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SCHOOL and CONFERENCE
on
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q-Expectation Values in Nonextensive Statistical Mechanics

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Ⅰ. Introduction

Two "Assumptions" in Nonextensive Statistical Mechanics

(i) Form of Entropy

$$S_q[p] = \frac{1}{1-q}\left[\sum_i (p_i)^q - 1\right]$$

(ii) q-Expectation Value

$$< H >_q = \sum_i P_i^{(q)} \varepsilon_i$$

where

$$P_i^{(q)} = \frac{(p_i)^q}{\sum_j (p_j)^q}$$: Escort Distribution

PURPOSE

To show that

(ii) is actually NOT an assumption

Ⅱ. Ordinary Expectation Values vs q-Expectation Values

Geometric Aspect of Maximum Entropy Principle

Functional to be maximized:

$$\Phi[p;\alpha,\beta]=\Sigma[p]-\alpha\left(\sum_i p_i-1\right)-\beta\left(\sum_i f(p_i)\varepsilon_i-U\right)$$

$\Sigma[p]$: a certain entropic measure

$f(p_i)$: some nonnegative function, satisfying $\sum_i f(p_i)=1$

α, β: Lagrange Multipliers

$T_i = \frac{\delta}{\delta p_i}$: **Translation**

$D = \sum_i p_i \frac{\delta}{\delta p_i}$: **Dilatation**

Closed Algebra

$$[T_i, T_j] = 0, \quad [T_i, D] = T_i, \quad [D, D] = 0.$$

Maximum Entropy Principle as an Invariance Principle

$T_i \Phi = 0$: **Maximization**

$D\Phi = 0$: **Elimination of** α

(i) Ordinary Expectation Value

$$\Phi[p;\alpha,\beta]=S_q[p]-\alpha\left(\sum_i p_i-1\right)-\beta\left(\sum_i p_i\varepsilon_i-U\right)$$

$$\Downarrow$$

$$T_i\Phi=0: \quad \frac{q}{1-q}\left(\tilde{p}_i^{(\mathrm{ord})}\right)^{q-1}-\alpha-\beta\varepsilon_i=0$$

$$D\Phi=0: \quad \alpha=\frac{q}{1-q}\left[1+(1-q)\,\tilde{S}_q^{(\mathrm{ord})}\right]-\beta\tilde{U}$$

∴

$$\tilde{p}_i^{(\mathrm{ord})} = \frac{1}{Z^{(\mathrm{ord})}(\beta)} \left[1 - \frac{q-1}{q} \beta' \left(\varepsilon_i - \tilde{U} \right) \right]_+^{1/(q-1)}$$

with

$$Z^{(\mathrm{ord})}(\beta) = \left[1 + (1-q) \tilde{S}_q^{(\mathrm{ord})} \right]^{-1/(q-1)}$$

$$= \sum_i \left[1 - \frac{q-1}{q} \beta' \left(\varepsilon_i - \tilde{U} \right) \right]_+^{1/(q-1)}$$

$$\beta' = \frac{\beta}{\sum_i \left(\tilde{p}_i^{(\mathrm{ord})} \right)^q}$$

(ii) q-Expectation Value

$$\Phi_q[p;\alpha,\beta]=S_q[p]-\alpha\left(\sum_i p_i-1\right)-\beta\left[\frac{\sum_i (p_i)^q\,\varepsilon_i}{\sum_j (p_j)^q}-U_q\right]$$

$$\Downarrow$$

$$T_i\Phi_q=0:\quad \frac{q}{1-q}\left(\tilde{p}_i\right)^{q-1}-\alpha$$

$$-q\beta^*\left(\varepsilon_i-\tilde{U}_q\right)\left(\tilde{p}_i\right)^{q-1}=0$$

$$D\Phi_q=0:\quad \alpha=\frac{q}{1-q}\left[1+(1-q)\,\tilde{S}_q\right]$$

∴

$$\tilde{p}_i = \frac{1}{Z_q(\beta)}\left[1-(1-q)\beta^*\left(\varepsilon_i - \tilde{U}_q\right)\right]_+^{1/(1-q)}$$

with

$$Z_q(\beta) = \left[1+(1-q)\tilde{S}_q\right]^{1/(1-q)}$$

$$= \sum_i \left[1-(1-q)\beta^*\left(\varepsilon_i - \tilde{U}_q\right)\right]_+^{1/(1-q)}$$

$$\beta^* = \frac{\beta}{\sum_i \left(\tilde{p}_i\right)^q}$$

In both (i) and (ii):

$$\frac{\partial \tilde{S}_q^{(\mathrm{ord})}}{\partial \tilde{U}^{(\mathrm{ord})}} = \beta$$

$$\frac{\partial \tilde{S}_q}{\partial \tilde{U}_q} = \beta$$

Therefore, the thermodynamic Legendre-transform structure exists in both cases.

Ⅲ. Generalized Relative Entropies

Two Different Definitions
in Information Theory

(i) Bregman Type:

$$I[p\|r]=\sum_i [f(p_i)-f(r_i)-(p_i-r_i)f'(r_i)]$$

(ii) Csiszár Type:

$$K[p\|r]=\sum_i p_i g(p_i/r_i)$$

where

f, g: having definite convexity

$\{r_i\}_i$: reference distribution (prior)

$\{p_i\}_i$: objective distribution (posterior)

Relative Entropies associated with Tsallis Entropy

(i) Bregman Type:

J. Naudts (2004).

Take $f(x) := \frac{1}{q-1}(x^q - x)$

$$\Downarrow$$

$$I_q[p \| r] = \frac{1}{q-1}\sum_i p_i\left[(p_i)^{q-1} - (r_i)^{q-1}\right]$$

$$-\sum_i (p_i - r_i)(r_i)^{q-1}$$

$$= \frac{q}{q-1}\sum_i \int_{r_i}^{p_i} ds\left[s^{q-1} - (r_i)^{q-1}\right]$$

(ii) Csiszár Type:

C. Tsallis (1998);
S. A. (1998).

Take $g(x) := \frac{1}{q-1}(x^{q-1} - 1)$

$$\Downarrow$$

$$K_q[p \| r] = \frac{1}{1-q}\left[1 - \sum_i (p_i)^q (r_i)^{1-q}\right]$$

Basic Properties

❶ Limiting Case: Kullback-Leibler Relative Entropy

$$I_q[p\|r], K_q[p\|r] \xrightarrow{q\to 1} \sum_i p_i \ln(p_i / r_i)$$

❷ Nonnegativity

$I_q[p\|r] \geq 0$ **&** $I_q[p\|r] = 0 \Leftrightarrow p_i = r_i$ **for** $\forall i$

$K_q[p\|r] \geq 0$ **&** $K_q[p\|r] = 0 \Leftrightarrow p_i = r_i$ **for** $\forall i$

❸ Convexity

* $I_q[p||r]$: **convex w.r.t.** $\{p_i\}_i$

but not in $\{r_i\}_i$

* $K_q[p||r]$: **jointly convex, i.e.,**

$$K_q\left[\sum_a \lambda_a p_{(a)} \middle\| \sum_a \lambda_a r_{(a)}\right] \le \sum_a \lambda_a K_q[p_{(a)}||r_{(a)}]$$

where

$\lambda_a > 0$ **and** $\sum_a \lambda_a = 1$

Stronger than individual convexity

in $\{p_i\}_i$ **and** $\{r_i\}_i$

❹ Composability

$$p_{ij}(A,B) = p_{(1)i}(A)\, p_{(2)j}(B)$$

$$r_{ij}(A,B) = r_{(1)i}(A)\, r_{(2)j}(B)$$

$$\Downarrow$$

$$K_q[p_{(1)}p_{(2)} \| r_{(1)}r_{(2)}] = K_q[p_{(1)} \| r_{(1)}] + K_q[p_{(2)} \| r_{(2)}]$$
$$+ (q-1) K_q[p_{(1)} \| r_{(1)}]\, K_q[p_{(2)} \| r_{(2)}]$$

No such relations exist for $I_q[p \| r]$.

❺ Free Energy Difference

(~: stationary quantities)

$$* \quad I_q[p \| \tilde{p}^{(\mathrm{ord})}] = \beta(F - \tilde{F})$$

where

$$F = U - \frac{1}{\beta} S_q \quad \textbf{and} \quad \tilde{F} = \tilde{U} - \frac{1}{\beta} \tilde{S}_q$$

$$* \quad K_q[p \| \tilde{p}] = \frac{\hat{\beta}}{\sum_i (\tilde{p}_i)^q} (F_q - \tilde{F}_q)$$

where

$$\hat{\beta} = \beta^* \sum_i (p_i)^q$$

$$F_q = U_q - \frac{1}{\hat{\beta}} S_q \quad \textbf{and} \quad \tilde{F}_q = \tilde{U}_q - \frac{1}{\hat{\beta}} \tilde{S}_q$$

$I_q[p\|r]$: **Relative entropy associated with the ordinary expectation value formalism**

$K_q[p\|r]$: **Relative entropy associated with the q-expectation value formalism**

IV. Shore-Johnson Theorem

Answer to the question:

> "why the correct rule of inference is to minimize relative entropy, in conformity with a vindication of Jaynes' claim that every other rule will lead to contradiction"

J. Uffink (1995).

5 Axioms

J. E. Shore and R. W. Johnson (1980, 1981, 1983).

[I] Uniqueness:

If the same problem is solved twice, then the same answer is expected to result both times.

[II] Invariance:

The same answer is expected when the same problem is solved in two different coordinate systems, in which the posteriors in the two systems should be related by the coordinate transformation.

[Ⅲ] System Independence:

It should not matter whether one accounts for independent information about independent systems separately in terms of their marginal distributions or in terms of the joint distribution.

[Ⅳ] Subset Independence:

It should not matter whether one treats independent subsets of the states of the systems in terms of their separate conditional distributions or in terms of the joint distribution.

[V] Expansibility:

In the absence of new information, the prior (i.e., the reference distribution) should not be changed.

Shore-Johnson Theorem

The relative entropy $J[p \| r]$ with the prior $\{r_i\}_i$ and the posterior $\{p_i\}_i$ satisfying the axioms [I]-[V] has the following form:

$$J[p \| r] = \sum_i p_i h(p_i / r_i)$$

- Such h exists for $K_q[p\|r]$:

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

- Such h does not exist for $I_q[p\|r]$:

$I_q[p\|r]$ violates [Ⅲ]!

∴

The q-expectation value formalism is consistent, whereas the ordinary expectation value formalism is inconsistent.

V. Concluding Remarks

- Geometric Aspect of Maximum Entropy Principle

- Generalized Relative Entropies and Their Properties

- Shore-Johnson Theorem:
  Consistency between Maximum Entropy Principle and Minimum Relative Entropy Principle

- Consistency of the q-Expectation Value Formalism and Inconsistency of the Ordinary Expectation Value Formalism

Reference

S. A. and G. B. Bagci, Phys. Rev. E 71, 016139 (2005).