一般化熱統計学における Legendre 構造と情報幾何

The Legendre structures in generalized thermostatistics and related information geometries

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Collaboration with
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sul 17 dicembre 2010 a Tohoku Gakuin University, Tagajo

Outline

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Nonextensive statistical mechanics

C. Tsallis, *Introduction to Nonextensive Statistical Mechanics* (2009).

Tsallis' generalized entropy:

$$S_q[\mathbf{p}] \equiv \frac{\sum_i p_i^q - 1}{1-q} \quad \underset{q \to 1}{\longrightarrow} \quad S^{\mathrm{BGS}} = -\sum_i p_i \ln p_i,$$

Introducing the so-called escort probabilities, w.r.t. p_i,

$$P_i \equiv \frac{p_i^q}{\sum_j p_j^q},$$

and the escort average of energy

$$U_q[\mathbf{p}] \equiv \sum_i E_i P_i,$$

Power law distribution

MaxEnt

$$\frac{\partial}{\partial p_i}\left(S_q[\mathbf{p}] - \beta^{\mathrm{T}} U_q[\mathbf{p}] - \gamma^{\mathrm{T}} \sum_j p_j\right) = 0.$$

leads to the asymptotic power-law distribution:

$$p_i \propto \exp_q\left[-\frac{\beta^{\mathrm{T}}}{\sum_j p_j^q}\left(E_i - U_q\right)\right], \quad \underset{E_i >> U_q}{\longrightarrow} E_i^{\frac{1}{1-q}}, \text{ power law!}$$

q-logarithmic and q-exponential functions:

$$\ln_q(x) \equiv \frac{x^{1-q}-1}{1-q} \quad \underset{q\to 1}{\longrightarrow} \quad \ln(x).$$

$$\exp_q(x) \equiv (1+(1-q)x)^{\frac{1}{1-q}} \quad \underset{q\to 1}{\longrightarrow} \quad \exp(x).$$

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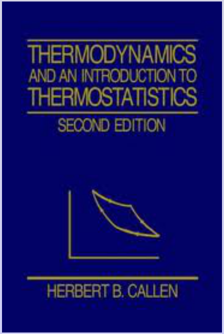
Generalized thermostatistics

H.B. Callen's book (John Wiley & Sons 1985)



From Chap. 21

Thermostatistics characterizes the equilibrium state of microscopic systems without reference either to the specific forces or to the laws of mechanical response.

Instead thermostatistics characterizes the equilibrium state as the state that maximizes the disorder, a quantity associated with a conceptual framework ("information theory") outside of conventional physical theory.

the disorder $\Leftrightarrow$ Shannon entropy

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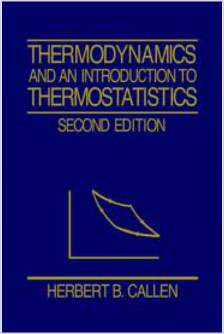

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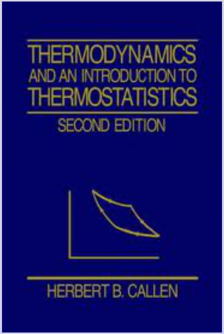

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Generalized thermostatistics

J. Naudts, Physica A **340** (2004) 32.
A generalization of Callen's thermostatistics with a generalized entropy:

$$S_\phi = -\sum_i p_i \ln_\phi p_i \quad \underset{\phi(x)\to x}{\longrightarrow} \quad S^{\mathrm{BGS}},$$

where ϕ-log is introduced with a positive function $\phi(x)$

$$\ln_\phi x \equiv \int_1^x \frac{1}{\phi(x)} dx \quad \underset{\phi(x)\to x}{\longrightarrow} \quad \ln x.$$

Examples:

- Tsallis: $\phi_q(x) = x^q, \quad \ln_q(x) = \frac{x^{1-q}-1}{1-q}, \quad q > 0$
- Kaniadakis:
  $\phi_\kappa(x) = \frac{2x}{x^\kappa + x^{-\kappa}}, \quad \ln_{\{\kappa\}}(x) = \frac{x^\kappa - x^{-\kappa}}{2\kappa}, \quad |\kappa| < 1$

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Outline

Canonical ensemble

Starting from canonical probability distribution:

$$p_i = \frac{1}{Z(\beta^{\mathrm{BG}})} \exp\left[-\beta^{\mathrm{BG}} E_i\right], \quad \gamma^{\mathrm{BG}} + 1 = \ln Z(\beta^{\mathrm{BG}}),$$

$$p_i = \exp\left[-\gamma^{\mathrm{BG}} - 1 - \beta^{\mathrm{BG}} E_i\right] = \mathrm{e}^{-1} \exp\left[-\gamma^{\mathrm{BG}} - \beta^{\mathrm{BG}} E_i\right].$$

Useful relation:

$$\frac{d}{dx}(x \ln x) = \ln x + 1 = \ln \frac{x}{\mathrm{e}^{-1}}.$$

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Useful relation:

$$\frac{d}{dx}(x \ln x) = \ln x + 1 = \ln \frac{x}{\mathrm{e}^{-1}}.$$

MaxEnt

From the canonical probability distribution, we have

$$-\ln \frac{p_i}{\mathrm{e}^{-1}} - \beta^{\mathrm{BG}} E_i - \gamma^{\mathrm{BG}} = 0.$$

Utilizing the identity it follows

$$\frac{\partial}{\partial p_i}\Big(-\sum_j p_j \ln p_j - \beta^{\mathrm{BG}} \sum_j E_j p_j - \gamma^{\mathrm{BG}} \sum_j p_j \Big) = 0,$$

which is equivalent to the maximization of S^{BGS}

$$S^{\mathrm{BGS}} = -\sum_i p_i \ln p_i,$$

under the constraints of

$$\sum_i E_i p_i = U \,, \quad \text{and} \quad \sum_i p_i = 1.$$

Outline

S_{2-q}-formalism

T. Wada, A.M. Scarfone, Phys. Lett. A **335** (2005) 351.

Starting from the q-exponential probability distribution:

$$p_i = \alpha_q \exp_q[-\gamma - \beta E_i],$$

where α_q is a q-dependent constant,

$$\alpha_q \equiv \left(\frac{1}{2-q}\right)^{1-q} = \frac{1}{\exp_q(1)}.$$

Useful relation:

$$\frac{d}{dx} x \ln_q x = \ln_q \frac{x}{\alpha_q}.$$

S_{2-q}-formalism

From the q-distribution, we have

$$-\ln_q \frac{p_i}{\alpha_q} - \beta E_i - \gamma = 0.$$

Utilizing the identity it follows

$$\frac{\partial}{\partial p_i}\Big(- \sum_j p_j \ln_q p_j - \beta \sum_j E_j p_j - \gamma \sum_j p_j \Big) = 0,$$

which is equivalent to the maximization of S_{2-q}

$$S_{2-q} = - \sum_i p_i \ln_q p_i,$$

under the constraints of

$$\sum_i E_i p_i = U \,, \quad \text{and} \quad \sum_i p_i = 1.$$

Legendre structures 1

The q-exponential distribution can be written as

$$\begin{aligned} p_i &= \alpha_q \exp_q\left[-\beta E_i - \gamma\right] \\ &= \exp_q\left[-\frac{\beta}{2-q} E_i - \left(\frac{\gamma+1}{2-q}\right)\right] \end{aligned}$$

Here we introduced

$$\begin{aligned} \beta^N &\equiv \frac{\beta}{2-q} \\ \Phi_q^N &\equiv \frac{\gamma+1}{2-q}, \qquad \text{generalized Massiue potential} \end{aligned}$$

Legendre structures 1

$$p_i = \exp_q \left[-\beta^N E_i - \Phi_q^N \right].$$

By differentiating $\sum_i p_i = 1$ w.r.t. β^N, and using $d \exp_q(x)/dx = \exp_q(x)^q$, we have

$$0 = \sum_i \frac{dp_i}{d\beta^N} = -\sum_i (E_i + \frac{d\Phi_q^N}{d\beta^N}) p_i^q, \quad \Rightarrow \quad \frac{d\Phi_q^N}{d\beta^N} = -\frac{\sum_i E_i p_i^q}{\sum_j p_j^q}.$$

which leads to the Legendre relation:

$$\frac{d\Phi_q^N}{d\beta^N} = -U_q.$$

Note that the escort probabilities P_i are naturally appeared!

Legendre structures 1

The normalized Tsallis entropy

$$S_q^N = -\sum_i P_i \ln_q p_i .$$

Substituting

$$p_i = \exp_q \left[-\beta^N E_i - \Phi_q^N \right]$$

into S_q^N leads to

$$S_q^N = \sum_i P_i (\beta^N E_i + \Phi_q^N) = \beta^N U_q + \Phi_q^N .$$

S_q^N and Φ_q^N are Legendre duals each other.

Legendre structure 2

$$S_{2-q} = -\sum_i p_i \ln_q p_i, \quad p_i = \alpha_q \exp_q \left[-\gamma - \beta E_i \right].$$

Using the identity $\frac{d}{dx} x \ln_q x = \ln_q \frac{x}{\alpha_q}$, we have

$$\frac{dS_{2-q}}{d\beta} = -\sum_i \frac{dp_i}{d\beta} \frac{d}{dp_i} p_i \ln_q p_i = -\sum_i \frac{dp_i}{d\beta} \ln_q \frac{p_i}{\alpha_q}$$
$$= \sum_i \frac{dp_i}{d\beta} (\beta E_i + \gamma) = \beta \frac{dU}{d\beta}.$$

$$\frac{dS_{2-q}}{dU} = \beta.$$

Legendre structure 2

The q-exponential distribution

$$p_i = \exp_q \left[-\frac{\beta}{2-q} E_i - \left(\frac{1+\gamma}{2-q} \right) \right], \quad S_{2-q} = -\sum_i p_i \ln_q p_i.$$

$$\Rightarrow \quad \Phi_q^N = \frac{1+\gamma}{2-q} = S_{2-q} - \frac{\beta}{2-q} U.$$

$$\Phi_{2-q} \equiv \frac{1+\gamma}{2-q} - \left(\frac{1-q}{2-q} \right) \beta U.$$

$$\Phi_{2-q} = S_{2-q} - \beta U.$$

Legendre structure 2

$$\Phi_q^N = S_{2-q} - \frac{\beta}{2-q} U, \quad \Phi_{2-q} = \Phi_q^N - \left(\frac{1-q}{2-q}\right) \beta U.$$

$$\begin{aligned}
\frac{d\Phi_q^N}{d\beta} &= \frac{dS_{2-q}}{d\beta} - \frac{\beta}{2-q}\frac{dU}{d\beta} - \frac{U}{2-q} \\
&= \left(\frac{1-q}{2-q}\right) \beta \frac{dU}{d\beta} - \frac{1}{2-q} U. \\
\frac{d\Phi_{2-q}}{d\beta} &= \frac{d\Phi_q^N}{d\beta} - \left(\frac{1-q}{2-q}\right) \beta \frac{dU}{d\beta} - \left(\frac{1-q}{2-q}\right) U = -U.
\end{aligned}$$

Legendre structures (summary)

Two different sets:

$$\Phi_q^N \equiv \frac{1+\gamma}{2-q},$$

$$\Phi_q^N = S_q^N - \beta^N U_q, \quad \frac{d\Phi_q^N}{d\beta^N} = -U_q, \quad \frac{dS_q^N}{dU_q} = \beta^N.$$

$$\Phi_{2-q} \equiv \frac{1+\gamma}{2-q} - \left(\frac{1-q}{2-q}\right)\beta U,$$

$$\Phi_{2-q} = S_{2-q} - \beta U, \quad \frac{d\Phi_{2-q}}{d\beta} = -U, \quad \frac{dS_{2-q}}{dU} = \beta.$$

Outline

κ-entropy

G. Kaniadakis, PRE **72** (2005) 036108.

$$S_\kappa = -\sum_i p_i \ln_{\{\kappa\}} p_i, \quad \underset{\kappa\to 0}{\longrightarrow} S^{\mathrm{BGS}},$$

$$\ln_{\{\kappa\}}(x) = \frac{x^\kappa - x^{-\kappa}}{2\kappa}, \quad \underset{\kappa\to 0}{\longrightarrow} \ln(x),$$

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κ-MaxEnt

κ-exponential probability distribution:

$$p_i = \alpha_\kappa \, \exp_{\{\kappa\}} \left[-\frac{1}{\lambda_\kappa} (\gamma + \beta \, E_i) \right],$$

where α_κ and λ_κ are κ-dependent constants,

$$\alpha_\kappa = \left(\frac{1-\kappa}{1+\kappa} \right)^{\frac{1}{2\kappa}}, \quad \lambda_\kappa = \sqrt{1-\kappa^2}.$$

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$$\alpha_\kappa = \exp_{\{\kappa\}} \left(-\frac{1}{\lambda_\kappa} \right), \quad \underset{\kappa \to 0}{\longrightarrow} \exp(-1).$$

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Useful identity:

$$\frac{d}{dx} x \ln_{\{\kappa\}} x = \lambda_\kappa \ln_{\{\kappa\}} \frac{x}{\alpha_\kappa}.$$

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$$\frac{\partial}{\partial p_i}\Big(-\sum_j p_j \ln_{\{\kappa\}} p_j - \beta \sum_j E_j p_j - \gamma \sum_j p_j \Big) = 0.$$

with Kaniadakis' entropy $S_\kappa[p] = -\sum_i p_i \ln_{\{\kappa\}} p_i$

Legendre structure

A.M. Scarfone, T. Wada, Prog. Theor. Phys. Suppl. **162** (2006) 45.
κ-generalized Massiue potential:

$$\Phi_\kappa = S_\kappa - \beta U, \quad \frac{d\Phi_\kappa}{d\beta} = -U,$$

$$\Phi_\kappa = \mathcal{I}_\kappa + \gamma,$$

$$\text{with} \quad \mathcal{I}_\kappa[\mathbf{p}] \equiv \sum_i \frac{1}{2}\left(p_i^{1+\kappa} + p_i^{1-\kappa}\right).$$

Outline

Information geometry

Amari and Nagaoka, *Methods of Information Geometry*, (AMS 2001)

N-dimensional probability simplex:

$$\mathcal{S}^n \equiv \left\{ \mathbf{p} = (p_i) \middle| p_i > 0, \sum_{i=1}^{n+1} p_i = 1 \right\}.$$

The natural basis tangent vector fields are

$$\partial_i \equiv \frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_{n+1}}, \quad i = 1, \cdots, n.$$

Riemannian metric g on $\mathcal{S}^n$ is Fisher information matrix:

$$g_{ij}(\mathbf{p}) \equiv \frac{1}{p_i}\delta_{ij} + \frac{1}{p_{n+1}} = \sum_{k=1}^{n+1} p_k \left(\partial_i \ln p_k\right)\left(\partial_j \ln p_k\right),$$

$$i, j, k = 1, \cdots, n.$$

A dually-flat structure in escort distributions

Ohara, Matsuzoe, Amari, J. Phys.: Conf. Series **201** (2010) 012012.

The α-covariant derivative is given by

$$\nabla^{(\alpha)}_{\partial_i}\partial_j = \sum_{k=1}^{n} \Gamma^{(\alpha)k}_{ij}, \quad i, j = 1, \cdots, n,$$

$$\text{where} \quad \Gamma^{(\alpha)k}_{ij}(\mathbf{p}) = \frac{1+\alpha}{2}\left(-\frac{1}{p_k}\delta^k_{ij} + p_k g_{ij}\right).$$

α-immersion

The α-immersion f of $\mathcal{S}^n$ into $\mathbb{R}_+^{n+1}$ with $q = (1-\alpha)/2$:

$$f : \mathbf{p} = (p_i) \mapsto \mathbf{x} = (x^i) = L^{(\alpha)}(p_i) = \frac{p_i^q}{q}.$$

$f(\mathcal{S}^n)$ is a level hypersurface in $\mathbb{R}_+^{n+1}$:

$$\Psi(\mathbf{x}) = \frac{1}{1-q} \sum_{i=1}^{n+1} (q x_i)^{\frac{1}{q}}.$$

Choosing a transversal vector ξ on the level hypersurface by

$$\xi \equiv \sum_{i=1}^{n+1} \xi^i \frac{\partial}{\partial x^i}, \quad \xi^i = -q(1-q)x^i = -\kappa x^i,$$

then the affine immersion (f, ξ) realizes the α-geometry on $\mathcal{S}^n$.

Conormal map

Introducing the dual vector $\mathbf{x}^*$ by

$$x_i^*(\mathbf{p}) = L^{(-\alpha)}(p_i) = \frac{1}{1-q} p_i^{1-q},$$

which satisfies

$$x_i^*(\mathbf{p}) = \frac{\partial \Psi}{\partial x^i}(\mathbf{x}(\mathbf{p})),$$

$$-\sum_{i=1}^{n+1} \xi^i(\mathbf{p}) x_i^*(\mathbf{p}) = 1, \quad \sum_{i=1}^{n+1} x_i^*(\mathbf{p})\, X^i = 0,$$

for an arbitrary vector $X = \sum_i X^i \partial / \partial x^i$ at $\mathbf{x}(\mathbf{p})$ tangent to $f(\mathcal{S}^n)$.
Hence $-\mathbf{x}^*(\mathbf{p})$ is a conormal map.

The escort probability is

$$P_i(\mathbf{p}) = \frac{x^i}{Z_q}, \quad Z_q(\mathbf{p}) \equiv \sum_{i=1}^{n+1} x^i(\mathbf{p}) = \sum_{i=1}^{n+1} \frac{p_i^q}{q},$$

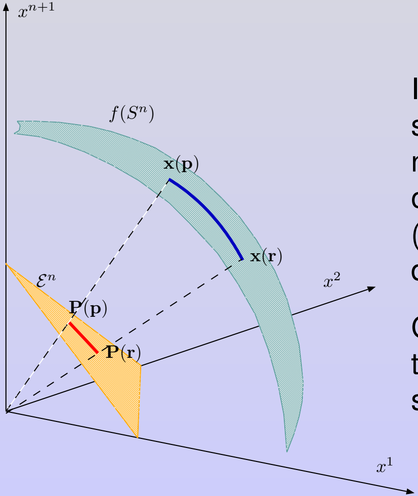
$$\lambda(\mathbf{p}) \equiv \frac{1}{Z_q(\mathbf{p})}.$$

The simplex

$$\mathcal{E}^n \equiv \left\{ \mathbf{x} = (x^i) \middle| x^i > 0, \sum_{i=1}^{n+1} x^i = 1 \right\}.$$

Outline

Conformal transformation



Introducing another immersion $\tilde{f} \equiv \lambda f$ and Riemannian metric $h \equiv \lambda g$, we can obtain a statistical manifold $(\mathcal{S}^n, h, \nabla, \nabla^*)$, which has a dually flat structure.

Conformal transformation to the dually-flat structure on the space of escort distributions.

Using the conormal map we can define the α-divergence as a contrast function on $(\mathcal{S}^n, g, \nabla^{(\alpha)})$:

$$D^{(\alpha)}(\mathbf{p},\mathbf{r}) = -\sum_{i=1}^{n+1} x_i^*(\mathbf{r})\big(x^i(\mathbf{p}) - x^i(\mathbf{r})\big) = \frac{1}{q}\sum_{i=1}^{n+1} r_i \ln_q \frac{p_i}{r_i}$$

$$= \frac{1}{q}\sum_{i=1}^{n+1} r_i \left(-\ln_{2-q}\frac{r_i}{p_i}\right). \quad \text{f-divergence}$$

The conformal divergence is a contrast function of $(\mathcal{S}^n, h, \nabla)$:

$$\rho(\mathbf{p},\mathbf{r}) = \lambda(\mathbf{r})D^{(-\alpha)}(\mathbf{p},\mathbf{r}) = \langle \mathbf{P}(\mathbf{r}), \mathbf{x}^*(\mathbf{p}) - \mathbf{x}^*(\mathbf{r})\rangle$$

$$= \sum_{i=1}^{n+1} P_i\big(\ln_q p_i - \ln_q r_i\big).$$

Using the conormal map we can define the α-divergence as a contrast function on $(\mathcal{S}^n, g, \nabla^{(\alpha)})$:

$$D^{(\alpha)}(\mathbf{p}, \mathbf{r}) = -\sum_{i=1}^{n+1} x_i^*(\mathbf{r})\big(x^i(\mathbf{p}) - x^i(\mathbf{r})\big) = \frac{1}{q}\sum_{i=1}^{n+1} r_i \ln_q \frac{p_i}{r_i}$$

$$= \frac{1}{q}\sum_{i=1}^{n+1} r_i \left(-\ln_{2-q} \frac{r_i}{p_i}\right). \quad \text{f-divergence}$$

The conformal divergence is a contrast function of $(\mathcal{S}^n, h, \nabla)$:

$$\rho(\mathbf{p}, \mathbf{r}) = \lambda(\mathbf{r}) D^{(-\alpha)}(\mathbf{p}, \mathbf{r}) = \langle \mathbf{P}(\mathbf{r}), \mathbf{x}^*(\mathbf{p}) - \mathbf{x}^*(\mathbf{r}) \rangle$$

$$= \sum_{i=1}^{n+1} P_i\big(\ln_q p_i - \ln_q r_i\big).$$

Using the conormal map we can define the α-divergence as a contrast function on $(\mathcal{S}^n, g, \nabla^{(\alpha)})$:

$$D^{(\alpha)}(\mathbf{p},\mathbf{r}) = -\sum_{i=1}^{n+1} x_i^*(\mathbf{r})\big(x^i(\mathbf{p}) - x^i(\mathbf{r})\big) = \frac{1}{q}\sum_{i=1}^{n+1} r_i \ln_q \frac{p_i}{r_i}$$
$$= \frac{1}{q}\sum_{i=1}^{n+1} r_i \left(-\ln_{2-q}\frac{r_i}{p_i}\right). \quad \text{f-divergence}$$

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$$= \sum_{i=1}^{n+1} P_i\big(\ln_q p_i - \ln_q r_i\big).$$

The mutually dual affine coordinate systems:

$$\eta_i = \frac{\partial \Psi}{\partial \theta^i}, \quad \theta^i = \frac{\partial \Psi^*}{\partial \eta_i}, \quad i = 1, \cdots, n,$$

for the potential function $\Psi(\theta)$ and its conjugate $\Psi^*(\eta)$.

Outline

Relations with S_{2-q}-formalism

$$\begin{aligned} p_i &= \exp_q\left[-\beta^N(E_i - E_{n+1}) - \Phi_q^N(\beta^N) - \beta^N E_{n+1}\right] \\ &= \exp_q\left[\theta^i - \Psi(\theta)\right], \end{aligned}$$

$$\begin{aligned} \theta^i &= -\beta^N(E_i - E_{n+1}), \\ \Psi(\theta) &= \Phi_q^N + \beta^N E_{n+1} \\ \eta_i = P_i &= \frac{p_i^q}{\sum_{j=1}^{n+1} p_j^q}, \\ \Psi^*(\eta) &= -S_q^N. \end{aligned}$$

Outlook

- Further study on the relations of q-thermostatistics with information geometries.
- What is the relation of κ-thermostatistics with information geometry?