

# Jaynes's principle and statistical mechanics

## Ulrich Schollwöck, Bayes Forum, 11.1.2019

$$I[P] = -k_B \sum_{\{P_i\}}^N P_i \ln P_i$$

*ignorance*

$$0 \leq I[P] \leq \ln N$$

- quantum case.

- continuous case (classical phase space)

$$I[P] \neq -k_B \int dx p(x) \ln p(x)$$

$\xrightarrow{N \rightarrow \infty}$

$$\Delta x \quad p(x) = (x_{i+1} - x_i) p_i$$

*well-defined*

point prob. density

$$q(x) \quad \int dx q(x) = 1$$

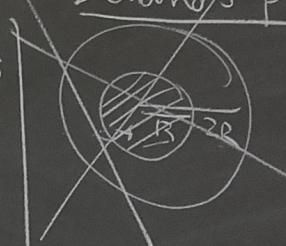
*PDFs*

$$I[P] = -k_B \int dx (p(x)) \ln \frac{(p(x))}{(q(x))}$$

What is  $q(x)$ ?

consistency argument:  
fixes  $q(x)$  in  
stat mech!

Bertrand's paradox



$$\text{data } D \rightarrow P = \arg \max_{Q|D} I[Q]$$

exact data  $\tilde{D}$   
means as data  $\bar{D}$

$$\underline{\langle g \rangle} \stackrel{!}{=} \langle g \rangle = \sum p_v g_v$$

$\underline{g}$ : time average

$$p_v = \frac{1}{Z(\beta)} e^{-\beta g_v} \quad Z(\beta) = \sum_v e^{-\beta g_v}$$

$$\underline{\langle g \rangle} \stackrel{!}{=} \langle g \rangle = - \frac{\partial}{\partial \beta} \ln Z(\beta)$$

$$\underline{\langle g \rangle} = \langle g \rangle(\beta)$$

$$\xrightarrow{\text{inv}} \beta = \beta(g)$$

$$-\frac{\partial g}{\partial \beta} = \frac{\partial^2}{\partial \beta^2} \ln Z(\beta) = \langle g^2 \rangle - \langle g \rangle^2 > 0$$

discussion:  $\boxed{g \rightarrow \beta}$      $\boxed{\beta \rightarrow g}$

$$I_{\max}(g) = \ln Z(\beta) - \beta \underbrace{\frac{\partial}{\partial \beta} \ln Z(\beta)}_{=g}$$

Legendre-Transfo  $I_{\max}[g]$   $\boxed{\text{concave}}$

$\ln Z(\beta)$  convex

# Stat. Phys.

data  $D$  macrodata fixing  
a TD equilibrium state | macrostate

proposition:  $X \in \text{Phase space}$  | microstate.  
 $| \psi \rangle \in \text{Hilbert space}$

a priori th: cl., /q. mech.

Post.  $S_{\text{eq}}(D) = \arg \max_{\rho|D} I[\rho]$

$$\hat{\rho} = \langle \hat{\rho} \rangle = \text{tr } S_{\text{eq}} \hat{\rho} \quad \text{prediction}$$

$$\langle \hat{\rho}^2 \rangle - \langle \hat{\rho} \rangle^2 =$$

$$\lambda \hat{\rho} / K(\hat{\rho})$$

predictability

$S_{\text{eq}}$  is not dist. of  
microstates.

$$\bar{\rho} = \frac{1}{T} \int_0^T \rho(t) dt$$



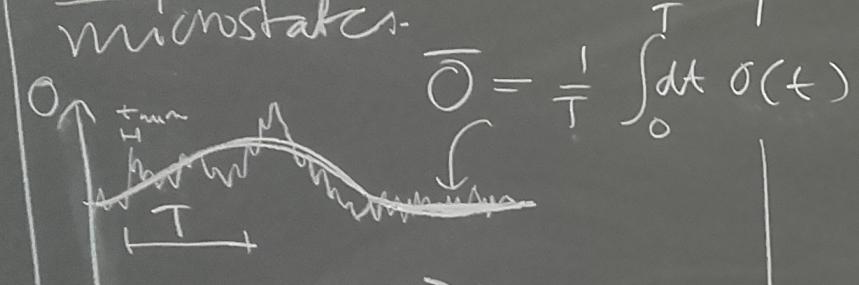
$$\bar{\rho} = \langle \rho \rangle$$

problem!  
 $T \rightarrow \infty$   
time-average = ensemble average

What is  $S$ ?

$$S_p[\rho] = I[\rho]$$

$S_{eq}$  is not dist. of microstates.



$$\boxed{\bar{O} = \langle O \rangle} \quad \text{problem!} \quad T \rightarrow \infty$$

time-average = ensemble average

What is  $S$ ?

$$S_p[S] = I[S]$$

$$S_{SP}(D)$$

$$= I[S_{eq}(D)] - \max_{S_{SP}} S_{SP}[S]$$

extremal principle

looks mathematically like  $S_{TD}$ .

show that  $S_{SP} = S_{TD}$  via

laws of thermodynamics

hypothesis

$$S_{TD}(D) \stackrel{T \rightarrow \infty}{=} S_{SP}(D).$$

2nd law

$$I[\rho] = -k_B \int d\mu(\underline{x}) \rho(\underline{x}) \ln \frac{\rho(\underline{x})}{\rho_0(\underline{x})} \quad \underline{x} = (q, p)$$

$$\rho_0(\underline{x}) = \text{const.}$$

$$I[\rho] = -k_B \int d\mu(\underline{x}) \rho(\underline{x}) \ln \rho(\underline{x})$$

Jacobi-det of can. trans = 1  $(q, p) \rightarrow (Q, P)$

$$\begin{aligned} \text{Ham. eq.} \\ \dot{P} &= \{H, q\} \\ \dot{q} &= \{H, P\} \end{aligned}$$

$K[\underline{S}(t_0)]$

If  $I[\underline{S}]$  is an information measure, then it must be t-indep under dynamics

$$\boxed{\frac{dI}{dt} = 0}$$

$$\underline{V} = \left( \frac{\partial H}{\partial P}, -\frac{\partial H}{\partial Q} \right)$$

Liouville:  $\boxed{\frac{\partial \rho}{\partial t} + \underline{V} \cdot \nabla \rho = 0}$



$$\rho_0(x, p)$$

$$\begin{aligned}
 0 &= \frac{dI}{dt} = - \int d\underline{x} \left( \frac{\partial \underline{S}}{\partial t} \ln \frac{\underline{S}}{\rho_0} + \frac{\partial \rho}{\partial t} \right) \\
 &\quad \text{[using } \frac{dI}{dt} = \int d\underline{x} \underline{V} \cdot \nabla \ln \underline{S} \text{]} \\
 &= + \int d\underline{x} (\underline{V} \cdot \nabla \rho) \ln \frac{\underline{S}}{\rho_0} \\
 &= - \int d\underline{x} \rho \underline{V} \cdot \nabla \ln \frac{\underline{S}}{\rho_0} \\
 &= - \int d\underline{x} (\underline{V} \cdot \nabla \underline{S} - \underline{S} \underline{V} \cdot \nabla \ln \rho_0) \\
 &= \left( \int d\underline{x} (\rho \underline{V} \cdot \nabla \ln \rho_0) \right) \\
 \Rightarrow \underline{V} \cdot \nabla \ln \rho_0 &= 0 \quad (\Rightarrow \sum \ln \rho_0 = 0)
 \end{aligned}$$

$\frac{d}{dt} \int d\underline{x} \rho = 0$

$\left(\frac{1}{X}\right)$

$$\bar{O} = \langle O \rangle = \text{avg } O = \frac{1}{N} \sum X_i$$

measure  $\langle \bar{O} \rangle = \cancel{\int_0^T dt \langle O(t) \rangle} = \langle O \rangle$

$$\bar{\bar{O}} \stackrel{?}{=} \langle O \rangle$$

$$\boxed{\langle \bar{O} \rangle = \langle O \rangle}$$

$$\langle \bar{O}^2 \rangle - \langle \bar{O} \rangle^2 \cancel{\approx \langle O^2 \rangle - \langle O \rangle^2}$$

$$\bar{\bar{O}} = \langle \bar{O} \rangle$$

$$\boxed{\bar{O} = \langle O \rangle}$$

$$\Delta^2 \bar{O} = \frac{1}{T^2} \iint_0^T dt_1 dt_2 (\langle O(t_1) O(t_2) \rangle - \langle O(t_1) \rangle \langle O(t_2) \rangle)$$

$$= \frac{2}{T^2} \int_0^T d\tau (T-\tau) C(\tau)$$

$$\sim \frac{1}{T} \left| \begin{matrix} E(t) \\ \downarrow \end{matrix} \right|$$

$$\rightarrow (\Delta \bar{O} \sim \frac{1}{\sqrt{T}})$$

$$\int_0^\infty C(t) dt < \infty$$

$$\int_0^\infty C(t) t dt < \infty$$

$$\Delta \bar{O} = \frac{1}{T} \int dt (O(t) - \bar{O})^2$$

$$\boxed{\langle \bar{\delta^2 O} \rangle = \Delta^2 O - \cancel{\bar{\delta^2 O}}}$$

$$\overbrace{C = \langle O(0) O(t) \rangle - \langle O \rangle^2}^? \\ (O(t) - \bar{O})(O(t') - \bar{O})$$