

$$F = U - TS \quad ^{-13-}$$

↓ ↑
 mean entropy
 energy
 (internal
 energy)

- $T = \frac{1}{\beta}$
 ↑
 temperature

Proof

$$\ell = F = -\frac{1}{\beta} \log Z(\beta) = -\frac{1}{\beta} \log \sum_i e^{-\beta E_i}$$

$$r = U - TS \quad \text{to show } \ell = r$$

$$p_i = \frac{1}{Z} e^{-\beta E_i}$$

$$\begin{aligned} \log p_i &= \log \frac{1}{Z} + \log (e^{-\beta E_i}) \\ &= -\log Z - \beta E_i \end{aligned}$$

$$\begin{aligned} \Rightarrow S &= - \sum_i p_i \log p_i \\ &= + \sum_i p_i (\log Z + \beta E_i) \\ &= \log Z \cdot 1 + \beta \underbrace{\sum_i p_i E_i}_U \end{aligned}$$

$$\begin{aligned} r &= U - TS = U - \frac{1}{\beta} S \\ &= \sum p_i E_i - \frac{1}{\beta} \log Z - \sum p_i E_i \end{aligned}$$

$$= -\frac{1}{\beta} \log \tilde{\mathcal{Z}} \quad \text{--- 74 ---}$$

q.e.d.

$$= F$$

Note that for the canonical ensemble

$$\Phi[\rho] = -S + \alpha + \beta U$$

$$\frac{1}{\beta} \Phi[\rho] = -TS + \frac{\alpha}{\beta} + U = F + \frac{\alpha}{\beta}$$

Φ has minimum

$\Leftrightarrow F$ has a minimum

$\Leftrightarrow S$ has a maximum

Generalized statistical mechanics

Start from more general information measures

$$I[\rho] = -S[\rho] = \sum_i p_i h(p_i)$$

Example: some function
Trallis entropy

$$S_q = \frac{1}{q-1} \left(1 - \sum_{i=1}^{q-1} p_i^q \right)$$

$$q \rightarrow 1 \Rightarrow S_q \rightarrow S = - \sum p_i \log p_i$$

✓

For this example

$$h(p_i) \approx \frac{p_i^{q-1} - 1}{q-1}$$

One defines a q -logarithm as

$$\log_q(x) = \frac{x^{1-q} - 1}{1-q}$$

[exercise : Show that

$$\lim_{q \rightarrow 1} \log_q(x) = \log x$$

The inverse function of the q -logarithm is the q -exponential

$$\exp_q(x) := (1 + (1-q)x)^{\frac{1}{1-q}}$$

$$q \rightarrow 1 \Rightarrow \exp_q(x) \rightarrow e^x$$

Now let's do generalized stab. mech.

$$\Psi[P] = \sum p_i h(p_i) + \alpha \sum p_i + \beta \sum p_i E_i$$

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$$\frac{\partial}{\partial p_i} \Psi [P] = 0$$

\Rightarrow we obtain

$$\underbrace{h(p_i) + p_i h'(p_i)}_{g(p_i)} + \alpha + \beta E_i = 0$$

$$g(p_i) = -\alpha - \beta E_i$$

$$p_i = g^{-1}(-\alpha - \beta E_i)$$

Nonextensive stat. mech.

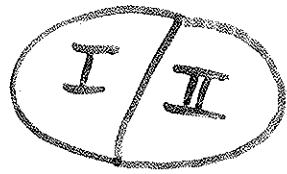
= generalized stat. mech. based
on maximization of Tsallis
entropies

Why that name?

Take two independent systems
I and II. Then the
Tsallis entropy of the

joint system I, II is non-additive:

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Theorem

$$S_q^{I,II} = S_q^I + S_q^II - (q-1) S_q^I \cdot S_q^II$$

Proof

$$\sum_i (p_i^I)^q = 1 - (q-1) S_q^I \quad (1)$$

$$\sum_j (p_j^II)^q = 1 - (q-1) S_q^II \quad (2)$$

$$\sum_{i,j} p_{ij}^q \underset{\text{independent}}{\uparrow} \sum_i (p_i^I)^q \sum_j (p_j^II)^q$$

independent

$$= 1 - (q-1) S_q^{I,II}$$

$$\text{eq. (1)} \times \text{eq. (2)}$$

$$\Rightarrow \sum_i (p_i^I)^q \cdot \sum_j (p_j^II)^q$$

$$= 1 - (q-1) S_q^I - (q-1) S_q^II$$

$$+ (q-1)^2 S_q^I \cdot S_q^II$$

$$S_q^{I, II} = S_q^I + S_q^{II} - (q-1) S_q^I S_q^{II}$$

q.e.d.

It has further (nice) properties of the Tsallis entropy

- convexity $S_q = \frac{1}{q-1} (1 - \sum p_i^q)$

$$\frac{\partial}{\partial p_i} S_q = -\frac{q}{q-1} p_i^{q-1}$$

$$\frac{\partial^2}{\partial p_i \partial p_j} S_q = -q p_i^{q-2} \delta_{ij}$$

$$\delta_{ij} = \begin{cases} 1 & i=j \\ 0 & \text{else} \end{cases}$$

- stability

Tsallis entropies are

Froche-stable, whereas

for example Rényi entropies

conlusion are not.

\Rightarrow After the Shannon entropy, the next-best entropy measures are the Tsallis entropies.

$$\frac{\partial}{\partial p_i} I[P] + \sum_{\beta} \beta \rho_i e^{\beta E_i} = 0$$

take now Tsallis information
For the canonical ensemble

$$\frac{\partial}{\partial p_i} I_q^T [P] = \frac{1}{q-1} p_i^{q-1}$$

$$\Rightarrow \frac{1}{q-1} p_i^{q-1} + \alpha + \beta E_i = 0$$

$$\Rightarrow p_i = \frac{1}{\sum_q} (1 - \beta(q-1)E_i)^{\frac{1}{q-1}}$$

Today's notation was $q' = 2-q$
and then renames $q' \rightarrow q$

$$\Rightarrow p_i = \frac{1}{\sum_q} (1 + \beta(q-1)E_i)^{-\frac{1}{q-1}}$$

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Further important entropy measures:

Tsallis entropy

$$S_x = - \sum_i \frac{p_i^{1+x} - p_i^{1-x}}{2x}$$

$x \rightarrow 0$ this again reduces to the Shannon entropy.

Sharma - Mittal entropies

$$S_{x,r} = - \sum_i p_i^r \left(\frac{p_i^x - p_i^{-x}}{2x} \right)$$

reduces to -Tsallis entropy
for $r=x$, $q=1-2x$

- Tsallis entropy
for $r=0$

- the entropy

$$\text{for } x = \frac{1}{2}(q - q^{-1})$$

$$r = \frac{1}{2}(q + q^{-1})$$

$$\overline{\log(p_1, \dots, p_n)} - ?$$