Due Wednesday November 25th, 2020.

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1. **MCMC updates: Heat bath, Glauber, Metropolis.**

   Consider the one-dimensional ferromagnetic Ising model

   $$H = -\sum_i \sigma_i \sigma_{i+1} - B \sum_i \sigma_i \ .$$

   The L classical spins σ_i, arranged linearly, can each take values ± 1. For this problem, we will not care about the boundaries.

   While performing Markov chain Monte Carlo, we are considering changing the spin at the site $i = \alpha$. The current values of the neighboring spins are such that $\sigma_{\alpha-1} + \sigma_{\alpha+1} = S_n$. ($S_n$ could be -2, 0 or $+2$.)

   Note: you don't have to worry about proposal probabilities in these problems, as you've already decided to consider the site $i = \alpha$ as the flip candidate for this step.

   (a) If you are using the heat bath update algorithm, what are the probabilities for choosing the next value of σ_α to be $+1$ or -1?

   (The heat bath algorithm does not care about the current value of σ_α, but the probabilities will depend on the current values of the neighboring spins, through S_n.)

   (b) If you are using the Glauber update algorithm and the current value is $\sigma_\alpha = -1$, what are the probabilities for flipping and for not flipping?

   (c) If you are using the Glauber update algorithm and the current value is $\sigma_\alpha = +1$, what are the probabilities for flipping and for not flipping?

   (d) If you are using the Metropolis algorithm and the current value is $\sigma_\alpha = -1$, what are the probabilities for flipping and for not flipping?

   Find the Metropolis acceptance probabilities specifically for the following values of (S_n, B):

   $$(-2, -1.5), \quad (0, -1.5), \quad (+2, -1.5), \quad (-2, +1.5),$$

   (e) From your calculations, infer whether the heat bath algorithm is equivalent to the Glauber algorithm or/and to the Metropolis algorithm.

   Of course, any equivalence you find is only valid for the Ising model and unlikely to be true for another Stat-Phys Hamiltonian.

2. **Finite difference approximations for derivatives.**

Consider the spatial discretization with distance h between neighboring points.

(a) A symmetric finite difference approximation for the second derivative is

$$f''(x) \approx \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}$$

Show that the error in this approximation is of order h^2. You can do this by Taylor expanding $f(x \pm h)$ around x.

(b) The forward difference approximation for the first derivative is

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}.$$

Show that the error is linear in h. Show how things improve if you use the centered (symmetric) approximation

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

(c) You are using second-order discretization formulae to numerically solve a 1-dimensional boundary value problem. The error is $\approx 10^{-3}$ when you use step sizes $h = 0.01$ for your discretization. Explain what you expect the error to be when you use step sizes $h = 0.002$, i.e., if you increase the number of grid points fivefold.

(d) Wikipedia claims that

$$\frac{2f(x) - 5f(x+h) + 4f(x+2h) - f(x+3h)}{h^2}$$

is a forward difference approximation for the second derivative $f''(x)$, of second order. Prove or disprove.