HW3 due 15/12/2023

(+2 points for timely submission)

Q.1

Numerical integration with random distribution.

a) Compute the value of π in the following manner:

Perform N trials of this task: select two random numbers in the range of 0:1, accept the pairs if the sum of their square is smaller than 1.0. Finally, evaluate

$$A = \frac{N_{\text{accepted}}}{N_{\text{trials}}}.$$

What is the expected result?

b) Generate a non-uniform distribution of random number x ($N > 35000$) in the range of 0.0 : 4.0 according to the distribution

$$\rho(x) = e^{x}$$

Plot a normalized histogram H of your collection of x, and verify that it follows the distribution

$$H = \rho(x)/\text{norm}$$

where

$$\text{norm} = \int_0^4 dx \rho(x).$$

c) Use the random collection to compute an integral, i.e.,

$$\frac{1}{N}\sum \tilde{f}(x) \approx \frac{\int dx\, \tilde{f}(x)\, \rho(x)}{\int dx\, \rho(x)}.$$

Choose, e.g. $\tilde{f}(x) = e^{-2x}$ and verify that

$$\frac{\text{norm}}{N}\sum \tilde{f}(x) \approx \int_0^4 dx e^{-x}.$$

d) What do we get when we choose $\tilde{f} = \rho^{-1}$? Compute the result.

Q.2

If we randomly pick 2 points in an N-dim cube, what would be the average distance? (Take box size to be 1.0 for simplicity.)

a) For 1D, the analytic solution is given by

$$\frac{\int dx_1 dx_2 |x_1 - x_2|}{\int dx_1 \int dx_2}.$$

Compute the integral. (ans. 1/3) (OMG!)

Verify this result by random sampling.

b) Compute the results for N = 2 to 10. (List them in a table.)

Q.3

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Memorize the Gaussian integral formula to pass the QM exam!
-- advice from my tutor (when I was an undergraduate)
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Gaussian integrals, keep coming back for more.

a) The Gaussian integral, in the presence of an auxiliary field h,

$$Z(h) = \int_{-\infty}^{\infty} dx\, e^{-A\,x^2 + h\,x} = \sqrt{\frac{\pi}{A}}\, e^{\frac{h^2}{4A}}.$$

generalizes to

$$Z(\vec{h}) = \int dx_1\, dx_2, \dots dx_N\, e^{-\vec{x}^t A \vec{x} + \vec{h}^t \vec{x}} = \sqrt{\frac{\pi^N}{\mathrm{detA}}}\, e^{\frac{1}{4}\,\vec{h}^t\, A^{-1}\, \vec{h}}.$$

Here A is an $N \times N$, positive definite, and symmetric matrix. Write a program to verify the result for N = 2, 3, 6.

b) Show that

$$\frac{1}{Z(0)} \frac{\partial^2 Z(\vec{h})}{\partial h_i \partial h_j} = \langle x_i x_j \rangle = \frac{1}{2}\, A^{-1}[i, j].$$

Again, it is understood that we take $\vec{h} \to \vec{0}$ in the end.

c) Numerically demonstrates the following at N = 8.

$$\langle x_1 x_2 \rangle = \frac{1}{2}\, A^{-1}[1, 2]$$
$$\langle x_1 x_2 x_3 x_4 \rangle = \langle x_1 x_2 \rangle \langle x_3 x_4 \rangle + \text{permutations}.$$

These are called N-point functions in field theory. 2-point function is just the propagator. As expected the higher ones are more difficult to compute.

Q.4

The Vandermonde matrix naturally arises in approximating a function using a polynomial:

$$f(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_{N-1} x^{N-1}.$$

a) By sampling the functions at N distinct points, show that the coefficients a_n's satisfy

$$V \begin{bmatrix} a_0 \\ a_1 \\ \cdots \\ a_{N-1} \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \cdots \\ f(x_{N-1}) \end{bmatrix},$$

where

$$V = \begin{bmatrix} 1 & x_0 & x_0^2 & \ldots & x_0^{N-1} \\ 1 & x_1 & x_1^2 & \ldots & x_1^{N-1} \\ 1 & x_2 & x_2^2 & \ldots & x_2^{N-1} \\ & & \cdots & & \\ 1 & x_{N-1} & x_{N-1}^2 & \ldots & x_{N-1}^{N-1} \end{bmatrix}$$

b) Write a program to interpolate the function based on this method:

$$f(x) = \frac{1}{1+x^2}$$

.

Choose e.g. N = 20 points in the interval -2:2.

c) Take the complex-step derivative on $f(x)$ and its interpolated version. Plot and compare the results.

Q.5

Derivative and Fourier Transform.

a) Obtain the analytic expression of $\tilde{f}(k)$

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx\, e^{-x^2}\, e^{-ikx}.$$

Ans: $\tilde{f}(k) = \sqrt{\pi}\, e^{-k^2/4}$.

b) This means $f(x) = e^{-x^2}$ and $\tilde{f}(k) = \sqrt{\pi}\, e^{-k^2/4}$ is a pair of Fourier transform. Verify this numerically, i.e. compute

$$f_1(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx} f(x)$$
$$f_2(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ikx} \tilde{f}(k)$$

and compare with known results.

Can your code handle transformation back to the x-space based on the numerical k-space result? I.e.

$$f_{2num}(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ikx} f_1(k).$$

c) Compute

$$g(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \times (ik) \times \tilde{f}(k).$$

Show that $g(x) = f'(x)$. Verify this numerically.

d) Compute higher order derivatives this way (i.e. via Fourier transform) for $n = 2, 3, 4$. Compare with the exact results.