April 2018 - HPC-Monte Carlo problems

Day 1

Problem 1: Infinite variance distributions

A random variable ξ, a result of a given experiment, is distributed according to the Lorentzian distribution:

$$P(\xi) = \frac{1}{[\pi(1+\xi^2)]} \tag{1}$$

The mean value of the observable ξ is exactly zero, but its variance is infinite and the central limit theorem cannot be applied. Nevertheless a large number n of experiments are done under the same conditions and average is performed in the usual way:

$$\bar{\xi} = \frac{1}{n}\sum_{i=1}^{n} \xi_i \tag{2}$$

- Use that the characteristic function of $P(\xi)$ is $\exp(-|t|)$ and determine the probability $P(\bar{\xi})$ of the random variable $\bar{\xi}$ for $n \to \infty$.

- Using the form of $P(\bar{\xi})$, determine what kind of information can be obtained from the average of several measurements.

- Consider instead the distribution:

$$P(\xi) = \frac{2}{\pi}\frac{1}{(1+|\xi|)(1+\xi^2)} \tag{3}$$

It can be shown that the characteristic function $\phi_\xi(t) = 1 + \frac{4}{\pi}t^2\ln(t)$ for $t << 1$, namely it has infinite variance, because its second derivatives diverges, since $\ddot{\phi}_\xi(t) = -\int d\xi P(\xi)\xi^2 \to \infty$. In this case we consider first the auxiliary variable:

$$Y = \frac{1}{\sqrt{n\ln(n)}}\sum_{k=1}^{n}\xi_k = \sqrt{\frac{n}{\ln n}}\bar{\xi} \tag{4}$$

resulting form the average over several independent experiments.

- Does exist an asymptotic distribution $P(Y)$ for large n?
- Is this in contradiction with the central limit theorem and the fact that the variance of $\bar{\xi}$ is infinite for any n?
- Instead of the variance consider instead a measure of the fluctuations δx of a random variable x weaker than the standard deviation assumption ($\delta x = \sqrt{Var(x)}$), namely:

  $$\delta x = \langle |x - \langle x \rangle| \rangle = \int dx P(x) |x - \langle x \rangle| \tag{5}$$

  and show that it is well defined also in this case, when fat tails in the distribution do not allow the computation of the variance.
- Using the previous results compute instead $\delta\bar{\xi}$ for $n \to \infty$.
- As before, what kind of information can be obtained from the average of several independent measurements?

Problem 2: Sum of uniformly distributed random variables

Consider a large number of samples for the random variable:

$$X = \sqrt{\frac{12}{n}} \sum_{i=1}^{n} \xi_i \tag{6}$$

for $n = 4$ and $n = 6$ where ξ_i are independent random variables uniformly distributed in the interval $[-\frac{1}{2}, \frac{1}{2})$.

- Apply the central limit theorem and show that X is distributed according to the normal distribution $\mathcal{N}(0, 1)$.
- Compute the exact distribution for finite n by using that the characteristic function associated to ξ_i is given by $\frac{2}{t}\sin(\frac{t}{2})$ and show that the random variable $Y = \sqrt{\frac{n}{12}} X = \sum_{i=1}^{n} \xi_i$ is distributed according to:

  $$P(Y) = \frac{1}{(n-1)!} \sum_{k=0}^{n} \binom{n}{k} \Theta(Y + \frac{n-2k}{2})(Y + \frac{n-2k}{2})^{n-1}(-1)^k \tag{7}$$

  where Θ is the Heaviside step function ($\Theta(x) = 0$ for $x < 0$ and $\Theta(x) = 1$ otherwise). Hint: Compute the n^{th} derivative $P^n(Y)$ of $P(Y)$ and then integrate back using that for $Y < -n/2$ $P(Y) = 0$ identically.
- Make a plot for $n = 6$ and $n = 4$ of $P(X)$ vs $\mathcal{N}(0, 1)$ of the numerical evaluated distributions and the analitycal ones.
- Compute the maximum percentage error Ξ of $P(X)$ as compared with $\mathcal{N}(0, 1)$ in the interval $(-2, 2]$, and determine how large should be n to have $\Xi \leq 1\%$.

Day 2

Problem 3: Ising model with arbitrary range

Consider the classical Heisenberg model:

$$H = \sum_{i,j=1}^{N} J_{i,j}\sigma_i\sigma_j \tag{8}$$

where $\sigma_i = \pm 1$ are classical Ising variables defined on each of the N sites, $i = 1, 2, \cdots N$, and J_{ij} is an arbitrary $N \times N$ matrix which is vanishing in the diagonal, i.e. $J_{ii} = 0$.

- Define a Monte Carlo code using a finite number of independent walkers with independent seed initialization.
- Use multithreading option to speed up the calculation.
- Parallelize the code using the hybrid OpenMP-mpi paradigm.
- Study a possible phase transition as a function of temperature for :

$$J(i,j) = -\begin{cases} \left[\frac{N}{\pi}|\sin(\frac{\pi(i-j)|}{N})\right]^{-\gamma} & i \neq j \\ 0 & i = j \end{cases} \tag{9}$$

where $\gamma = 1.25$