PHYS 177
winter 2019

lecture 14: practical MCMC

learning goals
- state practical considerations for implementing an MCMC sampler

main rule of MC is to satisfy detailed balance

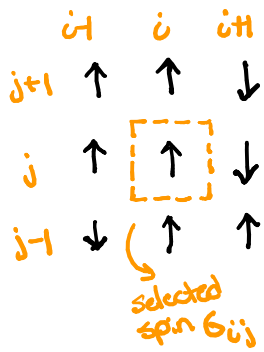
Metropolis rule gives

$$T_{ij} = \begin{cases} 1 & \text{if } E_j < E_i \\ e^{-\beta(E_j - E_i)} & \text{if } E_j > E_i \end{cases}$$

but how to put this into practice?

random transitions: use RNG to get a random # $[0,1)$, call it r
if random $r < T_{ij}$, change to new configuration

mechanics: probably need to make $T_{ij} = 0$ for almost all configurations i, j
make small moves with high probability of acceptance



in Ising model, select a spin at random to attempt to flip

change in energy is $E(\underline{\sigma}_{flip}) - E(\underline{\sigma}) = \Delta E$

$$\Delta E = -2J\sigma_{ij}(\sigma_{i-1j} + \sigma_{i+1j} + \sigma_{ij-1} + \sigma_{ij+1})$$

if $\Delta E < 0$, flip automatically
else flip w/ probability $e^{-\beta \Delta E}$

this means you will need to track and update parameters that represent the configuration

computations: as # samples $\to \infty$, the empirical distribution of configurations approaches the true distribution

if your system is small, you may be able to record an entire history of configurations throughout the simulation

if the system is large, may have to compute averages as you go along

in complex systems, early parts of simulation are often discarded (far from "equilibrium")

*notebook example, spin chain