2009
Computer Exercises
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Session 1 : simple sampling - correction

1 Calculation of π

1. Fraction=(Area of circle)/(Area of the square), then $\pi = 4 * \text{Fraction} * (l/d)^2$
2. see corrected code
3. if Fraction=n/N and p is the probability to hit the circle, $\sigma_\pi^2 = 16(l/d)^4/N^2 \times \sigma_n^2$. $\langle n \rangle = \sum_{n=0}^{N} nC_N^n p^n (1-p)^{N-n} = Np$ and $\langle n^2 \rangle = \sum_{n=0}^{N} n^2 C_N^n p^n (1-p)^{N-n} = pN(1+p(N-1))$. With $p = \pi/4 * (d/l)^2$, $\sigma_\pi^2 = \pi(4(l/d)^2 - \pi)/N$.
4. No, because the error scale as $N^{-1/2}$

2 $2D$-Ising model

1. $|M_{min,max}| = N$ and $|NNC_{min,max}| = 2N$
2. see corrected code
3. after each matrix generation, update a histogram H representing the relative density of state. If you know the exact value of D for a given pair (M_0, NNC_0), you can normalize H to get $D(M, NNC) = H(M, NNC) \times D(M_0, NNC_0)/H(M_0, NNC_0)$.
4. see corrected code
5. $\langle X \rangle(T') = (\sum_{M,NNC} X(M, NNC) D(M, NNC) e^{NNC/T'})(\sum_{M,NNC} D(M, NNC) e^{NNC/T'})$
6. the system is symmetric, then $\langle M \rangle = 0$
7. see corrected code
8. see corrected code
9. $P(M = M_{max}) = 1/2^N \approx 8.10^{-31}$ for $N = 100$, and $P(M = 0) = C_N^{N/2}/2^N \approx 8.10^{-2}$ for $N = 100$.
10. we do not generate states which are majority at low temperatures.

3 $3D$ Self-avoiding walks

1. $\mathcal{N}_{IW}(N) = z^N$ and $R_{rms}^{IW}(N) = N^{1/2}$
2. see corrected code
3. $\mathcal{N}_{SAW}(N) = z^N \times$ fraction. If fraction= M/P+idem than 1.3, $\sigma_{\mathcal{N}_{SAW}}/\mathcal{N}_{SAW} = \sqrt{(\mathcal{N}_{IW}/\mathcal{N}_{SAW} - 1)/P}$
4. $R_{rms}^2 = \langle r_e^2 \rangle = 1/M \sum_{well-growth} r_e^2$, $\sigma_{R_{rms}^2}^2 \sim 1/M$
5. see corrected code
6. As N increases, the probability to get a SAW from a IW rapidly decreases ($P \sim (4.68/6)^N \approx 10^{-11}$ for $N = 100$). Therefore we do not generate enough SAW to sample correctly the ensemble.