Computational Physics (Physics 760) Exercise #6

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Don't forget to make your code available to and useable by your tutor / grader!

6 [20 points] Critical Slowing Down

Consider the Ising model on a 2 dimensional square lattice with on N sites on a side (N^2 sites in total), and with periodic boundary conditions in both directions. Let the external magnetic field $h = 0$. The model is essentially indistinguishable from before

$$Z[\beta, J] = \sum_{\sigma} e^{-\beta H[J]} \qquad H[J] = -J \sum_{\langle \vec{x}, \vec{y} \rangle} \sigma_{\vec{x}} \sigma_{\vec{y}} \qquad \beta = 1/T \tag{1}$$

with dimensionful parameters (in units where $k_B = 1$). The difference from before is that x and y indicate positions on a 2D torus rather than a 1D ring. To pick a set of dimensionless units we can set $\beta = 1$, so that the only remaining parameter is J (if you prefer, in what follows everywhere you see J think to yourself 'oh yes, βJ').

Onsager showed that this model exhibits a phase transition: At high temperatures (small J) the system is disordered; at low temperatures (large J) the system is strongly correlated and spontaneously magnetizes. The transition happens at the *critical coupling*

$$J_c = \frac{1}{2} \log\left(1 + \sqrt{2}\right) \approx 0.4406867935097715\cdots \tag{2}$$

The net magnetization $M = \sum_{\vec{x}} \sigma_{\vec{x}}$, and the magnetization per site is $m = \frac{1}{N^2} M$. Onsager taught us that in the thermodynamic limit

$$\langle |m| \rangle = \begin{cases} 0 & J \leq J_c \quad \text{(warmer than critical)} \\ \left(1 - \frac{1}{\sinh^4(2J)}\right)^{1/8} & J > J_c \quad \text{(cooler than critical).} \end{cases} \tag{3}$$

We also know the energy per site

$$\epsilon = -J \coth(2J) \left(1 + \frac{2}{\pi}(2\tanh^2(2J) - 1) \times K\left(4\,\mathrm{sech}^2(2J)\tanh^2(2J)\right)\right) \tag{4}$$

where K is the *complete elliptic integral of the first kind*,

$$K(k^2) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2\theta}} \tag{5}$$

but be careful, sometimes that integral is called $K(k)$ without the square; it varies from package to package.

In Exercise 5 we studied a single $J = 0.5$ in the broken phase ($> J_c$). In this exercise we'll largely reuse code you've already written.

6.1 [5 points] Spontaneous Magnetization

- (2 points) Do an MCMC simulation with $N = 4$ for $J \in \{0.1, 0.2, J_c, 0.7, 0.8\}$. Pick a starting configuration that is checkerboarded with $+1$s and -1s, so that the starting m is close to 0. Make a histogram that shows the respective frequency of $|m|$.
- (1 point) Do it again for $N = 8$ and $N = 12$.
- (1 point) Using the already-generated ensembles, overlay the histograms for the different N at fixed J (one histogram per J).
- (1 point) Write a few sentences explaining the different tendencies as N grows. Can you see evidence for the thermodynamic limit? Of spontaneous magnetization?

6.2 [5 points] Scanning J

Perform importance-sampling via MCMC for $J^{-1} \in \{1.0, 1.1, 1.2, \cdots, 3.9, 4.0\}$ (a total of 31 different Js) for $N \in \{4, 8, 12\}$, generating at least 2000 configurations each time. Do some sort of uncertainty estimation, measuring $|m|$ and ϵ.

You'll reuse these ensembles below.

- (2 points) Plot $|m|$ with error bars indicating uncertainty as a function of J^{-1} (which is like T) over the exactly-known result.
- (2 points) Plot ϵ/J with uncertainties as a function of J^{-1} over the exactly-known result (don't miss the $/J$!)
- (1 point) Even though we know we have severe tunneling problems in the broken phase, these (should) come out basically OK. Explain this observation.

6.3 [5 points] The Spin-Spin Correlation Function

A *two-point correlation function* is an observable that depends on two spatial coordinates. The energy is built out of nearest-neighbor pairs, so is built from little short-range two-point functions.

The spin-spin two-point correlation function is[1]

$$C_{xy} = \langle \sigma_x \sigma_y \rangle \tag{6}$$

for all pairs of sites x and y (not just nearest neighbors). By translational invariance (leveraging pbcs) only the difference between x and y can matter, so we can define

$$C(\Delta x) = \frac{1}{\Lambda} \sum_x C_{x,x+\Delta x} \tag{7}$$

where $\Lambda = N^2$ is the 2-dimensional volume (number of sites).

- (1 point) What value should $C(0)$ take?
- (2 points) Implement it using Fourier acceleration (as in Exercise 4.3, but in 2 dimensions). Check your implementation produces the expected value at $\Delta x = 0$.
- (2 points) For each N (make 3 figures), plot the correlation function with uncertainties for $J^{-1} \in \{1.0, 2.0, 3.0, 4.0\}$ as a function of Δx. You can flatten it into a 1-dimensional figure, draw a 2- or 3-dimensional figure, whatever you think gets the message across.

(You might have to alter your bootstrap routine to handle an observable that isn't just a single number of every configuration.)

[1] It is common to only study the fluctuations from the mean value, in other words to study $\langle \sigma_x \sigma_y \rangle - \langle \sigma_x \rangle \langle \sigma_y \rangle$, or to study other cumulants for higher-order correlation functions.

6.4 [5 points] The Dynamical Exponent

The *dynamical exponent* z of a sampling algorithm for a physical system is defined through

$$\tau \propto \xi^z \tag{8}$$

where τ is the integrated autocorrelation time (a property of the Markov chain, and therefore algorithm-dependent) and ξ is the correlation length (an algorithm-independent property of the physics itself), and z indicates how well the proposal scheme makes big acceptable changes to the configurations (ie. how well it takes us through the whole probability space). Assuming $C \sim \#e^{-\Delta x/\xi}$, we can isolate ξ by computing

$$\xi = -\frac{1}{\partial_{\Delta x} \log C(\Delta x)} \qquad \text{or, equivalently} \qquad \xi = -\frac{C(\Delta x)}{\partial_{\Delta x} C(\Delta x)} \tag{9}$$

though which is more stable numerically may be context-dependent.

In this section you don't have to do any error analysis; just the gist is good enough.

Focus on C projected along one of the two axes of the lattice, so that we can think of it as one-dimensional.[2]

- (2 points) Actually, as written ξ depends on Δx. Implement one of formulations of the correlation length ξ (9), using one or the other right-hand sides.

ξ is only truly a constant on a pure exponential. This provides a good way to test if you've got your implementation right: put in a made-up pure-exponential-decay and see that you get out what you put in. However, real data is more complicated. Take as the 'true' ξ the value half-way between the origin ($\Delta x = 0$) and the boundary ($\Delta x = N/2$, for the one-dimensional projection).[3]

- (2 points) Compute ξ in this way on every ensemble you've got. Plot τ_m, the integrated autocorrelation time for the observable m (enforcing that $\langle m \rangle = 0$ no matter what the sample average is) against ξ.
- (1 point) Write a few sentences describing what you see. Do a rough estimate of z: eyeballing it is sufficient. Doesn't have to be anything fancy, as long as it's really based on what you see in your figure.

[2] This simplifies the finite differencing scheme you'll need, but is a perfectly valid thing to do—it just 'wastes' data in favor of easier thinking, a common trade. If you were spending huge quantities of computing time, though, you'd be crazy to throw away such juicy data.

[3] There are other ways to boil down the $\xi(\Delta x)$ function to a single estimate for ξ, but this one is easy.