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CP1: Monte Carlo Methods WS 2023/24

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9. Exercise: Autocorrelations

On the moodle page you find a file called `datafile`, which includes a Markov chain of 100000 numbers produced by some process. In the file `dataread.py` you see how it's read into a python array `data[]`.
Are there autocorrelations? Determine the average with statistical errors using the blocking method. How large do the blocks need to be?
Hint: in python you can do a blocking with blocksize `Nb` with the statement: `blockeddata= [ avr(data[i*Nb,(i+1)*Nb]) for i in range(int(len(data)/Nb)) ]` , as you also see in `dataread.py`
Hint 2: It's not necessary to calculate the autocorrelation function to solve this exercise.

10. Exercise: Jackknife

You will need a Jackknife subroutine in the future:
`def jackknife_estimation(func,data,jkn):`
where `data` is a list of numbers, `func` is a function that takes a list of numbers and calculates something from them, `jkn` is an integer number. The function splits the data into `jkn` blocks, and calculates jackknife errors and averages by considering each block as a jackknife sample. You can find such a function on the moodle page: `jackknife_mclect.py`, download it.

11. Exercise: π again

In exercise 2, we calculated π using the formula for the volume of a 10-ball: $V_{10}(r) = r^{10}\pi^5/120$. Suppose we generate N times $x_i,\ i = 1, \ldots, 10$ such that we can decide whether $\sum x_i^2 < 1$, as we did in exercise 2. We get thus a set $\{n_i\}$ of N numbers, $n_i = 1$ if $\sum x_i^2 < 1$, and $n_i = 0$ otherwise. An estimator for π is thus:

$$\pi = \left(2^{10} * 120 * \sum_i n_i/N\right)^{1/5} \tag{1}$$

Now we can continue with the analysis in different ways:

- We split our N numbers to N_{samp} blocks, and from each block we estimate π using the formula above. Finally we calculate the average and error from our N_{samp} estimates.
- We split our N numbers to N_{samp} blocks, and use Jackknife error estimation to get the average and an error estimate.
- In this case we can do a simplified estimate: we use the formula above to estimate π^5, the variance of which we can directly estimate from the variance of n_i. Finally we use standard error propagation to calculate errors for π.

Which one of the three ways is preferable? Is there a difference? Does it depend on how large N is?

12. Exercise: Generating random numbers with the Maxwell-Boltzmann Distribution – for the last time

Set up a Langevin equation to generate random numbers according to the Maxwell-Boltzmann distribution, given by (use $a = 1$)

$$P(x) = \sqrt{\frac{2}{\pi}} \frac{x^2 e^{-x^2/(2a^2)}}{a^3}, \qquad x > 0. \tag{2}$$

The discretised Langevin eq. for simulating $e^{-S(x)}$ is

$$x(\tau + \Delta\tau) = x(\tau) - \Delta\tau \partial_x S(x(\tau)) + \eta\sqrt{2\Delta\tau}, \tag{3}$$

where η is a Gaussian random variable with zero mean and unit variance. Use e.g. $\Delta\tau = 0.001$ to solve it numerically.
Wait until $\tau = 10$ before collecting averages to get rid of the initial thermalization of the process.
Calculate the mean and variance with errors (you can use e.g. blocked Jackknife with a large block to minimize correlations of the blocks) and verify that they agree with the exact results.

$$\mu = 2a\sqrt{\frac{2}{\pi}}, \qquad \sigma^2 = \frac{a^2(3\pi - 8)}{\pi}, \qquad \gamma_1 = \frac{2\sqrt{2}(16 - 5\pi)}{(3\pi - 8)^{3/2}} \tag{4}$$

Use $x(0) = 2$, and N_r runs with different seeds to calculate $\langle x(\tau) \rangle$. How does it depend on τ? Was it OK to wait until $\tau = 10$ to take averages?