Some discussion and/or hints on assignment 06.

There may be misprints, so use with care.

### 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,  $\sigma_1$  and  $\sigma_2$ , can each take values  $\pm 1$ .

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

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

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

(a) Write down the  $4 \times 4$  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.

### $Discussion/Hint \rightarrow$

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.

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

proposal prob × 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

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

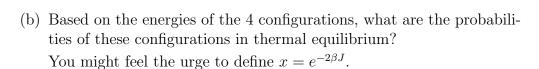
I think the second row of the matrix, representing probabilities from B to various states, is

$$1/2$$
 0 0  $1/2$ 

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but you will need to double-check.

The other two rows can be obtained using similar logic.



## $Discussion/Hint \rightarrow$

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

 $(1 \quad x \quad x \quad 1)$ 

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

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

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

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

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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