

1. Metropolis Simulation

1.a. MCMC transition matrix

The transition matrix W is written as

$$W(C \rightarrow C') = e^{-\beta(E(C')-E(C))} \quad (1.1)$$

$$W(C' \rightarrow C) = 1 \quad (1.2)$$

when $E(C') > E(C)$

1.a.1. Prove ergodicity

For ergodicity, it suffices to show that there exists one stationary probability.

$$P_{st}(C') = \sum_C P_{st}(C) W(C \rightarrow C') \quad (1.3)$$

Plugging in 1.1, one obtains

$$P_{st}(C') = e^{-\beta E(C')} \sum_C P_{st}(C) e^{\beta E(C)} \quad (1.4)$$

$$P_{st}(C') = e^{-\beta E(C')} \alpha \quad (1.5)$$

where α is just a constant.

1.a.2. Prove detailed balance w.r.t. equilibrium weight

$$\frac{W(C \rightarrow C')}{W(C' \rightarrow C)} = \frac{e^{-\beta(E(C')-E(C))}}{1} \quad (1.6)$$

Rearranging 1.6, one obtains

$$e^{-\beta E(C)} W(C \rightarrow C') = e^{-\beta E(C')} W(C' \rightarrow C) \quad (1.7)$$

1.b. Metropolis algorithm implementation

The code, `ising_MCMC.py`, is appended. For system sizes, 4×4 , 8×8 , and 32×32 , 2500-sweep runs were run at 1.5, 2.0, 2.2, 2.3, 2.6 and 3.0 kT (coupling constant $J = 1$). Plots of $E(\tau)$ and $M(\tau)$ are attached. To run the program:

```
for size in 4 8 32; do
  for temperature in 1.5 2.0 2.2 2.3 2.6 3.0; do
    ./ising_MCMC.py $size $temperature --verbose \
      --out-pkl 2500_sweeps_${size}x${size}_${temperature}kT.pkl \
      | tee 2500_sweeps_${size}x${size}_${temperature}kT.log
  done
done
```

1.c. Simulation results

χ in the limit of high temperatures. Using Mathematica,

1.d. Critical exponents

1.e. Finite size scaling

2. Swendsen-Ma MCRG