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*-Project 3 - FYS3150/FYS4150- By Simon Schrader (4150), Adrian Kleven (3150) - autumn 2019

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 Problem$_set_3.Tosolvethisintegral,twodifferent$ $Carlointegrationareused.IntroductionThepurposeofthisarticleistoapplydifferentversionsofGaussianquadratureand$ $Carlointegrationinsolvingasix-dimensionalintegral\int_{-\infty}^{\infty} \exp\left(-4\left(\sqrt{x_1^2+y_1^2+z_1^2}+\sqrt{x_2^2+y_2^2+z_2^2}\right)\right)\sqrt{(x_1-x_2)^2+($

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 devore2012modern,

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

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

Implementation 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 λ=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 press1992numerical 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,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x_1,x_2,y_1,y_2,z_1,z_2)dx_1dx_2dy_1dy_2dz_1dz_2$$

$$\approx \int_{-2}^{2}\int_{-2}^{2}\int_{-2}^{2}\int_{-2}^{2}\int_{-2}^{2}\int_{-2}^{2} f(x_1,x_2,y_1,y_2,z_1,z_2)dx_1dx_2dy_1dy_2dz_1dz_2$$

$$\approx \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N}\sum_{m=1}^{N}\sum_{n=1}^{N} \omega_i\omega_j\omega_k\omega_l\omega_m\omega_n f(x_i,x_j,x_k,x_l,x_m,x_n)$$

where x_i and ω_i where 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}. Laguerre and Legendre polynomials When transferred into spherical coordinates, the integral reads

$$\int_0^{\pi}\int_0^{\pi}\int_0^{2\pi}\int_0^{2\pi}\int_0^{\infty}\int_0^{\infty} r_1^2r_2^2sin(\theta_1)sin(\theta_2)e^{-4(r_1+r_2)}\sqrt{r_1^2+r_2^2-2r_1r_2cos(\beta)}dr_1dr_2d\phi_1d\phi_2d\theta_1d\theta_2$$

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, Lagrange-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 Lagrange polynomials for the angle θ (ω_θ, x_θ) and one using Lagrange 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

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

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

This integral is then approximated by the following sum:

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

Again, the risk of dividing by zero is averted when the denominator is lower than a threshold, which was chosen to be 10^{-8}. Monte Carlo integration without importance sampling The first approach is to use Monte Carlo with uniformely distributed values for each dimension in the range $[-\lambda, \lambda]$, as no uniform distributions for $(-\infty, \infty)$ exist. As for the Lagrange polynomials, the integration limits were changed to $[-2, 2]$ for all 6 integrands. Using the PDF p(x)=0.25 for $x \in [-2, 2]$, otherwise zero, the integral reads (BY FUNCTION XXX in the theory part)

$$\int_{-2}^2 \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 \int_{-2}^2 0.25^6 4^6 f(x_1, x_2, y_1, y_2, z_1, z_2) dx_1 dx_2 dy_1 dy_2 dz_1 dz_2$$

$$\approx 4^6 1N \sum_{i=1}^N f(x_{i,1}, x_{i,2}, x_{i,3}, x_{i,4}, x_{i,5}, x_{i,6})$$

where $x_{i,1}, ..., x_{i,6}$ are uniformely distributed in [-2,2]. Again, all function evaluations where the denominator is smaller than 10^{-8}, are ignored. Monte Carlo integration with importance sampling In polar coordinates, the polar part of the function resembles the PDF $p(r_1, r_2) = 16e^{-4(r_1+r_2)}$, where $p(r_1, r_2)$ is the product of two exponential distributions with parameter=4. Thus, it is possible to sample both r_1 and r_2 from that exponential distribution. The angles θ_1 and θ_2 can be sampled from a uniform distribution for values in $[0, \pi]$, while the angles ϕ_1 and ϕ_2 are taken from a uniform distribution for values in $[0, 2\pi]$. Doing this, the function that we want to get the expectation value from is given by

$$g(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) = \pi^4 2^2 4^2 r_1^2 r_2^2 sin(\theta_1) sin(\theta_2) \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos(\beta)}$$

with $cos(\beta)$ as defined earlier. Thus, the integral is approximated by

$$1N \sum_{i=1}^N g(r_{i,1}, r_{i,2}, \theta_{i,1}, \theta_{i,2}, \phi_{i,1}, \phi_{i,2})$$

where $r_{i,1}, r_{i,2}$ are exponentially distributed with a factor 4; $\theta_{i,1}, \theta_{i,2}$ are uniformely distributed in $[0, \pi]$, and $\phi_{i,1}, \phi_{i,2}$ are uniformely distributed in $[0, 2\pi]$. In order to create exponentially distributed random variables, we use that a variable x_i is exponentially distributed when

$$x_i = -14ln(1 - u_i)$$

where u_i is standard uniformely distributed. Again, all function evaluations where the denominator is smaller than 10^{-8}, are ignored. Results The results using Legendre polynomials for the two different methods and different values of n can be found in table 1: table[ht] tabular—l—l—l—l—l— n Result Relative Error time [s]

Conclusion

Critique

Appendix Proof that $F^{-1}(U)$ has cumulative function P(x) Let F(X) be a cumulative distribution function (CDF).

Tables

Lecture$_Notes_Fall_2015Problem_set_3Plain$

citations

comment

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