Random processes and Monte Carlo Simulation

- Importance Sampling and Statistical mechanics.
- Markov Chain Monte Carlo.
- Simulated Annealing

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- We can take the approach that we will calculate the sum via Monte Carlo (random sampling). In that case, we will chose N random states, $k = 1 \ldots N$ and calculate:

$$\langle X \rangle \simeq \frac{\sum_{k=1}^{N} X_k P(E_k)}{\sum_{k=1}^{N} P(E_k)}$$

The denominator is needed to normalize the weighted average correctly..

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- That is most of the states we choose will have have very little contribution to the original average.
- Typically, only a small fraction of states will actually contribute significantly to the value of the sum – and choosing states at random, we are unlikely to pick these important states and hence get a poor estimate of the true value.
- But this is ideally suited for importance sampling!

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- Making the particular choice $g_i = X_i P(E_i)/w_i$:

$$\left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w = \frac{\sum_i X_i P(E_i)}{\sum_i w_i} = \frac{\langle X \rangle}{\sum_i w_i}$$

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- Then:

$$\langle X \rangle = \left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w \sum_i w_i$$

- We can evaluate this expression approximately by selecting a set of N sample states randomly but non-uniformly such that the probability of choosing a state i is:

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- In this case, we get:

$$\langle X \rangle \simeq \frac{1}{N} \sum_{k=1}^{N} \frac{X_k P(E_k)}{w_k} \sum_i w_i$$

Note that the first sum is only over the states that we sample, but the second sum is over all states i and has to be calculated analytically!

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- In other words, we just choose N states in proportion to their Boltzmann probabilities and take the average of X over them..
- Unfortunately, we are not done yet – The catch is that it is not easy to pick states with probability $P(E_i)$. This is because to calculate $P(E_i)$, we need to know the partition function, Z.

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- For the new state, instead of choosing randomly, we will make some change (usually small) to the state i so as to create a new state.
- The choice of the new state is determined probabilistically by a set of transition probablilities T_{ij} that give the probability of changing from state i to j.

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- When we take many steps and generate the entire chain, the complete set of states that we move through is a correct sample of the Boltzmann distribution and we can average any quantity we like over these states.

- The trick lies in choosing T_{ij}:

$$\sum_j T_{ij} = 1$$

and also

$$\frac{T_{ij}}{T_{ji}} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j}/Z}{e^{-\beta E_i}/Z} = e^{-\beta(E_j - E_i)}$$

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  In other words, we are choosing a particular value for the ratio of the probability to go from i to j and the probability to go back from j to i.
- The Boltzmann distribution is a fixed point of the Markov chain.

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- We will accept or reject the new state with probability P_a:

$$P_a = \begin{cases} 1 \quad \text{if } E_j \leq E_i, \\ e^{-\beta(E_j - E_i)} \quad \text{if } E_j > E_i \end{cases}$$

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- This scheme will satisfy all the criterion of the transition probability: $\frac{T_{ij}}{T_{ji}} = e^{-\beta(E_i - E_j)}$

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6. Go to step 2.

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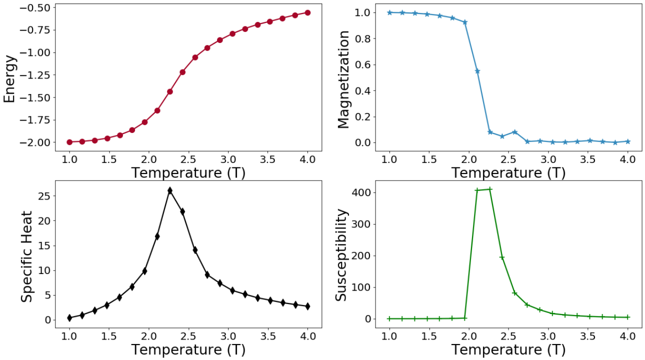
- One has to choose a move set such that every possible state is reachable.
- That the Markov chain will go to Boltzmann distribution is proved but, how long will it to take to reach equillibrium is not known.

$$E = -\sum_{\langle ij \rangle} s_i s_j$$



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- Then in the limit $T \to 0$, $\beta \to \infty$ and $e^{-\beta E_i} \to 0$ except in the ground state where $e^0 = 1$.
- This in this limit:

$$P(E_i) = \begin{cases} 1 & \text{for } E_i = 0 \\ 0 & \text{for } E_i > 0 \end{cases}$$

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- As one lowers the temperature, the system should land in the ground-state!