Dynamics of Uncertainty

Piotr Garbaczewski, University of Zielona Góra

TERMINOLOGY

QUANTUM $\longrightarrow$ (statistical) mechanics $\longleftarrow$ **CLASSICAL**

state (of the system)

statistics

Cramér-Rao inequalities

Fisher information/state estimation

information theory

entropy

information and entropy

QUANTUM $\longrightarrow$ entropy and **uncertainty** $\longleftarrow$ **CLASSICAL**

OBJECTS OF INTEREST

$\sum_{j=1}^{N} \mu_j = 1 \quad \to$ **Shannon entropy**: $\quad \mathcal{S}(\mu) = -\sum_{j=1}^{N} \mu_j \ln \mu_j$

$\int \rho(x)\, dx = 1 \quad \to$ **differential entropy**: $\quad \mathcal{S}(\rho) = -\int \rho(x) \ln \rho(x) dx$

PROBLEM ADDRESSED

dynamics of densities $\to$ **dynamics** of differential entropy

$$\rho(x) \to \rho(x,t) \Longrightarrow \mathcal{S}(\rho) \to \mathcal{S}(\rho)(t)$$

SHANNON ENTROPY $\longrightarrow$ DIFFERENTIAL ENTROPY

Long **message** (n "entries"); an **"alphabet"** ($N << n$ "letters");

$\mu_j, 1 \leq j \leq N$ - probability of the $j-th$ "letter" , $\mu = (\mu_1, ..., \mu_N)$

$$\sum_1^N \mu_j = 1 \rightarrow \int \rho dx = 1$$

$$? \quad \Downarrow \quad ?$$

$$\mathcal{S}(\mu) = -\sum_1^N \mu_j \ln \mu_j \longrightarrow S(\rho) = -\int \rho(s) \ln \rho(s) ds$$

Pedestrian argument (see e.g. standard coarse-graining methods):

- Take an interval of length L on a line and the partition unit $\Delta s = L/N$
- Define $\mu_j \doteq p_j \Delta s \Rightarrow$:

$$\mathcal{S}(\mu) = -\sum_j (\Delta s) p_j \ln p_j - \ln(\Delta s)$$

- Fix L and allow N to grow, so that Δs decreases

$$0 \leq \mathcal{S}(\mu) = -\sum_j (\Delta s) p_j \ln p_j - \ln L + \ln N \leq \ln N$$

$$\Downarrow$$

$$\ln(\Delta s) \ \leq \ -\sum_j (\Delta s) p_j \ln p_j \ \leq \ \ln L$$

$$\Downarrow$$

$$(\mathcal{S}(\rho) = -\int \rho(s) \ln \rho(s) ds$$

In the infinite volume $L \rightarrow \infty$ and infinitesimal grating $\Delta s \rightarrow 0$ limits, the differential entropy may be unbounded both from below and above. **Bad news ? Not quite...**

Note: properly executed coarse-graining implies:

$$\mathcal{S}(\rho) - \ln \Delta s \leq \mathcal{S}(\mu) \textbf{ and } \mathcal{S}(\mu) - \mathcal{S}(\mu') \sim \mathcal{S}(\rho) - \mathcal{S}(\rho')$$

DIFFERENTIAL ENTROPY (pedestrian approach plus comments).

- Gaussian density

$$\rho(x) = \frac{1}{[2\pi\sigma^2]^{1/2}} \exp\left[- \frac{(x-x_0)^2}{2\sigma^2}\right]$$
$$\Downarrow$$
$$\mathcal{S}(\rho) = \frac{1}{2}\ln(2\pi e\sigma^2)$$

- Harmonic oscillator in quantum mechanics

$$\rho(x,t) = \left(\frac{2\pi D}{\omega}\right)^{-1/2} \exp\left[-\frac{\omega}{2D}\ (x - q(t))^2\right]$$
$$d\mathcal{S}/dt = 0$$

- Free quantum dynamics for a Gaussian wave-packet

$$\rho(x,t) = \frac{\alpha}{[\pi(\alpha^4 + 4D^2t^2)]^{1/2}} \exp\left(-\frac{x^2\alpha^2}{\alpha^4 + 4D^2t^2}\right) . \tag{1}$$

$$\mathcal{S}(t) = \frac{1}{2}\ln\left[e\pi \left\langle X^2\right\rangle(t)\right]$$

$$\left\langle X^2\right\rangle \doteq \int x^2\rho dx = (\alpha^4 + 4D^2t^2)/2\alpha^2$$

- Squeezed state of the oscillator (atomic units)

$$\sigma^2 \to \sigma^2(t) = \frac{1}{2}\left(\frac{1}{s^2}\sin^2 t + s^2\cos^2 t\right)$$

- Non-quantum example: free Brownian motion; $D = k_BT/m\beta$

$$\sigma^2 \to \sigma^2(t) = 2Dt$$

Comment (i):
For general continuous probability distributions $\rho(x)$ with an arbitrary finite mean value, whose variance is **fixed** at σ^2 we have

$$\mathcal{S}(\rho) \leq \frac{1}{2}\ln(2\pi e\sigma^2)$$

$\mathcal{S}(\rho)$ becomes maximized if and only if ρ is a Gaussian.

Comment (ii):
We address a general **time-dependent setting**, before exemplified by admitting $\sigma = \sigma(t)$,

Comment (iii):
Recall the Fourier transform for normalized Schrödinger wave functions, together with the notions of **position and momentum representation** wave packets.
Given any, real (!) or complex function in $\psi(x) \in L^2(R)$. Let $(\mathcal{F}\psi)(p)$ be its Fourier transform. The corresponding probability densities follow:

$$\rho(x) = |\psi(x)|^2 \quad \text{and} \quad \tilde{\rho}(p) = |(\mathcal{F}\psi)(p)|^2.$$

Denote:

$$S_q = -\int \rho(x)\ln\rho(x)dx \qquad \text{and} \qquad S_p = -\int \tilde{\rho}(p)\ln\tilde{\rho}(p)dp$$

There holds the **entropic uncertainty relation** (Białynicki-Birula/Mycielski) between two forms (position and momentum respectively) of the information entropy:

$$S_q + S_p \geq (1 + \ln\pi)$$

Note:
In view of $\int \rho(x)dx = 1$, any continuous probability density can be rewritten as $\rho \doteq (\sqrt{\rho})^2$, i.e. in terms of $L^2(R)$ functions. The previous argument, of seemingly pure quantum provenance, undoubtedly works for $\psi \doteq \sqrt{\rho}$, hence in non-quantum settings as well.

MEASURES OF LOCALIZATION, MORE ENTROPIC INEQUALITIES

For an ρ with finite mean and variance fixed at σ^2, we have:

$$\mathcal{S}(\rho) \leq \frac{1}{2}\ln\left(2\pi e\sigma^2\right)$$

$$\Downarrow$$

$$\frac{1}{\sqrt{2\pi e}}\exp[\mathcal{S}(\rho)] \leq \sigma$$

We consider $\rho_\alpha \doteq \rho(x-\alpha)$ and fix at σ^2 the value $\langle (x-\alpha)^2\rangle = \langle x^2\rangle - \alpha^2$ of the variance. Let us define the Fisher information (localization measure) of ρ_α:

$$\mathcal{F}_\alpha \doteq \int \frac{1}{\rho_\alpha}\left(\frac{\partial \rho_\alpha}{\partial \alpha}\right)^2 dx \geq \frac{1}{\sigma^2}$$

INEQUALITIES OF VARIOUS SORTS FOLLOW

$$\frac{1}{\sigma^2} \leq (2\pi e)\,\exp[-2\mathcal{S}(\rho)] \leq \mathcal{F}_\alpha$$

Under an additional decomposition/factorization ansatz (of the quantum mechanical $L^2(R^n)$ provenance) that $\rho(x) \doteq |\psi|^2(x)$, where a real or complex function $\psi = \sqrt{\rho}\exp(i\phi)$ is a normalized element of $L^2(R)$,we have:

$$\mathcal{F}_\alpha = 4\int\left(\frac{\partial\sqrt{\rho}}{\partial x}\right)^2 dx \leq 16\pi^2\tilde{\sigma}^2$$

$$\frac{1}{\sigma^2} \leq \mathcal{F}_\alpha \leq 16\pi^2\tilde{\sigma}^2$$

$$\frac{1}{4\pi\tilde{\sigma}} \leq \frac{1}{\sqrt{2\pi e}}\exp[\mathcal{S}(\rho)] \leq \sigma$$

Outcome: the differential entropy $\mathcal{S}(\rho)$ typically may be expected to be a well behaved quantity: with finite both lower and upper bounds.

DYNAMICS OF INFORMATION $\rightarrow$ DYNAMICS OF LOCALIZATION

Smoluchowski diffusion process

We consider **time-dependent** probability densities $\rho \doteq \rho(x,t)$, whose evolution is governed by the **Fokker-Planck equation**:

$$\partial_t \rho = D \triangle \rho - \nabla \cdot (\rho b)$$

with the drift $b = b(x) = (1/m\beta)F, \quad F = -\nabla V, \quad D = k_B T/m\beta$. Set:

$$u(x,t) = D\nabla \ln \rho(x,t) \text{ and } v(x,t) = b(x,t) - u(x,t)$$

$$\Downarrow$$

$$\partial_t \rho = -\nabla(v\rho)$$

Now the **differential entropy**, typically is **not** a conserved quantity.

$$\mathcal{S}(t) = -\int \rho(x,t)\, \ln \rho(x,t)\, dx$$

$$\Downarrow$$

(with boundary restrictions that $\rho, v\rho, b\rho$ vanish at spatial infinities or finite interval borders)

$$\frac{d\mathcal{S}}{dt} = \int [\rho\,(\nabla \cdot b) + D \cdot \frac{(\nabla\,\rho)^2}{\rho}]\, dx$$

Remembering that $v = b + u$ and $u = D\nabla \ln \rho$, we have:

$$\frac{d\mathcal{S}}{dt} = \int [\rho\,(\nabla \cdot b) + D \cdot \frac{(\nabla\,\rho)^2}{\rho}]\, dx$$

$$\Updownarrow$$

$$D\dot{\mathcal{S}} \doteq D\,\langle \nabla \cdot b \rangle + \left\langle u^2 \right\rangle = -\,\langle v \cdot u \rangle$$

$$\Updownarrow$$

$$D\dot{\mathcal{S}} = \left\langle v^2 \right\rangle - \langle b \cdot v \rangle$$

$$D\dot{\mathcal{S}} = \left\langle v^2 \right\rangle - \langle b \cdot v \rangle$$

$$\Downarrow$$

"Thermodynamic" formalism

$$\frac{d\mathcal{S}}{dt} = \frac{d\mathcal{S}_{prod}}{dt} - \frac{d\mathcal{Q}}{dt}$$

where:

$$\frac{d\mathcal{S}_{prod}}{dt} \doteq \frac{1}{D} \left\langle v^2 \right\rangle \geq 0$$

while

$$\frac{d\mathcal{Q}}{dt} \doteq \frac{1}{D} \int \frac{1}{m\beta} F \cdot j \, dx = \frac{1}{D} \langle b \cdot v \rangle$$

Note:

$$k_B T \dot{\mathcal{Q}} = \int F \cdot j \, dx$$

$V = V(x)$ does not depend on time, define:

$$j = \rho D F_{th}$$

with:

$$k_B T F_{th} = F - k_B T \nabla \ln \rho \doteq -\nabla \Psi$$

Consider:

$$\Psi = V + k_B T \ln \rho$$

$$\Downarrow$$

$$\langle \Psi \rangle = \langle V \rangle - T\, \mathcal{S}'$$

where $\mathcal{S}' \doteq k_B \mathcal{S}$.

Minor surprise: $\langle\Psi\rangle = \langle V\rangle - T\,\mathcal{S}'$

(1) $< \Psi >$ stands for the**Helmholtz free energy**
(2) $< V >$ stands for the (mean) **internal energy**

$$\Downarrow$$

($\rho V v$ needs to vanish at the integration volume boundaries).

$$\frac{d}{dt}\langle\Psi\rangle = -k_B T\int F_{th}\cdot j\,dx = -(m\beta)\left\langle v^2\right\rangle = -k_B T\,\frac{d\mathcal{S}_{prod}}{dt} \leq 0$$

The "Helmholtz free energy" either remains constant or decreases as a function of time towards its minimum (which equals $-\infty$ when there is no external forces)

Note: Of particular interest is the case of constant differential entropy $\dot{\mathcal{S}} = 0$ which amounts to the existence of steady states. In the simplest case, when the diffusion current vanishes, we encounter the primitive realization of the state of equilibrium with an invariant density ρ. Then, $b = u = D\nabla\ln\rho$ and we readily arrive at the classic equilibrium identity for the Smoluchowski process:

$$-(1/k_B T)\nabla V = \nabla\ln\,\rho \qquad (2)$$

which determines the functional form of the invariant density:

$$\rho = \tfrac{1}{Z}\exp[-V/k_B T]$$

$$\Psi = V + k_B T\ln\rho$$

$$\Downarrow$$

$$\Psi = -k_B T\ln Z$$

MORE ABOUT LOCALIZATION DYNAMICS

In the absence of external forces, the de Bruijn identity tells us that:

$$\frac{d\mathcal{S}}{dt} = \frac{1}{D} \cdot \mathcal{F} \doteq D \cdot \int \frac{(\nabla\rho)^2}{\rho} dx > 0$$

Define:

$$Q = 2D^2 \frac{\Delta\rho^{1/2}}{\rho^{1/2}} = \frac{1}{2}u^2 + D\nabla \cdot u$$

$$\mathcal{F} \doteq \langle u^2 \rangle = -2\langle Q \rangle > 0$$

Variational arguments (with respect to ρ and $s(x,t)$ such that $v = \nabla s$) yield:

$$\mathcal{L} = -\int \rho \left[\partial_t s + \tfrac{1}{2}(\nabla s)^2 - \left(\tfrac{u^2}{2} + \Omega\right)\right] dx$$

$$\mathcal{H} \doteq \int \rho \cdot \left[\tfrac{1}{2}(\nabla s)^2 - \left(\tfrac{u^2}{2} + \Omega\right)\right] dx$$

$$\Downarrow$$

$$\partial_t s + \tfrac{1}{2}(\nabla s)^2 - (\Omega - Q) = 0$$

(plus the continuity equation) where:

$$\Omega = \tfrac{1}{2}\left(\tfrac{F}{m\beta}\right)^2 + D\nabla \cdot \left(\tfrac{F}{m\beta}\right)$$

We have:

$$\mathcal{H} = (1/2)(\langle v^2 \rangle - \langle u^2 \rangle) - \langle \Omega \rangle = -\langle \partial_t s \rangle$$

But:

$$\dot{\Psi} = \tfrac{k_B T}{\rho} \nabla(v\rho) \to \langle \dot{\Psi} \rangle = 0$$

in view of $v\rho = 0$ at the integration volume boundaries. Since $v = -(1/m\beta)\nabla\Psi$, we define

$$s(x,t) \doteq (1/m\beta)\Psi(x,t) \Longrightarrow \langle \partial_t s \rangle = 0$$

so that $\mathcal{H} \equiv 0$ identically.

$$\mathcal{H} \equiv 0$$

$$\Downarrow$$

$$\left(\frac{dS}{dt}\right)_{prod} = \frac{2}{D} \int \rho \left(\frac{\vec{u}^2}{2} + \Omega\right) \, dx = \frac{1}{D} \langle v^2 \rangle = \dot{\mathcal{H}}_c(t) \geq 0$$

Recall:

$$\mathcal{F} = \langle v^2 \rangle - 2\langle \Omega \rangle \geq 0$$

and exploit:

$$\partial_t(\rho v^2) = -\nabla \cdot [(\rho v^3)] - 2\rho v \cdot \nabla(Q - \Omega)$$

We get:

$$\frac{1}{2} \frac{d}{dt} \langle v^2 \rangle = -\langle v \nabla (Q - \Omega) \rangle$$

and

$$\frac{d}{dt}\mathcal{F} = \frac{d}{dt}[\langle v^2 \rangle + 2\langle \Omega \rangle] = -2\langle v \cdot \nabla Q \rangle$$

which is the general equation for the **localization/uncertainty dynamics** in the course of the Smoluchowski process.

Notice:

If together with $\rho(t) \to \rho_*$ we have $\dot{\mathcal{H}}_c(t) \to 0$ as $t \to \infty$, this implies $\mathcal{F} \to -2\langle \Omega \rangle_*$.

Reminders:

(*) $D\dot{\mathcal{S}} = \left\langle v^2 \right\rangle - \langle b \cdot v \rangle$

(**) $\frac{1}{\sigma^2} \leq (2\pi e) \exp[-2\mathcal{S}(\rho)] \leq \frac{1}{D^2}\mathcal{F}$

Reference: P. G., "Differential entropy and dynamics of uncertainty", quant-ph/0408192; see also Acta Phys. Pol. **B 36**, (2005), 1561-1577 and Phys. Lett. **A 341**, (2005), 33-38.