Computational Science 2

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Seminar Exercises

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Exercise 4 (16.4.2019):

Integration using the Metropolis algorithm

from ***An Introduction to Computer Simulation Methods***,
Chapter 11, Problem 11.18

a) Use the Metropolis algorithm to estimate the average

$$\langle x \rangle = \frac{\int_0^\infty x p(x) dx}{\int_0^\infty p(x) dx}, \tag{1}$$

with $p(x) = e^{-x}$ for $x \geq 0$ and $p(x) = 0$ for $x < 0$. Compute the histogram $H(x)$ showing the number of points in the random walk in the region x to $x + \Delta x$, with $\Delta x = 0.2$. Begin with $n \geq 1000$ and maximum step size $\delta = 1$. Allow the system to equilibrate before computing the averages. Is the integrand sampled uniformly? If not, what is the approximate region of x where the integrand is sampled more often?

b) Calculate analytically the exact value of $\langle x \rangle$ using Eq. (1). How do your Monte Carlo results compare with the exact value for $n = 100$ and $n = 1000$ with $\delta = 0.1, 1,$ and 10? Estimate the standard error of the mean. Does this error give a reasonable estimate of the error? If not, why?

c) In part (b) you should have found that the estimated error is much smaller than the actual error. The reason is that the x_i are not statistically independent. The Metropolis algorithm produces a random walk whose points are correlated with each other over short times (measured by the number of steps of the random walker). The correlation of the points decays exponentially with a characteristic time τ. If τ is the characteristic time for this decay, then only points separated by approximately 2 to 3 times τ can be considered statistically independent. Compute the autocorrelation function

$$C(j) = \frac{\langle x_{i+j} x_i \rangle_{(n-j)} - \langle x_i \rangle_n^2}{\langle x_i^2 \rangle_n - \langle x_i \rangle_n^2} \tag{2}$$

using the arithmetic mean $\langle . \rangle_n$ and make a rough estimate of τ . Rerun your program and compute $n = 1000$ points. Group the data into 20 sets of 50 points each and 10 sets of 100 points each. If the averages of the sets of 50 points each are statistically independent (that is, if τ is significantly smaller than 50), then your estimate of the error for the two groupings should be approximately the same.