

A Microscopic Interpretation of the Entropy Increase Rate

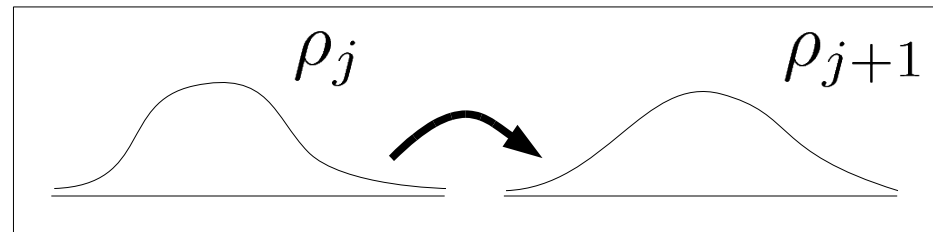
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For two probability densities ρ, ρ_0 on \mathbb{R}^d :

$$I_h(\rho; \rho_0) := \int \rho(x) \log \rho(x) dx + \frac{1}{2h} d(\rho, \rho_0)^2$$

$$\begin{aligned} \rho_1 &:= \arg \min_{\rho} I_h(\rho; \rho_0) \\ \rho_2 &:= \arg \min_{\rho} I_h(\rho; \rho_1) \\ &\vdots \end{aligned}$$



Th. (*R. Jordan, D. Kinderlehrer, F. Otto 1998*)

$$\rho_{t/h} \xrightarrow{h \rightarrow 0} u \quad \text{in } L^1(\mathbb{R}^d \times (0, \infty))$$

where u is the solution of the diffusion equation:

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u, & \mathbb{R}^d \times (0, \infty) \\ u = \rho_0, & \mathbb{R}^d \times \{t = 0\} \end{cases}$$

$$I_h(\rho; \rho_0) = \underbrace{\int \rho(x) \log \rho(x) dx}_{\text{driving force: (negative) entropy}} + \underbrace{\frac{1}{2h} d(\rho, \rho_0)^2}_{\text{brake: Wasserstein distance}}$$

How can we interpret this functional microscopically?

Look for a similar functional in ρ and ρ_0 such that the minimisers converge to u (the solution of the diffusion eq.)

ρ_0 initial probability density of particles

X_i random position of particle i at time h ,
with probability density $k_h(x, x_0) = \frac{1}{(4\pi h)^{d/2}} \exp\left(-\frac{|x-x_0|^2}{4h}\right)$

$L_n(x) := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}(x)$ particle density at time h

Th. (*Strong Law of Large Numbers*)

$$L_n \xrightarrow{n \rightarrow \infty} u \quad a.s.$$

where u is the solution of the diffusion equation:

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u, & \mathbb{R}^d \times (0, \infty) \\ u = \rho_0, & \mathbb{R}^d \times \{t = 0\} \end{cases}$$

We loose too much information in this limit!

Def. $\mathbb{P}(L_n)$ satisfies a Large Deviation Principle with rate functional J iff:

- (i) $J \neq \infty$ and has compact level sets
- (ii) $\frac{1}{n} \log \mathbb{P}(L_n) \xrightarrow{n \rightarrow \infty} -J$ (weak convergence by duality with continuous bounded functions)

Informally, this means that for large n :


$$\mathbb{P}(L_n \sim \rho) \sim e^{-nJ(\rho; \rho_0)}$$

Note that J is minimised by the most likely particle density ρ !

$$S(\rho) := \int \rho(x) \log \rho(x) dx$$
$$H(q|\mu) := \iint q(x, y) \log \frac{q(x, y)}{\mu(x, y)} dx dy$$

The rate functional is given by:

connection
for small h ?

$$J_h(\rho; \rho_0) = \inf_{q \in \Gamma(\rho, \rho_0)} H(q|\rho_0 k_h)$$
$$I_h(\rho; \rho_0) = S(\rho) + \frac{1}{2h} d(\rho, \rho_0)^2$$


Th. (*Adams, Dirr, Peletier, Zimmer; forthcoming*)

$$J_h(\cdot; \rho_0) - \frac{1}{4h} d(\cdot, \rho_0)^2 \xrightarrow{h \rightarrow 0} \frac{1}{2} S(\cdot) - \frac{1}{2} S(\rho_0)$$

- The Entropy-Wasserstein functional reflects the (infinitely small) probability that the system deviates from diffusion!
- Currently, my research focuses on extending this result to:
 - diffusion with drift
 - diffusion with death
 - diffusion with birth