Divergences via generalized statistical mechanics

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Collaborators

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https://complex.pfi.uem.br/

Timeline

- 1995 -> Tsallis went to Maringá.
- 1996 -> I arrived here.
- 1998 -> 2sd master’s committee
- 2002 -> 1st PhD committee
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This presentation

Divergences from the Shannon entropy.

Divergences related to the Rényi entropy.

Divergences from free energies.

Introduction

Shannon entropy: $$S = \int_{-\infty}^{\infty} \rho(x) \ln \frac{1}{\rho(x)} dx$$

Kullback-Leibler divergence (relative entropy):

$$D_{KL}(\rho, \rho_0) = -\int_{-\infty}^{\infty} \rho(x) \ln \left(\frac{\rho_0(x)}{\rho(x)} \right) dx$$

Property: $D(\rho, \rho_0) \geq 0$ $\qquad \ln(x) \leq x - 1$

Kullback and Leibler, On the information and sufficience, *Ann. Math. Statist*. 22:79, 1951

Tsallis divergence

Tsallis entropy: $$S_q(\rho) = \int \rho(x) \ln_q \frac{1}{\rho(x)}\, dx$$

q-logarithm: $$\ln_q(x) = \frac{x^{1-q} - 1}{1 - q}$$

Tsallis divergence: $$D_q(\rho, \rho_0) = -\int \rho(x) \ln_q \left(\frac{\rho_0(x)}{\rho(x)} \right) dx$$

Tsallis, Generalized entropy-based criterion for consistent testing. *Phys. Rev.* E, 58:1442–1445, 1998.

Generalized logarithm

Generalized logarithm: $$\mathrm{Ln}(x) = \int_1^x \frac{dy}{g(y)}$$

$$g(y) > 0 \quad g'(y) > 0 \quad g(1) = 1$$

Usual logarithm: $g(y) = y$

q-logarithm: $g(y) = y^q$

Naudts, Generalized thermostatistics based on deformed exponential and logarithmic functions, *Physica A*, 340:32–40, 2004.

Generalized divergence

Generalized entropy: $\mathbb{S}(\rho) = \int_{-\infty}^{\infty} \rho(x) \, \mathrm{Ln}\left(\frac{1}{\rho(x)}\right) \, dx$

Generalized divergence:

$$\mathbb{D}(\rho, \rho_0) = -\int_{-\infty}^{\infty} \rho(x) \, \mathrm{Ln}\left(\frac{\rho_0(x)}{\rho(x)}\right) \, dx$$

Inequality: $\mathrm{Ln}(x) \leq x - 1$

Dem.: $\mathrm{Ln}(x) = \int_1^x \frac{1}{g(y)} dy \leq \int_1^x 1 dy = x - 1$

f-divergence

$$D_f(\rho, \rho_0) = \int_{-\infty}^{\infty} \rho(x) f\left(\frac{\rho_0(x)}{\rho(x)}\right) dx$$

$$\mathbb{D}(\rho, \rho_0) = -\int_{-\infty}^{\infty} \rho(x) \,\mathrm{Ln}\left(\frac{\rho_0(x)}{\rho(x)}\right) dx$$

Rényi, On measures of entropy and information. *In Proceedings of the fourth Berkeley symposium on mathematical statistics and probability*, vol 1, Berkeley, California, USA, 1961.

Rényi divergence

Rényi entropy:

$$H_\alpha(\rho) = \frac{1}{1-\alpha} \ln \left(\int_{-\infty}^{\infty} [\rho(x)]^\alpha dx \right)$$

Rényi divergence:

$$D_\alpha(\rho, \rho_0) = \frac{1}{\alpha - 1} \ln \left(\int_{-\infty}^{\infty} \frac{[\rho(x)]^\alpha}{[\rho_0(x)]^{\alpha-1}} dx \right)$$

Rényi, On measures of entropy and information.
In Proceedings of the fourth Berkeley symposium on mathematical statistics and probability, vol 1, Berkeley, California, USA, 1961.

Generalized Rényi divergence

Rényi entropy:

$$\mathbb{H}_\alpha(\rho) = \frac{1}{1-\alpha} \mathrm{Ln} \left(\int_{-\infty}^{\infty} [\rho(x)]^\alpha dx \right)$$

Rényi divergence:

$$\mathbb{D}_\alpha(\rho, \rho_0) = \frac{1}{\alpha - 1} \mathrm{Ln} \left(\int_{-\infty}^{\infty} \frac{[\rho(x)]^\alpha}{[\rho_0(x)]^{\alpha-1}} dx \right)$$

Ex.: Rényi-Tsallis framework

Rényi-Tsallis entropy:

$$\mathbb{H}_{q,\alpha}(\rho) = \frac{1}{1-\alpha} \ln_q \left(\int_{-\infty}^{\infty} [\rho(x)]^\alpha dx \right)$$

Rényi-Tsallis divergence:

$$\mathbb{D}_{q,\alpha}(\rho, \rho_0) = \frac{1}{\alpha - 1} \ln_q \left(\int_{-\infty}^{\infty} \frac{[\rho(x)]^\alpha}{[\rho_0(x)]^{\alpha-1}} dx \right)$$

Kullback-Leibler divergence as free energy

$$D_{KL}(\rho, \rho_0) = -\int_{-\infty}^{\infty} \rho(x) \ln\left(\frac{\rho_0(x)}{\rho(x)}\right) dx$$

$$\rho_0 = \frac{1}{Z} e^{-\beta V} \rightarrow \boxed{D_{KL}(\rho, \rho_0) = \beta F - \beta F_0}$$

where

$$F = \int \rho V \, dx + \frac{1}{\beta} \int \rho \ln \rho \, dx$$

$$F_0 = -\frac{1}{\beta} \ln Z$$

Usual *H*-theorem

Fokker-Planck equation:

$$\frac{\partial \rho}{\partial t} = D_0 \frac{\partial^2 \rho}{\partial x^2} - \frac{\partial}{\partial x}(\rho A)$$

where

$$D_0 = 1/\beta \qquad\qquad A = -dV/dx$$

H-theorem:

$$\frac{dF}{dt} \leq 0$$

Generalized *H*-theorem (I)

"Free energy":

$$\mathcal{F}[\rho] = \int_{-\infty}^{\infty} \phi(\rho, x)\, dx$$

"Fokker-Planck" equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\omega(\rho, x)\frac{\partial}{\partial x}\frac{\delta \mathcal{F}[\rho]}{\delta \rho}\right)$$

$\omega(\rho, x)$ is a non-negative function

The usual case:

$$\omega(\rho, x) = D_0 \rho \text{ and } \mathcal{F}[\rho] = F/D_0$$

Frank, Nonlinear Fokker-Planck equations: fundamentals and applications. Springer Science & Business Media, 2005.

Generalized *H*-theorem (II)

Time derivative: $$\frac{d\mathcal{F}[\rho]}{dt} = \int_{-\infty}^{\infty} \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \frac{\partial \rho}{\partial t} \, dx$$

Integration by parts:

$$\frac{d\mathcal{F}[\rho]}{dt} = \int_{-\infty}^{\infty} \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \frac{\partial}{\partial x} \left(\omega(\rho, x) \frac{\partial}{\partial x} \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \right) dx$$

$$= \int_{-\infty}^{\infty} \frac{\partial}{\partial x} \left(\omega(\rho, x) \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \frac{\partial}{\partial x} \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \right) dx - \int_{-\infty}^{\infty} \omega(\rho, x) \left| \frac{\partial}{\partial x} \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \right|^2 dx$$

$$\frac{d\mathcal{F}[\rho]}{dt} = -\int_{-\infty}^{\infty} \omega(\rho, x) \left| \frac{\partial}{\partial x} \frac{\delta \mathcal{F}[\rho]}{\delta \rho} \right|^2 dx \leq 0$$

Divergence:: $$\mathcal{D}(\rho, \rho_0) = \mathcal{F}(\rho, \rho_0) - \mathcal{F}(\rho_0, \rho_0)$$

Ex.: Tsallis context (I)

Free energy:

$$\mathcal{F} = \frac{1}{D}\int_{-\infty}^{\infty} \rho(x)V(x)dx - \int_{-\infty}^{\infty} \rho(x)\ln_q \frac{1}{\rho(x)}dx$$

$$\omega = D\rho$$

Fokker-Planck equation:

$$\frac{\partial \rho(x)}{\partial t} = -\frac{\partial}{\partial x}[A\rho(x)] + D\frac{\partial^2}{\partial x^2}\rho^q(x)$$

Plastino and Plastino, Non-extensive statistical mechanics and generalized Fokker-Planck equation. *Physica A*, 222:347, 1995.

Ex.: Tsallis context (II)

Stationary solution: $\rho_0(x) = N e_{2-q}^{-\beta V}$

Eliminating V:

$$\mathcal{F}_q[\rho] = \int_{-\infty}^{\infty} \rho \left[-\ln_q \frac{1}{\rho} + q \ln_q \frac{1}{\rho_0} + qK \ln_q N \right] dx$$

The divergence:

$$\mathcal{D}_q(\rho, \rho_0) = -S_q(\rho) + (1-q) S_q(\rho_0) + q \int_{-\infty}^{\infty} \rho \ln_q \left(\frac{1}{\rho_0} \right) dx$$

Conclusions

We discuss three distinct ways to obtain divergences.

We verified that it is possible to connect these ways with *H*-theorems and Fokker-Planck equations.

Thank you