Entropy and Recurrence with applications to Statistical Physics

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February 22, 2021

Overview

Definition ($\sigma-$ *algebra*)

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- $\bigcup_{n=1}^{\infty} B_n \in \mathcal{A}$ whenever $B_n \in \mathcal{A}$ for every $n \in \mathbb{N}$

Definition (Measure space)

Let $\mathcal{A}$ be a $\sigma -$ *algebra* of X. We say that a function $\mu : \mathcal{A} \to [0, +\infty]$ is a measure in X if:

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- If $B_n \in \mathcal{A}$ for every $n \in \mathcal{A}$ and $B_m \cap B_n = \emptyset$ whenever $m \neq n$, then
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$$\mu\left(\bigcup_{n=1}^{\infty} B_n\right) = \sum_{n=1}^{\infty} \mu(B_n).$$
- $(X, \mathcal{A}, \mu)$ is called a measure space.

Definitions (Measurable Transformations)

Let $(X, \mathcal{A}, \mu)$ a measure space.

- A function $\phi : X \to \mathbb{R}$ is measurable if $\phi^{-1}B \in \mathcal{A}$ whenever $B \in \mathcal{B}$, where $\mathcal{B}$ is the Borel $\sigma -$ *algebra* in $\mathbb{R}$, i.e, the $\sigma -$ *algebra* generated by the open sets in $\mathbb{R}$.

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- A transformation $f : X \to X$ is measurable if

$$f^{-1}B = \{x \in X : f(x) \in B\} \in \mathcal{A}$$

for every $B \in \mathcal{A}$.

Definition (Invariant Measure)

- Given $f : X \to X$, a measurable transformation, we say that μ is $f-$ *invariant* and that f preserves μ if

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- We notice that when f is invertible with measurable inverse the condition on this last definition is equivalent to

$$\mu(f(B)) = \mu(B)$$

for every $B \in \mathcal{A}$.

Recurrence

In this section we show that invariant finite measures origin recurrence, i.e, that almost every point of a set returns infinitely many times to that set, whenever this set is in the $\sigma - algebra$

Theorem (Poincaré's Recurrence Theorem)

Given $f : X \to X$ a measurable transformation and μ an $f - invariant$ finite measure in X. Then

$$\mu(\{x \in A : f^n(x) \in A \; for \; infinitely \; many \; values \; n\}) = \mu(A)$$

whenever $A \in \mathcal{A}$.

Poincaré's Recurrence Theorem Proof

Proof.

Let $B = \{x \in A : f^n(x) \in A \textit{ for infinitely many values } n\}$. We have that

$$B = A \cap \bigcap_{n=1}^{\infty} A_n = A \setminus \bigcup_{n=1}^{\infty} (A \setminus A_n),$$

where

$$A_n = \bigcup_{k=n}^{\infty} f^{-k}A.$$

Notice that

$$A \setminus A_n \subset A_0 \setminus A_n = A_0 \setminus f^{-n}A_0.$$

As $f^{-n}A_0 = A_n \subset A_0$ and μ is finite, then since μ is $f - \textit{invariant}$

$$0 \leq \mu(A \setminus A_n) \leq \mu(A_0 \setminus f^{-n}A_0) = \mu(A_0) - \mu(f^{-n}A_0) = 0,$$

and thus $\mu(B) = \mu(A)$. □

Birkhoff's Ergodic Theorem

Formulation of the Theorem

Let $f : X \to X$ be a measurable transformation and $A \subset X$ be a measurable set. Given $x \in X$ and $n \in \mathbb{N}$, we define

$$\tau_n(A, x) = card\Big\{k \in \{0, ..., n-1\} : f^k(x) \in A\Big\}.$$

Note that $\tau_1(A, x) = \mathcal{X}_A(x)$ and thus,

$$\tau_n(A, x) = \sum_{k=0}^{n-1} \tau_1(A, f^k(x)) = \sum_{k=0}^{n-1} \mathcal{X}_A(f^k(x)).$$

When the limit

$$\lim_{n\to\infty} \frac{\tau_n(A, x)}{n} = \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \mathcal{X}_A(f^k(x))$$

exists, it gives the frequency with which the orbit of x visits the set A.

Birkhoff's Ergodic Theorem

If μ is a finite $f-invariant$ measure in X, Poincaré's recurrence theorem says that $\tau_n(A, x) \to \infty$ when $n \to \infty$, for $\mu - almost$ every $x \in A$. Birkhoff's ergodic theorem gives us information about the existence of the limit above.

Theorem

(Birkhoff's ergodic theorem) Let $f : X \to X$ be a measurable transformation and μ a finite $f-invariant$ measure in X. Given a $\mu-integrable$ function $\phi : X \to \mathbb{R}$, the limit

$$\phi_f(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \phi(f^k(x))$$

exists for almost every point $x \in X$ and we have

$$\int_X \phi_f \, d\mu = \int_X \phi \, d\mu.$$

Entropy

The notion of metric entropy with respect to a measurable partition is introduced. Let $(X, \mathcal{A}, \mu)$ be a probability space, i.e, a measure space with $\mu(X) = 1$. $0 \log 0 = 0$ is used as a convention.

Definition

It is said that a finite collection $\xi \subset \mathcal{A}$ is a partition of X with relation to the measure μ if:
a) $\mu\left(\bigcup_{C\in\xi} C\right) = 1$;
b) $\mu(C \cap D) = 0$ for any $C, D \in \xi$ whenever $C \neq D$.

Definition

The entropy of a partition ξ of X with respect to μ is given by

$$H_\mu(\xi) = \sum_{C\in\xi} \mu(C) \log \mu(C).$$

Boltzmann's Entropy

In physics, entropy measures the level of disorder and chaos in a system. Boltzmann came up with the formula for the entropy of a physical system.

$$S = k_B \log W$$

where k_B is the Boltzmann constant, and W is the number of micro-states corresponding to the macro-state. Given a partition $\xi = \{A_1, ..., A_N\}$ with probability measure $\mu(A_i) = p_i$, the entropy of the partition is

$$H_\mu(\xi) = -\sum_{i=1}^{N} p_i \log(p_i).$$

Boltzmann's Entropy

Then for a system with a discrete set of micro-states, if E_i is the energy of a micro-state i, and p_i is the probability that it occurs, then the entropy of the system is

$$S = -k_B \sum_{i=1}^{W} p_i \log(p_i).$$

A fundamental postulate in physical statistics states that for an isolated system with an exact macro-state, every micro-state that is consistent with the macro-state should be found with equal probability. Therefore if $p_i = W^{-1}$ for all i, then

$$S = -k_B \sum_{i=1}^{W} \frac{1}{W} \log \frac{1}{W} = k_B \log W$$

which is exactly the Boltzmann's entropy.

Definition Hamiltonian

The energy of a system of N particles is a function of the positions and momentum of these particles, called the Hamiltonian. The Hamiltonian is a function given by

$$H(q,p) = \sum_{i=1}^{n} \left(\frac{p_i^2}{2m} + W(q_i) \right) + \sum_{i<j} V(|q_i - q_j|),$$

where $q = (q_1, ..., q_n)$, $p = (p_1, ..., p_n)$ and W, V are the external and the pair potential that come from external forces and forces that one particle exerts on the other, respectively.

Micro-canonical Measure

We have an insulated box Λ.
The phase space, denoted as Γ is the set of all spatial positions and momenta of these particles, so

$$\Gamma = (\Lambda \times \mathbb{R}^d)^N$$

For any $E \in \mathbb{R}_+$, the energy surface Σ_E for a given Hamiltonian H is defined as

$$\Sigma_E = \{(p, q) \in \Gamma : H(p, q) = E\}.$$

Micro-canonical Measure

If $\omega(E) = \mu'_E(\Gamma) < \infty$, then μ'_E can be normalized as

$$\mu_E = \frac{\mu'_E}{\omega(E)}$$

which is a probability measure on $(\Gamma, \mathcal{B}_\Gamma)$, called the micro-canonical measure or microcanonical ensemble. The micro-canonical measure can also be defined explicitly using polar coordinates. Let $d\sigma_E$ be the surface area element of Σ_E, then

$$d\mu'_E = \frac{d\sigma_E}{\|\nabla H\|}, \omega(E) = \int_{\Sigma_E} \frac{d\sigma_E}{\|\nabla H\|}$$

The function $\omega(E)$ is called the micro-canonical partition function. From the definition above, $\omega(E)$ is the number of microstates on the energy surface, so $W = \omega(E)$. From Boltzmann's Entropy $S = k_B \log \omega(E)$.

Ideal Gas in a Micro-canonical Ensemble

N identical particles, mass m in d-dimensions in a box Λ of volume $V = |\Lambda|$.

The Hamiltonian is given by

$$H_\Lambda(x) = \sum_{i=1}^{n} \frac{p_i^2}{2m}$$

with gradient

$$\nabla H_\Lambda(x) = \frac{1}{m}(0, ..., 0, p_1, ..., p_n).$$

Note that

$$|\nabla H_\Lambda(x)| = \frac{1}{m^2}\sum_{i=1}^{n} p_i^2 = \frac{2}{m}H(x).$$

For every $x \in \Sigma_E, H(x) = E$ and

$$|\nabla H_\Lambda| = \sqrt{\frac{2E}{m}}.$$

Ideal Gas in a Micro-canonical Ensemble

Notice that

$$|(p_1, ..., p_n)| = m|\nabla H_\Lambda(x)| = \sqrt{2mE}.$$

Since the norm of p is constant, the energy surface Σ_E can be expressed as

$$\Sigma_E = \Lambda^N \times S_n(\sqrt{2mE})$$

where $S_d(r)$ is the hyper sphere of radius r in dimension d. The surface area of a hyper-sphere with dimension d is

$$A = c_d r^{d-1}$$

where c_d is constant. Therefore,

$$\omega(E) = \int_{\Sigma_E} \frac{d\sigma_E}{|\nabla H_\Lambda|} = \sqrt{\frac{m}{2E}} \int_{\Sigma_E} d\sigma_E = mV^N c_{Nd}(2mE)^{\frac{1}{2}Nd-1}.$$

From Boltzman's entropy formula,

$$S = k_B \log \omega(E) = k_B \log \left(mV^N c_{Nd}(2mE)^{\frac{1}{2}Nd-1} \right).$$

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