Assignment VIII: Monte Carlo Integration

Due 10/31/2016

1. Multi-Dimensional Integration

Using Monte-Carlo integration evaluate the 10-dimensional integral

$$I = \int_0^1 dx_1 \int_0^1 dx_2 \cdots \int_0^1 dx_{10} (x_1 + x_2 + \cdots + x_{10})^3. \tag{1}$$

(a) Conduct 16 trials and take the average as your answer.

(b) Try sample sizes of N= 64, 128, 256, 512, ... 8192.

(c) Tabulate and plot the absolute value of the error versus $1/\sqrt{N}$ and try to identify linear behavior.

2. Integration with Importance Sampling: Ground State Correlation between two Electrons in a Helium Atom

Let us assume that the wave function of each electron in the helium atom can be modeled like the single-particle wave function of an electron in the hydrogen atom. The single-particle wave function for an electron i in the $1s$ state is given in terms of a dimensionless variable (The wave function here is not properly normalized, but should not be a concern in this calculation.)

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

as

$$\psi_{1s}(\mathbf{r}_i) = e^{-\alpha r_i}, \tag{3}$$

where α is a parameter, and

$$r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}. \tag{4}$$

We will fix $\alpha = 2$, which should correspond to the charge of the helium atom $Z = 2$.

The ansatz for the wave function for two electrons in the ground state is then given by the product of two so-called $1s$ wave functions as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{-\alpha(r_1 + r_2)}. \tag{5}$$

Note that it is not possible to find a closed-form solution to the Schrödinger differential equation for two interacting electrons in the helium atom.

The integral that needs to be calculated is the quantum mechanical expectation value of the correlation energy between two electrons which repel each other via the classical Coulomb interaction, namely

$$\langle\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\rangle \equiv \int d^3r_1 d^3r_2 \; e^{-2\alpha(r_1+r_2)} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{6}$$

Note that there is a normalization factor missing, but for this problem you do not need to worry about that.

To calculate the integral of Eq. (6) change to spherical coordinates

$$d^3r_1 d^3r_2 = r_1^2 dr_1 \; r_2^2 dr_2 \; d\cos(\theta_1) \; d\cos(\theta_2) \; d\phi_1 \; d\phi_2, \tag{7}$$

with

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \equiv \frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\beta}}, \tag{8}$$

where

$$\cos\beta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2) \tag{9}$$

Calculate this variable transformation and document it. The integral of Eq. (6) can now be rewritten with appropriate integration limits. Write down explicitly the limits of the integration for all variables.

Evaluate the integral with Monte Carlo techniques.

(a) Evaluate the integral using the compiler built in random number generator. Conduct at least 8 runs. Tabulate your answers and plot them as function of $1/\sqrt{N}$.
(b) Employ importance sampling (for which variables will that be useful?) Use that

$$\int dy e^{-y} = e^{-y}. \tag{10}$$

Assess how much the importance sampling improves your calculation, i.e. determine if a smaller number of N is sufficient to reach the same result as in **(a)**.