Computational Physics II

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Spring term 2021
Project 3, due March 24, 2021 at 11:55 pm
to be uploaded to https://moodle.jacobs-university.de

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(all projects parts carry 100 points each)

3. Integration using Metropolis algorithm [100 points]

a) Implement the Metropolis algortihm for performing a one-dimensional integral. Use it to determine the integral

$$\int_1^5 (x^2+x)e^{-x}dx \; .$$

To this end, try three different distributions to speed up the integration., i.e., $p_a(x) = 1$, $p_b(x) = e^{-x}$ and $p_c(x) = (x^2+x)e^{-x}$ for $x \geq 0$ and $p(x) = 0$ for $x < 0$. Please do not forget to normalize these distributions before you use them. Compute the histograms $H(x)$ showing the number of points in the random walk in the region x to $x+\Delta x$ with $\Delta x = 0.1$. Try three different but reasonable values of the maximum step size δ.

b) Calculate analytically the exact value of the integral . How do your Monte Carlo results compare with the exact value for increasing values of n ? Plot the dependence of the integral as a function of n for all nine cases above (in one plot if possible).

General remarks for all Projects

You will have to (i) analyze the problem, (ii) select an algorithm (if not specified), (iii) write a Python program, (iv) run the program, (v) visualize the data numerical data, and (vi) extract an answer to the physics question from the data.
Which checks did you perform to validate the code? State the results you got for these tests.
For each project you will submit a short report describing the physics problem, your way of attacking it, and the results you obtained. Provide the documented Python code in such a form that we can run the code. A Jupyter Notebook including the code and report is fine but not necessary.