Some discussion and/or hints on assignment 08.

There may be misprints, so use with care.

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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.)

   Discussion/Hint $\longrightarrow$

   Heat bath algorithm: the current value of σ_α does not matter.

   If the new value of σ_α is 1, then the energy terms involving this spin is

$$E_{(+1)} \;=\; -\,1\cdot\sigma_{\alpha-1} - 1\cdot\sigma_{\alpha+1} - B(1) = -S_n - B.$$

   There are other terms in the energy, of course, but they do not involve this spin. Since we are thinking about flipping the $i = \alpha$ spin, those terms are not going to be affected in this step.

   If the new value of σ_α is -1, then the energy terms involving this spin is

$$E_{(-1)} \;=\; -\,(-1)\cdot\sigma_{\alpha-1} - (-1)\cdot\sigma_{\alpha+1} - B(-1) = S_n + B.$$

So the thermal probabilities of the two choices are $\propto e^{-\beta E_{(+)}}$ and $\propto e^{-\beta E_{(-)}}$. Including a normalization constant we write the probabilities as

$$\frac{1}{N}e^{-\beta(-S_n-B)} \quad \text{and} \quad \frac{1}{N}e^{-\beta(S_n+B)}$$

with $N = e^{\beta(S_n+B)} + e^{-\beta(S_n+B)}$. The normalization constant should ensure that the sum of probabilities is 1.

Therefore, the probabilities of choosing $+1$ and -1 as the next value of σ_α are

$$\frac{e^{\beta(S_n+B)}}{e^{\beta(S_n+B)} + e^{-\beta(S_n+B)}} \quad \text{and} \quad \frac{e^{-\beta(S_n+B)}}{e^{\beta(S_n+B)} + e^{-\beta(S_n+B)}}$$

irrespective of the current value of σ_α. Do check that the sum of these probabilities are 1. They can also be written as

$$\frac{1}{1+\exp\big[-2\beta(S_n+B)\big]} \quad \text{and} \quad \frac{1}{1+\exp\big[2\beta(S_n+B)\big]}. \tag{1}$$

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(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?

Discussion/Hint $\longrightarrow$

The Glauber algorithm involves a proposal probability and an acceptance probability. We have already chosen this spin and are considering whether to flip. So only the acceptance probability is relevant. This is given by $1/(1+e^{\beta\Delta H})$.

If we flip from $\sigma_\alpha = -1$ to $\sigma_\alpha = +1$, the energy changes by

$$\Delta H = \big(-S_n - B\big) - \big(S_n + B\big) = -2(S_n + B)$$

So the probability for flipping to $\sigma_\alpha = +1$ is

$$\frac{1}{1+\exp\big[-2\beta(S_n+B)\big]}$$

and the probability for not flipping is

$$1-\frac{1}{1+\exp\big[-2\beta(S_n+B)\big]}=\frac{1}{1+\exp\big[2\beta(S_n+B)\big]}.$$

Note that the probabilities of ending up with $\sigma_\alpha=+1$ or with $\sigma_\alpha=-1$ are exactly the same as would be the case if we used the heat bath algorithm.

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(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?

Discussion/Hint $\longrightarrow$

Should be able to do yourself based on previous question. You should obtain exactly the same probabilities for ending up with $\sigma_\alpha=+1$ or with $\sigma_\alpha=-1$.

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(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):

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

Discussion/Hint $\longrightarrow$

The probability for flipping, i.e., accepting the move $-1\to+1$ for the $i=\alpha$ spin, is

$$\min\left(1,\frac{e^{-\beta E_{(+1)}}}{e^{-\beta E_{(-1)}}}\right)=\min\left(1,\frac{e^{-\beta(-S_n-B)}}{e^{-\beta(S_n+B)}}\right)=\min\left(1,e^{2\beta(S_n+B)}\right).$$

We can't tell whether $e^{2\beta(S_n+B)}$ is larger or smaller than 1, unless we know the values of S_n and B. But you can of course calculate this for every set of values given for (S_n, B).
The probability of not flipping (rejecting the proposed flip) is

$$1 - \min\left(1, e^{2\beta(S_n+B)}\right).$$

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(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.

Discussion/Hint $\longrightarrow$

The heat bath algorithm gives the probabilities listed in Eq. (1) for obtaining $+1$ or -1 in the next step, irrespective of the value in the current step.
The Glauber algorithm chooses $+1$ or -1 with the same probabilities, if the current value is -1 (shown explicitly) and also if the current value is $+1$ (left as an exercise). Thus the Glauber and heat bath algorithm happen to be identical for the Ising Hamiltonian.
This is accidentally true for the Ising model; it is not true, e.g., for the Potts model or the XY model.

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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.

Discussion/Hint $\longrightarrow$

Let's Taylor exapand:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + O(h^4)$$
$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + O(h^4)$$

The notation $O(h^4)$ means that the terms dropped involve h to the power 4 or higher. It also means that we do not care to write down or work out the exact coefficients of h^4. Hopefully you are familiar with this notation from somewhere. This is sometimes called Big-O notation.

Adding the two expressions and subtracting $2f(x)$ from the result,

$$f(x+h) + f(x+h) - 2f(x) = h^2 f''(x) + O(h^4)$$

You might be tempted to write $2O(h^4)$. That would defeat the purpose of the O-notation. We have already decided to ignore the coefficients of the dropped terms. It makes no sense to start adding them again.

Dividing by h^2 gives us

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

In other words, the error of the approximation is of order h^2.

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(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

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

Discussion/Hint $\longrightarrow$

Same calculation as before. The centered approximation has error of second order.

When we say that this is a second-order approximation, we mean that the error is of second order.

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(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.

Discussion/Hint $\longrightarrow$

If h is decreases fivefold, the error should decrease by a factor of $5^2 = 25$. This is the benefit of using a higher-order approximation.

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(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.

Discussion/Hint $\longrightarrow$

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