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Introduction to Computer Simulation I

Homework 10

Due: Wednesday, 22 January 2020
(Along with answers submit the codes you used)

19. **One-dimensional random walk with continuous step width**

    The step widths s_i of a one-dimensional random walk shall be uniformly distributed between -1 and 1, i.e., $w(s_i) = 1$ for $s_i \in [-1, 1]$ and $w(s_i) = 0$ otherwise. The distance to the origin after N steps is then given by $x_N = \sum_{i=1}^{N} s_i$.

    Calculate first the expectation value and the variance of s_i with "paper and pencil". Next perform simulations of $10\,000 - 100\,000$ realisations of this random walk and measure $\langle x_N \rangle$, $\langle x_N^2 \rangle$, and $\langle x_N^2 \rangle - \langle x_N \rangle^2$ numerically. Determine in particular the probability distribution $P(x_N)$ of x_N for $N = 2$, 4, 8, and 12. Which known function resembles $P(x_N)$ for large N? Show them via plotting on the same graph.

20. **2D self-avoiding walks (SAWs)**

    Write a computer program for the exact enumeration of all self-avoiding random walks (SAWs) with up to $N = 20$ steps on a two-dimensional (2D) square lattice. In a relatively simple implementation one may simply work with N nested "do loops". On a "normal" PC the counting of all possible SAWs with up to $N = 20$ steps should not take longer than about 30 seconds.

    Use this exact method to determine the number Z of SAWs and their mean squared end-to-end distance $\langle R_{ee}^2 \rangle$ from the starting point (chosen to be the origin (0,0)) in dependence of N. Plot $\ln \sqrt{\langle R_{ee}^2 \rangle}$ against $\ln N$ and verify the scaling law $\sqrt{\langle R_{ee}^2 \rangle} \propto N^\nu$ with $\nu = 3/4$ in 2D. Similarly also the scaling law for Z can be tested. Show the corresponding plots.