The Gibbs distribution

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Overview

Let Ω be a finite configuration space of a physical system. The energy of the configuration $\omega \in \Omega$ is $H(\omega)$.

Example: Ising model on a finite graph (V, E):

$$\Omega = \{-1, +1\}^V, \qquad H(\omega) := -\sum_{\{x,y\}\in E} \omega_x \omega_y \,.$$

Gibbs distribution: probability measure μ on Ω that has fixed energy and maximal entropy.

Entropy

Quantify the disorder or "mixed-up-ness" [Gibbs, 1903] of the measure μ. Informally:

$$S = \log \big|\{\text{microstates giving rise to the observed macrostate}\}\big|.$$

If μ is the uniform distribution on Ω (all configurations of Ω are equally likely) then

$$S(\mu) = \log |\Omega|.$$

Why log?

Entropy should be extensive. Putting two systems, 1 and 2, together amounts to $\Omega = \Omega_1 \times \Omega_2$ and $\mu = \mu_1 \otimes \mu_2$. Hence, $S(\mu) = S(\mu_1) + S(\mu_2)$.

How to define S for general μ? Simple model: put n balls into the boxes of Ω:

$$\text{microstate} = \text{individual balls' locations}$$

$$\text{macrostate} = \text{number of balls in each box.}$$

More formally: To $\mathbf{b} = (b_1, b_2, \dots, b_n) \in \Omega^n$ (individual balls' locations) assign $N_\omega(\mathbf{b}) := |\{1 \leqslant i \leqslant n : b_i = \omega\}|$ (number of balls in box ω).

Then $\mathbf{b}$ is the microstate and $\mathbf{N}(\mathbf{b}) = (N_\omega(\mathbf{b}))_{\omega \in \Omega}$ is the associated macrostate.

For $\mathbf{N} \in \mathbb{N}^\Omega$ define

$$W(\mathbf{N}) := |\{\mathbf{b} \in \Omega^n : \mathbf{N}(\mathbf{b}) = \mathbf{N}\}| \,.$$

Exercice. Suppose that $b_1, b_2, \dots$ are i.i.d. random variables in Ω with law μ. Then, almost surely as $n \to \infty$,

$$\frac{1}{n} \log W(\mathbf{N}(\mathbf{b})) \longrightarrow S(\mu) := -\sum_{\omega \in \Omega} \mu(\omega) \log \mu(\omega) \,.$$

The quantity

$$S(\mu) = -\sum_{\omega \in \Omega} \mu(\omega) \log \mu(\omega)$$

is the (Boltzmann-Gibbs-Maxwell-Shannon) entropy of the probability measure μ.

Exercise.

- $0 \leqslant S(\mu) \leqslant \log|\Omega|$.
- $S(\mu) = 0$ if and only if $\mu = \delta_{\omega_0}$ for some $\omega_0 \in \Omega$.
- $S(\mu) = \log|\Omega|$ if and only if μ is uniform on Ω.

The Gibbs measure

Define the energy of the distribution μ as

$$U(\mu) := \sum_{\omega \in \Omega} H(\omega)\, \mu(\omega)\,.$$

Maximize the entropy $S(\mu)$ under fixed energy $U(\mu)$.

Exercise.

$$\mu(\omega) = \frac{1}{Z} \mathrm{e}^{-\beta H(\omega)}\,, \qquad Z := \sum_{\omega \in \Omega} \mathrm{e}^{-\beta H(\omega)}\,.$$

- β is a Lagrange multiplier with the interpretation of the inverse temperature, $\beta = 1/T$.
- Z is the partition function.
- The (Helmholtz) free energy is $F := -T \log Z$. We obtain the thermodynamic relation

$$F = U - TS\,.$$

Infinite configuration space

In most interesting applications, Ω is infinite, and the notion of Gibbs measure is much more subtle.

It is best formulated in the framework of spin systems: A probability space (S, λ) is assigned to each site of a lattice L. The configuration space is $\Omega = S^L$ with configuration $\omega = (\omega_x)_{x \in L}$.

Notations: Let $\Lambda \subset L$.

- $\omega_\Lambda = (\omega_x)_{x \in \Lambda}$ and $\omega = \omega_\Lambda \omega_{\Lambda^c}$.
- $\lambda(\mathrm{d}\omega_\Lambda) = \prod_{x \in \Lambda} \lambda(\mathrm{d}\omega_x)$.

For each finite $A \subset L$, introduce a potential Φ_A that depends only on ω_A.

Defining $H(\omega) := \sum_{A \subset L} \Phi_A(\omega)$, we want to define the Gibbs measure

$$\mu(\mathrm{d}\omega) = \frac{1}{Z} \, \mathrm{e}^{-\beta H(\omega)} \, \lambda(\mathrm{d}\omega) \,, \qquad Z := \int \lambda(\mathrm{d}\omega) \, \mathrm{e}^{-\beta H(\omega)}$$

Only makes sense for finite L.

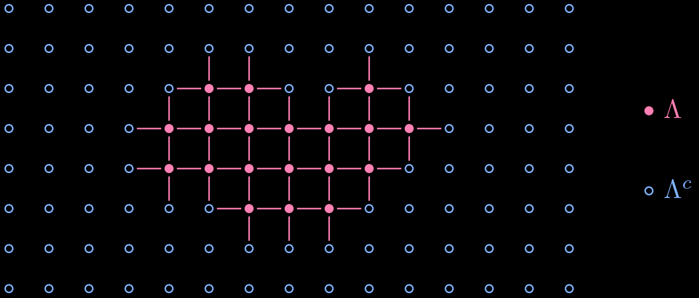
The Dobrushin-Lanford-Ruelle (DLR) equation

Let $\Lambda \subset L$ be finite. For a boundary condition $\eta \in S^L$ define the conditional energy

$$H(\omega_\Lambda | \eta_{\Lambda^c}) := \sum_{A \subset L : A \cap \Lambda \neq \emptyset} \Phi_A(\omega_\Lambda \eta_{\Lambda^c})$$

and the conditional partition function

$$Z_\Lambda^\eta := \int \lambda(\mathrm{d}\omega_\Lambda)\, \mathrm{e}^{-\beta H(\omega_\Lambda | \eta_{\Lambda^c})}\,.$$



Exercise. For finite L and bounded $f : \Omega \to \mathbb{R}$ we have

$$\int \mu(\mathrm{d}\omega)\, f(\omega) = \int \mu(\mathrm{d}\eta)\, \frac{1}{Z_\Lambda^\eta} \int \lambda(\mathrm{d}\omega_\Lambda)\, \mathrm{e}^{-\beta H(\omega_\Lambda | \eta_{\Lambda^c})}\, f(\omega_\Lambda \eta_{\Lambda^c})\,. \qquad \text{(DLR)}$$

For infinite L, take (DLR) as the definition of a Gibbs measure:

Definition. A probability measure μ satisfying (DLR) for all finite $\Lambda \subset L$ and f of bounded support is called a Gibbs measure associated with (Φ_A).

Existence is easy under a general locality assumption on (Φ_A) (weak compactness argument).

Uniqueness is delicate and in general wrong: coexistence of phases (dependence on boundary conditions).