Lec 15

Last Topic - More Monte Carlo

- To simulate Stochastic i.e. random process, we need to encode/approximate it.
- We use the Markov Chain approximation, considering it is a Markovian process.
    - Let us consider a dynamical system that evolves through states $S_1, S_2, \cdots, S_n$ at time-points $t_1, t_2, \cdots, t_n$
    - Ergocidity from Stat Mech : Ensemble average (average over a large number of states) = time average (average over a long time evolution of a system)
        - Effectively means that a system chaotically and effectively visits all points, or a point close to it.
    - Say a system occupies a state $x_{t_n} = s_n$ at t_n. Thus the probability that the system occupies a paricular state s' at time t_n is conditional on it's history

$$P(x_{t_n} = s' | x_{t_{n-1}} = s_{n-1}, x_{t_{n-2}} = s_{n-2}, \cdots)$$

    - However, it is cumbersome to store the entire history of the system. Most systems also don't show such deep hysterical behavior. Thus we can approximate to just last state dependence.

$$P(x_{t_n} = s' | x_{t_{n-1}} = s_{n-1})$$

        - This is the Markov Chain of states.
    - We can use a weight matrix to denote this : $W_{ij} = W(S_i \to S_j) \equiv P(x_{t_n} | s_j | x_{t_{n-1}} = s_i)$, where $\{s_i\}_i$ is our sample space of states, phase space.
    - If $P(x_{t_n} = s_j), P(x_{t_n} = s_i)$ are the total probability, then

$$P(x_{t_n} = s_i) = \sum_j P(x_{t_n} = s_j | x_{t_{n-1}} = s_i) P(x_{t_{n-1}} = s_i)$$

    - This leads to the master equation of probabilites.

$$\frac{dP(s_i, t)}{dt} = -\sum_j W_{i \to j} P(s_j, t) + \sum_j W_{j \to i} P(s_i, t)$$

        - At equilibrium, the we reach the low energy solution. This is called Detailed Balance.

$$\sum_j W_{i \to j} P_{eq}(s_j, t) = \sum_j W_{j \to i} P_{eq}(s_i, t)$$

            - Sir says that actually a strong condition, $W_{i \to j} P_{eq}(s_j, t) = W_{j \to i} P_{eq}(s_i, t)$ holds, but I don't follow on how this comes about.
    - Sir is talking about states and their evolution being like $(1_1\ 2_2\ 3_3\ 4_4\ 5_5\ 6_6) \to (1_1\ 2_2\ 3_3\ 4_4\ 5_6\ 6_5)$, where 5_6 means particles 5 being in position 6/site 6. Thus $5 \to 6$ is particle at site 5 going to site 6, so no summations are required. I am considering it to be like non-interacting particles evolving, basically an ensemble. I don't know why he is making this so confusing with the notation.

- We get this kind of a probability matrix

$$W_{i\to j} = \begin{bmatrix} 0.1 & 0.5 & 0.4 & 0 & 0 & 0 \\ 0.3 & 0.3 & 0 & 0 & 0.4 & 0 \\ 0.1 & 0 & 0.2 & 0 & 0 & 0.7 \\ 0 & 0.3 & 0 & 0.2 & 0.4 & 0.5 \\ 0 & 0.4 & 0 & 0 & 0 & 0.6 \\ 0 & 0 & 0.2 & 0.2 & 0.2 & 0.4 \end{bmatrix}$$

- It has a few properties, e.g. it is always square with non-negative entries, and sum over a row, $\sum_j W_{i\to j} = 1$ is 1, so probability is conserved.

- Then we discussed the Metropole Algorithm again.
  - The system is in the n-th state $p_n = e^{-E_n/k_BT}/Z$, $\frac{W_{n\to m}}{W_{m\to n}} = \frac{P_m}{P_n} = e^{-\Delta E/k_BT}$
  - Metropolis(?) Algorithm
    - If the energy of the new state is of lower energy, we accept it.
    - If the energy of the new state is slightly higher $E_f < E_i + \delta$, then we accept the state with the probability $\propto e^{-\beta(E_f-E_i)}$, $p = \frac{e^{-\beta(E_f-E_i)}}{1+e^{-\beta(E_f-E_i)}}$
    - ~~If $E_f \gg E_i$, then reject outright. This prevents random fluctuations to shoot us very high in the energy landscape.~~ Nope, accept anyway.
    - Keep repeating
- Endsem
  - 1 page of formulae allowed
  - Everything since Midsem.