Exercises 2 for Computational Physics (physik760)
WS 2017/2018

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Further probability theory

1: For n independent random variables $X_i \sim \mathcal{N}_{\mu,\sigma_i}$, $i = 1, \ldots, n$ show that the weighted sum $Z = w_1 X_1 + \cdots + w_n X_n$ is normally distributed. What is its variance in terms of $\sigma_1, \ldots, \sigma_n$? Taking $w_1 + \cdots + w_n = 1$, for which system of weights does Z have minimal variance?

Demonstration of the central limit theorem

2: A direct practical application of the central limit theorem is the generation of random variables, whose distribution is a systematically improvable approximation of the normal distribution. To demonstrate this, draw N samples of K independent random variables $X_1, X_2 \ldots X_K$ from $\mathcal{U}_{[-1,1]}$ and look at the sums

$$Z_K = \sum_{k=1}^{K} \frac{X_k}{\sqrt{n}\sigma_k} \,.$$

(a) Derive the pdf for Z_2 analytically.

(b) For each $K = 2$, 4, 8, 12 sample $N = 10^6$ random numbers and plot a histogram of your observed distribution.

For a random variable X with cumulative distribution function F_X the Q-quantile μ_Q is defined implicitly by $F_X(\mu_Q) = Q$ for $0 \leq Q \leq 1$. In a QQ-plot the quantiles for two distributions are plotted against each other.

(c) Employ a QQ-plot to visually check how closely this approximates the implementation of normally distributed random numbers in your chosen programming language.

(d) How does this relate to example *2.5.1* from the lecture?

Box-Muller method

3: Show (analytically) that the algorithm

step 1: generate U, $V \sim \mathcal{U}\left([-1, 1]\right)$ until $S = U^2 + V^2 \leq 1$;

step 2: define $Z = \sqrt{-2\log(S)/S}$ and $X_1 = Z\,U$ and $X_2 = Z\,V$

is an alternative to the Box-Muller algorithm Example 3.2.4 in the lecture.

(a) What is the average number of generations in step 1?

(b) Implement the algorithm and compare it to the one above using QQ-plots or otherwise.

(c) Which algorithm is more efficient and why?

Simulation of the Ising model in two dimensions

Add to your simulation package for the Ising model.

4: Implement the *estimate* $|\bar{m}|$ of $\langle |m| \rangle$ by randomly drawing N spin configurations $s^{(1)}, \ldots, s^{(N)}$ according to the uniform distribution, i.e. the probabilty for drawing any individual configuration s is $\mathrm{P}_{\text{draw}}\,(s) = 1/2^{L_\sigma L_\tau}$, and using the weighted sum

$$\bar{m} = \frac{\sum\limits_{i=1}^{N} \exp\left(-\mathcal{H}(s^{(i)})/(k_B T)\right)\, |m|(s^{(i)})}{\sum\limits_{i=1}^{N} \exp\left(-\mathcal{H}(s^{(i)})/(k_B T)\right)} \,.$$

For $L_\sigma = L_\tau = 4,\, 5,\, 6$ observe the dependence of $\bar{m}$ on the number of samples N.

5: Implement the estimate $|\bar{m}|$ of $\langle |m| \rangle$ by using the *Metropolis algorithm* below to generate spin configurations $s^{(0)},\, s^{(1)},\, s^{(2)}, \ldots, s^{(N)}$. The algorithm will be covered in detail later in the lecture, for now we just want to have it ready to generate spin configurations efficiently.

step 1: given $s^{(i)}$ for $i \geq 0$, select a lattice site $y \in \mathbb{L}$, uniformly distributed, i.e. with probability $\mathrm{P}_{\text{select}}(x) = 1/\left(L_\sigma\, L_\tau\right)$ for all $x \in \mathbb{L}$;

step 2: make a trial configuration $\tilde{s}$ from $s^{(i)}$ by flipping the spin at y, i.e.

$$\tilde{s}_x = \begin{cases} s_x^{(i)} & x \neq y \\ -s_x^{(i)} & x = y \end{cases}$$

step 3: calculate the energy change $\Delta\mathcal{H}\left(\tilde{s}, s^{(i)}\right) = \mathcal{H}\left(\tilde{s}\right) - \mathcal{H}\left(s^{(i)}\right)$

- think about the difference in spin configurations to compute $\Delta\mathcal{H}$

step 4: calculate the acceptance probability $\mathrm{P}_{\text{accept}} = \min\left\{1,\, \exp\left(-\Delta\mathcal{H}\left(\tilde{s}, s^{(i)}\right)\right)\right\}$;
draw a random number r from the uniform distribution on the unit interval and set

$$s^{(i+1)} = \begin{cases} \tilde{s} & \text{if } r < \mathrm{P}_{\text{accept}} \\ s^{(i)} & \text{else} \end{cases} .$$

6: Estimate the magnetisation from the simple average over spin configurations, i.e. $|\bar{m}| = \sum\limits_{i=1}^{N} |m\left(s^{(i)}\right)|/N$

(a) take $J/T = 1/5$ on a $L_\sigma = L_\tau = 4$ lattice

(b) start with a random spin configuration

(c) check if you can reproduce your exact result by using every 10^{th} measurement, assuming no residual auto-correlation

(d) what about an $L_\sigma = L_\tau = 10$ lattice?

As a reference:

L	J/T	$\lvert\bar{m}\rvert$
4	1/5	0.337(5)
10	1/5	0.134(2)