Some discussion and/or hints on assignment 06.

There may be misprints, so use with care.

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1. **python etc**

2. **Transition matrix for a Metropolis chain**

Consider the 2-site Ising model

$$H \;=\; -J\sigma_1\sigma_2$$

where the two classical spins, σ_1 and σ_2, can each take values ± 1.

We are performing Markov chain Monte Carlo on this (admittedly toy) model for inverse temperature β. At every step, one proposes a flip of one of the two spins chosen at random. The state space consists of 4 configurations:

$$A = (+,+) \qquad B = (+,-) \qquad C = (-,+) \qquad D = (-,-)$$

where, e.g., $(+,-)$ means $\sigma_1 = +1$ and $\sigma_2 = -1$.

(a) Write down the 4×4 transition matrix, also known as the row stochastic matrix or the Markov matrix.

Hint 1: In the Metropolis process, a transition probability is the product of the proposal probability and the acceptance probability. Make sure to work out both, for each pair of states.

Hint 2: Each row should sum to 1.

Discussion/Hint $\longrightarrow$

Let's first think of proposal probabilities.

If we are state A, then we could propose to flip the first spin (i.e., propose a move to C) or propose to flip the second spin (propose a move to B). So the proposal probabilities for $A \to B$ and $A \to C$ are each half, and the proposal probability for $A \to D$ is zero.

For $A \to B$, the Metropolis acceptance probability is x. Thus the $A \to B$ probability is

$$\text{proposal prob} \times \text{acceptance prob} = (1/2) \times x = x/2.$$

Similarly the $A \to D$ probability is $x/2$. The probability of remaining at A is therfore

$$1 - x/2 - x/2 = 1 - x.$$

So the first row of the stochastic matrix is

$$1-x \qquad x/2 \qquad x/2 \qquad 0.$$

I think the second row of the matrix, representing probabilities from B to various states, is

$$1/2 \qquad 0 \qquad 0 \qquad 1/2$$

but you will need to double-check.
The other two rows can be obtained using similar logic.

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(b) Based on the energies of the 4 configurations, what are the probabilities of these configurations in thermal equilibrium?
You might feel the urge to define $x = e^{-2\beta J}$.

Discussion/Hint $\longrightarrow$

In thermal equilibrium, the probability for finding the system in one of the high-energy states (B or C) must be x times the probability of finding the system in one of the low-energy states (A or D). This is because $x = e^{-\beta(dE)}$ where dE is the energy difference between the two types of states.
So the probability vector must be proportional to

$$\begin{pmatrix} 1 & x & x & 1 \end{pmatrix}$$

I hope this makes sense — please let me know if it doesn't.

This is unnormalized. To interpret the elements as probabilities, their sum would have to be unity. Thus the probability vector is

$$\frac{1}{2+2x}\begin{pmatrix}1 & x & x & 1\end{pmatrix} = \begin{pmatrix}\frac{1}{2+2x} & \frac{x}{2+2x} & \frac{x}{2+2x} & \frac{1}{2+2x}\end{pmatrix}$$

Note that normalization just means that the sum should be 1. (This is unlike normalization in quantum mechanics, where the sum of $||^2$ is 1, rather than the sum itself.)

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(c) Form a row vector combining the probabilities in the stationary (thermal) state.

Check that this is the left eigenvector of your stochastic matrix, corresponding to eigenvalue 1.

Discussion/Hint $\longrightarrow$

Note left eigenvector, not normal eigenvector.

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3. **QR method for eigenvalues**

The eigenvalues of a matrix can be found by successive QR decompositions. In an earlier assignment, you showed that if A is QR-decomposed as $A = Q_1R_1$, then the matrix $A^{(1)} = R_1Q_1$ has the same eigenvalues as A. We could do this repeatedly: We define $A^{(0)} = A$ and the sequence of matrices $A^{(k)}$ as

$$A^{(k-1)} = Q_kR_k \qquad \text{(QR decomp of } A^{(k-1)}\text{)}$$
$$A^{(k)} = R_kQ_k \qquad \text{(inverting order: next matrix defined)}$$

The $A^{(k)}$ each have the same eigenvalues. In addition, they have the property that successive $A^{(k)}$ are more and more diagonally dominant. If A is hermitian, for large k the iteration gives diagonal matrices. (If A is not hermitian, the large-k result might be instead a triangular matrix, which is good enough for obtaining eigenvalues.)

This is known as the QR method for obtaining eigenvalues. .....

(a) ....

(b) ....

(c) In the QR iteration, *why* do the matrices approach diagonal form?

Discussion/Hint $\longrightarrow$

I don't have a simple answer to this unfortunately. But watching the off-diagonals vanish is pretty remarkable.

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