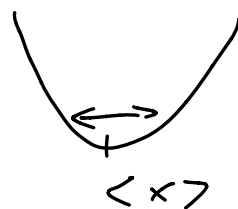


HW-1 ideas

Limit theorems, law of large numbers

$$X = \frac{X_1 + X_2 + \dots + X_N}{N} \quad I(x)$$

$$P(X=x) \sim e^{-N I(x)}$$



$$e^{-N}$$

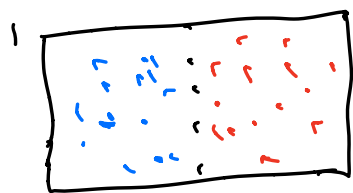
$$I(x) = I''(x_0)(x-x_0)^2$$

$$P(f) = e^{-N(f-1/2)^2}$$

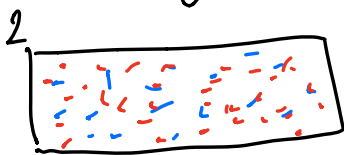
$$B_N(n) = \frac{N!}{n!(N-n)!}$$

$$\ln N! \approx \int_1^N \ln x dx = N \ln N - N$$

$$\ln B_N(n) = -N \left(f \ln f + (1-f) \ln(1-f) + \ln 2 \right) \\ -N \quad I(f)$$



\Downarrow

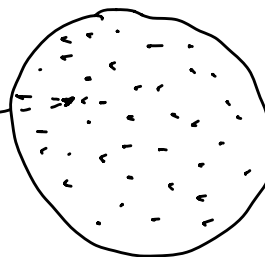


$$S' = k_B \ln \Omega(N, V, E)$$



Ω_1

\Rightarrow



Ω_2

$\Omega(N, V, E)$

$$S_2 > S_1$$

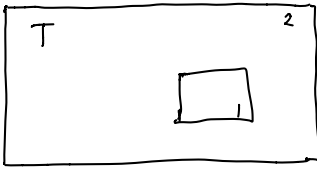
$$\rho = \frac{1}{\Omega}$$

Lattice models

$$N, \Omega = \frac{N!}{n!(N-n)!}$$

$$\begin{array}{l} \epsilon \text{ ————— } n \\ 0 \text{ ————— } N-n \\ E = n\epsilon \end{array}$$

$$\begin{array}{l} (N, V, E) \quad (N, V, T) \\ (N, P, T) \end{array}$$



$$E_0 = E_1 + E_2 \quad \begin{array}{l} \text{total energy} \\ \text{distributed between} \\ E_1 \text{ and } E_2 \end{array}$$

$$\Omega(E_0) = \sum_{\epsilon=0}^{E_0} \Omega_1(\epsilon) \Omega_2(E_0 - \epsilon)$$

$$\ln \Omega_2(E_0 - \epsilon) \approx \ln \Omega_2(E_0) - \frac{\partial \ln \Omega_2(E_0 - \epsilon)}{\partial (E_0 - \epsilon)} \epsilon$$

$$= \ln \Omega_2(E_0) - \epsilon \left(\frac{\partial \ln \Omega_2(E_0)}{\partial E_2} \right) + \dots$$

$$= \ln \Omega_2(E_0) - \frac{\epsilon}{k_B T} = \frac{S_2(E_0)}{k_B} - \beta \epsilon \quad \beta = \frac{1}{k_B T}$$

$$\Omega(E_0) e^{-S'_2(E_0)} = \sum_{\epsilon} \Omega_1(\epsilon) e^{-\frac{\epsilon}{k_B T}}$$

$$S(E_0) - S_2(E_0) = k_B \ln Z(\beta)$$

$\left(\begin{array}{l} \text{thermodynamics} \\ \text{ensemble} \end{array} \right) \rightarrow S(E_0) = S_1(\bar{E}) + S_2(E_0 - \bar{E})$
 \bar{E} - thermodyn. average energy

$$S'_1(\bar{E}) + S_2(E_0 - \bar{E}) - S_2(E_0) = k_B \ln Z(\beta)$$

$$S_1(\bar{E}) - \frac{\bar{E}}{T} = k_B \ln Z(\beta)$$

$$- \frac{(\bar{E} - TS)}{T} = k_B \ln Z(\beta)$$

$$- \frac{A}{T} = k_B \ln Z(\beta)$$

$$A = -k_B T \ln Z(\beta, N, V) \quad NVT$$

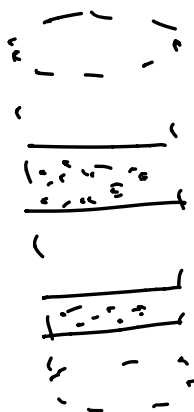
$$S = k_B \ln \Omega(N, V, E) \quad NVE$$

$$Z_\beta = \sum_{\epsilon} e^{-\beta \epsilon} \quad \text{vs } \Omega(E)$$

$$P(E) \sim \Omega(E_0 - \varepsilon) \Omega(\varepsilon) \sim e^{-\beta \varepsilon}$$

$$Z_\beta = \sum_i e^{-\beta \varepsilon_i} = \sum_{E_v} \Omega(E_v) e^{-\beta E_v}$$

$$Z_\beta = \int dE \Omega(E) e^{-\beta E}$$

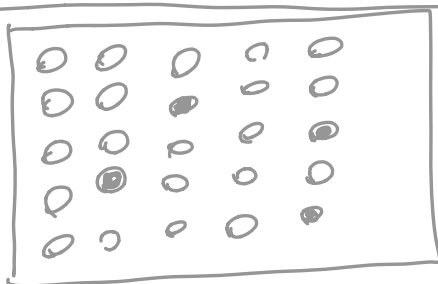


$$\frac{n(h+\Delta h)}{n(h)} \sim e^{-\beta (mg\Delta h)}$$

$$P(E) \sim \Omega(E) e^{-\beta E}$$

$$\sim e^{-\beta E} e^{\frac{S}{k_B}} = e^{-\beta(E - TS)}$$

$$e^{-\beta N(\varepsilon - TS)} = e^{-\beta N I}$$



N - sites

n - defects

$$E = n \varepsilon$$

$$\Omega(E) = \frac{N!}{n! (N-n)!}$$

$$\begin{aligned}
Z(\beta) &= \sum_{n=0}^N \Omega(n) e^{-\beta n E} = \\
&= \sum_n \frac{N!}{n! (N-n)!} e^{-\beta n E} = \\
&= \sum_n \frac{N!}{n! (N-n)!} p^n q^{N-n} = \\
&= \sum_n \frac{N!}{n! (N-n)!} (e^{-\beta E})^n 1^{N-n} = \\
&= (1 + e^{-\beta E})^N
\end{aligned}$$

$$\begin{aligned}
Z(\beta) &= \sum_{\substack{\epsilon_1 = \epsilon \\ \epsilon_1 = 0}} \sum_{\substack{\epsilon_2 = \epsilon \\ \epsilon_2 = 1}} \dots e^{-\beta \sum \epsilon_i} = \\
&= (1 + e^{-\beta E})^N = Z_1^N
\end{aligned}$$

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

$$Z(\beta) = \int \Omega(E) e^{-\beta E} dE \sim \langle e^{-\beta E} \rangle$$

$$\sum_i E_i P(E_i) = \langle E \rangle = \frac{\sum E_i e^{-\beta E_i}}{Z}$$

$$= -\frac{1}{Z_\beta} \frac{\partial}{\partial \beta} Z_\beta = -\frac{\partial}{\partial \beta} \ln Z_\beta = \langle E \rangle$$

Z_β - moment generating function

$$\sum p_i E_i^2 - \left(\sum p_i E_i \right)^2 = \frac{\partial^2}{\partial \beta^2} \ln Z$$
$$= - \frac{\partial}{\partial \beta} \langle E \rangle$$

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

$$\langle E^2 \rangle - \langle E \rangle^2 = k_B T C_V \sim O(N)$$

$$\frac{(\langle E^2 \rangle - \langle E \rangle^2)^{1/2}}{\langle E \rangle} \sim \frac{\sqrt{k_B T C_V}}{\langle E \rangle} \sim O(N^{-1/2})$$