Exercises

8.6 **Metropolis.**[1] (Mathematics, Computation) ①

The heat-bath algorithm described in the text thermalizes one spin at a time. Another popular choice is the Metropolis algorithm, which also flips a single spin at a time:

(1) pick a spin at random;

(2) calculate the energy $\Delta \mathbf{E}$ for flipping the spin;

(3) if $\Delta \mathbf{E} < 0$ flip it; if $\Delta \mathbf{E} > 0$, flip it with probability $e^{-\beta \Delta \mathbf{E}}$.

Show that Metropolis satisfies detailed balance. Note that it is ergodic and Markovian (no memory), and hence that it will lead to thermal equilibrium. Is Metropolis more efficient than the heat-bath algorithm (fewer random numbers needed to get to equilibrium)?

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[1]From *Statistical Mechanics: Entropy, Order Parameters, and Complexity* by James P. Sethna, copyright Oxford University Press, 2007, page 176. A pdf of the text is available at pages.physics.cornell.edu/sethna/StatMech/ (select the picture of the text). Hyperlinks from this exercise into the text will work if the latter PDF is downloaded into the same directory/folder as this PDF.