PHYS-E0412 Computational Physics :: Homework 3

Due date 29.1.2019 at 10 am

Metropolis importance sampling

Let us consider two Gaussian charge distributions in three dimensions, i.e. each with density

$$\rho(\mathbf{r}) \propto e^{-x^2-y^2-z^2}. \tag{1}$$

The total charge of each cloud is assumed to be one. Furthermore, to make things more interesting, we separate the charge clouds by a distance d. We are then asking what is the Coulomb interaction energy between the two charge clouds. This is effectively to evaluate the six-dimensional integral

$$U(d) := \frac{\int dx_1 dy_1 dz_1 \int dx_2 dy_2 dz_2 \; e^{-x_1^2-y_1^2-z_1^2} \frac{1}{\|\mathbf{r}_1-\mathbf{r}_2\|} e^{-(x_2-d)^2-y_2^2-z_2^2}}{\int dx_1 dy_1 dz_1 \int dx_2 dy_2 dz_2 \; e^{-x_1^2-y_1^2-z_1^2} \; e^{-(x_2-d)^2-y_2^2-z_2^2}} \;, \tag{2}$$

which is to be done by the Metropolis Monte Carlo integration.

Hint. The integral can be cast to the average

$$U(d) \approx \left\langle \frac{1}{\|\mathbf{r}_1 - \mathbf{r}_2\|} \right\rangle, \tag{3}$$

given that $\mathbf{r}_1$ and $\mathbf{r}_2$ are sampled according to the Gaussian distributions centered at $(0,0,0)$ and $(d,0,0)$. Alternatively, one can evaluate $\left\langle \frac{1}{\|\mathbf{r}_1-\mathbf{r}_2-d\hat{e}_x\|} \right\rangle$ with both Gaussians at the origin. In the Metropolis part of the algorithm, the random moves can be made in one of the six dimensions at a time. Then, the formula for the acceptance is simple.

(i) Write a code that evaluates $U(d)$ using the Metropolis Monte Carlo integration algorithm described in the lectures and lecture slides. Evaluate the integral numerically at points $U(0)$ and $U(1)$. Report acceptance rates for these two calculations. (2p)

(ii) Calculate numerical error estimates for values at $U(0)$ and $U(1)$. Make sure that the error estimates are reasonable. Exact value for $U(0)$ is known to be $\sqrt{\frac{2}{\pi}}$. (2p)

(iii) Investigate if the large d the interaction energy $U(d)$ follows the $1/d$-law. (1p)

(iv) How many hours you used for problems in this exercise set?