PHYS 177
winter 2019

lecture 13: Markov chain Monte Carlo

learning goals
- apply MCMC to sample from probability distributions

equilibrium properties determined by average over $P(\underline{\sigma})$, but this is impossible to do when variables are coupled and N is large

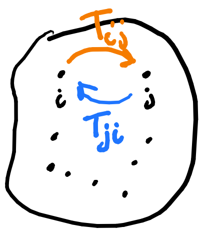
we can solve this problem by <u>randomly sampling</u> from $P(\underline{\sigma})$, but this is also hard because

$$P(\underline{\sigma}) = \frac{e^{-\beta E(\underline{\sigma})}}{Z}$$

normalization also requires sum over $\underline{\sigma}$!

arbitrary!

<u>solution</u>: start with a probability distribution $P_0(\underline{\sigma})$ and write down dynamics to evolve it towards $P(\underline{\sigma})$



call the transition probability from the configuration labeled i to the one labeled j T_{ij}, then we want

$$\frac{dP_i}{dt} = \underbrace{\sum_j T_{ji} P_j}_{\text{flux in}} - \underbrace{\sum_j T_{ij} P_i}_{\text{flux out}}$$

Gibbs distribution

to be $\emptyset$ for all configurations i <u>if</u> $P = P(\underline{\sigma})$

<u>detailed balance</u> ensures that this is true, set

$$P_i T_{ij} = P_j T_{ji}$$ so that all probability fluxes balance exactly

this is satisfied if we choose $$\frac{T_{ij}}{T_{ji}} = \frac{P_j}{P_i} = \frac{e^{-\beta E_j}/Z}{e^{-\beta E_i}/Z} = e^{\beta(E_i - E_j)}$$

tricky normalization Z <u>cancels</u>!

detailed balance only sets the ratio of transition probabilities, so we can choose

common choice is the Metropolis rule : $$T_{ij} = \begin{cases} 1 & \text{if } E_j < E_i \\ e^{-\beta(E_j - E_i)} & \text{if } E_j > E_i \end{cases}$$

<u>note</u>: $T_{ij} = T_{ji} = 0$ also ok, all possible transitions need not have T_{ij} nonzero

*notebook example, two spin system