2}\right)\right)}{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}} dx_1 dx_2 dy_1 dy_2 dz_1 dz_2 \quad (12)$$

The Gauss- Legendre quadrature relies on the orthogonality of the Legendre polynomials in the domain $x \in \{-1, \dots, 1\}$. Therefore it's necessary to replace infinity with other bounds that still yield suitable results. Then, only a simple change of variables is required to bring the integration bounds to $[-1, 1]$:

$$\lim_{t \rightarrow \pm\infty} f(t) \approx f(\pm\lambda)$$

change of variable $t = \lambda\tau$:

$$\int_{-\lambda}^{\lambda} f(t)dt = \lambda \int_{-1}^1 f(\lambda\tau)d\tau$$

Using this fact for integral 12 gives

$$\lambda^5 \iiint_{-1}^1 \iiint_{-1}^1 \frac{\exp\left(-4\lambda\left(\sqrt{\chi_1^2 + v_1^2 + \zeta_1^2} + \sqrt{\chi_2^2 + v_2^2 + \zeta_2^2}\right)\right)}{\sqrt{(\chi_1 - \chi_2)^2 + (v_1 - v_2)^2 + (\zeta_1 - \zeta_2)^2}} d\chi_1 d\chi_2 dv_1 dv_2 d\zeta_1 d\zeta_2$$

and then renaming the integrand

$$g(\chi_1, \chi_2, v_1, v_2, \zeta_1, \zeta_2) = \frac{\exp\left(-4\lambda\left(\sqrt{\chi_1^2 + v_1^2 + \zeta_1^2} + \sqrt{\chi_2^2 + v_2^2 + \zeta_2^2}\right)\right)}{\sqrt{(\chi_1 - \chi_2)^2 + (v_1 - v_2)^2 + (\zeta_1 - \zeta_2)^2}} \quad (13)$$

gives the final equation

$$\lambda^5 \iiint_{-1}^1 \iiint_{-1}^1 g(\chi_1, \chi_2, v_1, v_2, \zeta_1, \zeta_2) d\chi_1 d\chi_2 dv_1 dv_2 d\zeta_1 d\zeta_2. \quad (14)$$

As long as the function g can be approximated with a polynomial P_{2N-1} of degree $2N-1$ or lower on the interval $[-1, 1]$, this integral can be approximated by

$$\lambda^5 \sum_{i_1=1}^N \dots \sum_{i_6=1}^N \omega_{i_1} \dots \omega_{i_6} g(x_{i_1}, \dots, x_{i_6}) \quad (15)$$

where ω_{ik} for $k \in \{1, \dots, 6\}$ are the weights and x_{ik} for $k \in \{1, \dots, 6\}$ are the zeros of the Legendre polynomial \mathcal{L}_N of degree N .

$\mathcal{L}_N(x_{ik})$ can be gotten by simply using the recursion relation

$$(n+1)\mathcal{L}_{n+1}(x_{ik}) + n\mathcal{L}_{n-1}(x_{ik}) - (2n+1)x_{ik}\mathcal{L}_n(x_{ik}) = 0 \quad (16)$$

given by [?] and the requirement that $\mathcal{L}_0 = 1$.

The zeros of \mathcal{L}_N , x_{ik} are found by any root- finding algorithm, such as Newton's method.

3.1.2 Gauss- Laguerre quadrature

The Gauss- Legendre quadrature in this case, got a little ugly. A different approach would be to transform the integral with polar coordinates and using

the Laguerre polynomials that are orthogonal on the interval $[0, \infty]$. Looking again at equation 1, and applying the change of variables given in the Project 3 Problem set [?] section 3b):

$$\int_0^\pi \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} \int_0^\infty \int_0^\infty \frac{r_1^2 r_2^2 \sin(\theta_1) \sin(\theta_2) e^{-4(r_1+r_2)}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\beta)}} dr_1 dr_2 d\phi_1 d\phi_2 d\theta_1 d\theta_2$$

with

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

r_1 and r_2 in this case, are integrated from 0 to ∞ , suitable for the Gauss-Laguerre quadrature.

The Gauss- Laguerre quadrature carries the weight function

$$W(x) = x^\alpha e^{-x} \quad (17)$$

[?]. α being the exponent of x in an integral of the form

$$\int_0^\infty x^\alpha e^{-x} f(x). \quad (18)$$

For simplicity, lets isolate one of the r 's in the integrand, as the other will be treated as a constant. let's pick r_1 :

$$C \int_0^\infty \frac{r_1^2 e^{-4r_1}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\beta)}} dr_1 \quad (19)$$

where

$$C = \int_0^\pi \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} \int_0^\infty r_2^2 \sin(\theta_1) \sin(\theta_2) e^{-4r_2} dr_2 d\phi_1 d\phi_2 d\theta_1 d\theta_2.$$

The integral 19, can then be written as

$$C \int_0^\infty W(r_1) g(r_1) dr_1 \quad (20)$$

with

$$W(r_1) = r_1^2 e^{-r_1}$$

and

$$g(r_1) = \frac{e^{-3r_1}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\beta)}}.$$

Integral 20, neglecting C for just a bit, can now be approximated according to the Gauss- Laguerre quadrature:

$$\int_0^\infty W(r_1) g(r_1) dr_1 \approx \sum_{i=1}^N \omega_i g(x_i) \quad (21)$$

ω_i being the weights acquired by inverting the matrix (see appendix 7.1)

$$\mathbf{L} = \begin{bmatrix} e^{-x_1} L_0(x_1) & e^{-x_1} L_1(x_1) & \cdots & \cdots & e^{-x_1} L_{N-1}(x_1) \\ e^{-x_2} L_0(x_2) & e^{-x_2} L_1(x_2) & \cdots & \cdots & e^{-x_2} L_{N-1}(x_2) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ e^{-x_{N-1}} L_0(x_{N-1}) & e^{-x_{N-1}} L_1(x_{N-1}) & \cdots & \cdots & e^{-x_{N-1}} L_{N-1}(x_{N-1}) \\ e^{-x_N} L_0(x_N) & e^{-x_N} L_1(x_N) & \cdots & \cdots & e^{-x_N} L_{N-1}(x_N) \end{bmatrix} \quad (22)$$

and $x_i | i \in \{1, \dots, N\}$ being the zeros of the Laguerre polynomial L_N of degree N .

3.2 Monte Carlo Integration

A different approach to solving integrals numerically is the use of Monte Carlo integration, where properties of probability distribution functions (PDFs) are used to approximate the solution. For any integral $\int_a^b f(x)dx$, one can find a PDF $p(x)$ that fulfills $\int_a^b p(x)dx = 1$ that is nonzero $\forall x \in [a, b]$. Then by the law of large numbers [?],

$$\int_a^b f(x)dx = \int_a^b p(x) \frac{f(x)}{p(x)} dx = E\left[\frac{f(x)}{p(x)}\right] \approx \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p(x_i)}$$

where N is a very large number and x_i are random samples from the given PDF. The variance is then given by

$$\sigma^2 = \frac{1}{N} \sum_{i=1}^N \left(\left(\frac{f(x_i)}{p(x_i)} \right)^2 - E\left[\frac{f(x)}{p(x)}\right]^2 \right) p(x_i) = E\left[\left(\frac{f(x)}{p(x)}\right)^2\right] - E\left[\frac{f(x)}{p(x)}\right]^2$$

It can then be shown [?] that the standard error of the mean is

$$\sigma_N \approx \frac{\sigma}{\sqrt{N}}$$

Thus, the error is a function of $\frac{1}{\sqrt{N}}$. This does not depend on the dimensionality of the integral to be evaluated, making Monte Carlo methods very effective for integrals in higher dimensions. The appropriate choice of a fitting PDF is crucial. Even though the above equations hold true for any PDF, choosing a PDF $p(x)$ that closely follows our function $f(x)$, leads to a better sampling of x_i [?] and decreases the standard deviation. Thus, the real integral is approached much faster.

3.3 Implementation

3.3.1 Legendre polynomials

The first approach to solving the integral is to use Legendre polynomials. As Legendre polynomials cannot be properly mapped to $(-\infty, \infty)$, it is necessary to define a threshold λ where the function is "sufficiently" zero. Thus, the integral is only evaluated for $(-\lambda, \lambda)$. As can be seen in FIGURE XXX, the function approaches zero rather quickly, and $\lambda=2$ seems to be an appropriate choice. The integration limit is then changed to $[-2, 2]$ for all 6 integrands. Numerical recipe's gauleg-function [?] then maps the weights from $[-1, 1]$ to $[-2, 2]$. Because any all the 6 variables in the integral are freely interchangeable, the the approximation then reads,

$$\begin{aligned} & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x_1, x_2, y_1, y_2, z_1, z_2) dx_1 dx_2 dy_1 dy_2 dz_1 dz_2 \\ & \approx \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 f(x_1, x_2, y_1, y_2, z_1, z_2) dx_1 dx_2 dy_1 dy_2 dz_1 dz_2 \\ & \approx \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N \sum_{l=1}^N \sum_{m=1}^N \sum_{n=1}^N \omega_i \omega_j \omega_k \omega_l \omega_m \omega_n f(x_i, x_j, x_k, x_l, x_m, x_n) \end{aligned}$$

where x_i and ω_i were created using the gauleg-function. Computationally, this will lead to a total of N^6 function evaluations. A possible problem to face is that one will end up dividing by zero N^3 times. This problem can be faced by ignoring all function evaluations where the function's denominator is lower than a threshold, which was chosen to be 10^{-8} .

3.3.2 Laguerre and Legendre polynomials

When transferred into spherical coordinates, the integral reads

$$\int_0^\pi \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} \int_0^\infty \int_0^\infty \frac{r_1^2 r_2^2 \sin(\theta_1) \sin(\theta_2) e^{-4(r_1+r_2)}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\beta)}} dr_1 dr_2 d\phi_1 d\phi_2 d\theta_1 d\theta_2$$

with

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

This has the advantage that infinity only has to be faced twice, and Laguerre-Polynomials can be used for that. Laguerre-polynomials are defined for $[0, \infty)$ and have a weight function $W(x) = e^{-x}$. This is relevant for r_1 and r_2 , as the integration limits go from 0 to ∞ . The angles θ_1 and θ_2 lie in $[0, \pi]$, and the angles ϕ_1 and ϕ_2 lie in $[0, 2\pi]$. Here, Legendre-Polynomials can be used again. Because each of the θ , ϕ and r are interchangeable, it is necessary to create 3 types of mesh points and weights: One using the Laguerre polynomials (ω_r , x_r), one using Legendre polynomials for the angle θ (ω_θ , x_θ) and one using Legendre polynomials for the angle ϕ (ω_ϕ , x_ϕ). The function to be evaluated changes slightly due to the Laguerre-polynomials weight function, the exponent goes from -4 to -3, leading to

$$g(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) = \frac{r_1^2 r_2^2 \sin(\theta_1) \sin(\theta_2) e^{-3(r_1+r_2)}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\beta)}}$$

$$\int_0^\pi \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} \int_0^\infty \int_0^\infty g(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) dr_1 dr_2 d\phi_1 d\phi_2 d\theta_1 d\theta_2$$

This integral is then approximated by the following sum:

$$\approx \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N \sum_{l=1}^N \sum_{m=1}^N \sum_{n=1}^N \omega_{r,i} \omega_{r,j} \omega_{\theta,k} \omega_{\theta,l} \omega_{\phi,m} \omega_{\phi,n} g(x_{r,i}, x_{r,j}, x_{\theta,k}, x_{\theta,l}, x_{\phi,m}, x_{\phi,n})$$

4 Results

5 Conclusion

6 Critique

7 Appendix

7.1 Proof that \mathbf{L} is invertible

For the matrix \mathbf{L} in equation 22; each column is constructed of constants multiplied with the Laguerre polynomial L_n for each row in column n . With the

Laguerre polynomials being orthogonal with respect to the inner product

$$L_n|L_m = \int_0^{\infty} e^{-x} L_n(x) L_m(x) dx = \delta_{mn} \quad (23)$$

no column can be expressed as a linear combination of any of the others (at least not for $x \in [0, \infty]$, so \mathbf{L} is an $N \times N$ matrix with N linearly independent columns. As such it is necessarily non-singular and therefore, must be invertible.

7.2 List of programs

All programs can be found on https://github.com/adrian2208/FYS3150_collab in the folder "project 3".

- 1.

7.3 Tables

[?] [?]