36 Thermodynamic formalism

36.1-36.8 summarize the Gibbs measure theory on 1D lattice (for disordered systems). Mathematically, this measure and the observable measure for chaotic dynamical systems are closely related. Here, we wish to maximally abuse functional analysis and to respect theoretical physics aesthetics.

36.1 Preparatory comments on measures

Let $M(X)$ be the set of all the Borel measures on X.
Let T be an automorphism on X. Then, T induces a map T^* on $M(X)$: for $\mu \in M(X)$

$$\mu(T^{-1}E) = (T^*\mu)(E) = T^*\mu(E). \tag{36.1}$$

Since $T^{-1}(E)$ the totality of the points coming to E after one time step, $T^*\mu = \mu$ means the preservation of measure.

We may introduce a weak topology on $M(X)$. Actually,
Proposition: $M(X)$ is a compact convex metrizable space.

36.2 Invariant measure set is nonempty and closed

Proposition: Let $M_T(X)$ be the set of all the invariant measures. Then, it is nonempty and is closed in $M(X)$.

[Demo] Let

$$\mu_n = \frac{1}{n}(\mu_0 + T\mu_0 + \cdots + T^n\mu_0). \tag{36.2}$$

Since $M(X)$ is compact, we can always take a converging subsequence. The result is invariant.

$\mu \in M_T(X)$ means

$$\int (f \circ T) d\mu = \int f d\mu. \tag{36.3}$$

36.3 Lattice states

Let $x_i \in \{0, 1, \cdots, n-1\}$ be a state at a single lattice point. A lattice state is described by $\{x_k\}_{k=-\infty}^{\infty}$. The totality of these sequences is Σ_n.

36.4 Energy function

To do study statistical mechanic on the lattice we need an energy function $\varphi : \Sigma_n \to \mathbb{R}$. It is the 1/2 of the total interaction and the self energy of a spin. We impose the following constraint on ϕ. Let

$$\mathrm{var}_k \phi = \sup\{|\phi(x) - \phi(y)| \, : x_i = y_i \text{ for } |i| \le k\}. \tag{36.4}$$

Our constraint is

$$\mathrm{var}_k \varphi \le b\alpha^k, \tag{36.5}$$

where $b > 0$ and $\alpha \in (0, 1)$. Let us explicitly write

$$\mathcal{F}_A = \{\phi \,|\, \Sigma_A \to \mathbb{R}, \mathrm{var}_k \varphi \le b\alpha^k, \forall k \in \mathbb{N}\}. \tag{36.6}$$

Here Σ_A is a Markov subshift with matrix A.

36.5 Gibbs measure

For any Hamiltonian $\phi \in \mathcal{F}_A$, there is a unique shift invariant measure μ_ϕ satisfying the following inequality for some positive constants C_1, C_2 and A (= free energy per spin)

$$C_1 \le \frac{\mu\{y \, : y_i = x_i, \forall i \in \{0, 1, \cdots, n\}}{\exp(-An + \sum_{k=0}^{n-1} \phi(\sigma^k x))} \le C_2, \tag{36.7}$$

36.6 Transfer operator

Consider the totality of the states on the right-half lattice S_A^+.[401] and $\phi \in C(\Sigma_A^+$. Define the transfer operator T_ϕ as

$$[T_\phi f](x) = \sum_{y \in \sigma^{-1} x} e^{\phi(y)} f(y). \tag{36.8}$$

Notice that $y = x_* x_1 x_2 \cdots$.

[401] If you read the original math paper, there is a long discussion about how to justify considering of Σ^+ instead of Σ_A.

36.7 Ruelle-Perron-Frobenius theorem

Let Σ_A be mixing and $\phi \in \mathcal{F}_A \cap C(\Sigma_A^+)$. There is a unique positive eigenvalue λ_ϕ of T_ϕ, and the Gibbs measure is obtained from the partition function and the normalization obtained from λ_ϕ

$$\mu([x]_n) \simeq \frac{1}{\lambda_\phi^n} \exp\left(\sum_{i=1}^n \phi(x_i)\right), \tag{36.9}$$

where $[x]_n = x_1 \cdots x_n$ is a cylinder set.

36.8 Variational principle for Gibbs measure

The Gibbs measure μ_ϕ is the unique measure satisfying the following variational principle:

$$s(\mu) + \int \phi d\mu = \tilde{A}(\phi). \tag{36.10}$$

where s is the entropy per spin, and $\tilde{A} = (1/N) \log Z = \log \lambda_\phi$ (that is, $-\beta A/N$ in the standard statistical thermodynamic notation).

The T-invariant measure satisfying the variational principle is called an equilibrium state wrt to T and ϕ.[402]

36.9 Large deviation and thermodynamics

In the following we assume H is bounded from above.

The partition function

$$Z(\beta) = \sum e^{(-\beta) \sum_h} \tag{36.11}$$

may be interpreted as the generating function for energy with respect to the Liouville measure (the uniform or equal probability) measure. We ask the energy fluctuation with respect to this measure (for a portion of the system containing N subsystems which are assumed to be more or less statistically independent. We assume the LD principle:

$$P\left(\frac{1}{N} \sum h \sim e\right) \approx e^{-NI(e)}. \tag{36.12}$$

[402] Th 2.7

Its generating function may be written as

$$\frac{Z(\beta)}{Z(0)} = \left\langle e^{(-\beta)\sum h} \right\rangle_0, \tag{36.13}$$

where $\langle\ \rangle_0$ denotes the expectation value with respect to the uniform measure.

(36.13) may be rewritten as

$$\begin{aligned} \frac{Z(\beta)}{Z(0)} &= \left\langle e^{(-\beta)\sum h} \right\rangle_0 = \int dy \left\langle \delta\left(y - \frac{1}{N}\sum h\right)\right\rangle_0 e^{(-\beta)Ny} && (36.14) \\ &= \int dy\, P\left(\frac{1}{N}\sum h \sim y\right) e^{(-\beta)Ny} = \int dy e^{-NI(y)} e^{(-\beta)Ny}. && (36.15) \end{aligned}$$

Using the Laplace-type approximation, we have

$$\frac{1}{N}\log(Z(\beta)/Z(0)) = \sup_y[(-\beta)y - I(y)]. \tag{36.16}$$

Introduce

$$[-a](-\beta) = \frac{1}{N}\log(Z(\beta)). \tag{36.17}$$

(36.16) reads

$$[-a](-\beta) - [-a](0) = \sup_y[(-\beta)y - I(y)]. \tag{36.18}$$

In terms of the usual thermodynamic quantity $[-a](-\beta) = -\beta A/N$, $y = E/N = e$. Also so $[-a](0) = -\lim_{\beta\to 0}\beta A/N = -\lim_{T\to\infty} A/T = \lim_{T\to\infty}(S - E/T)$, but if we assume H to be bounded (as magnets), this converges to $S(\infty)$, the log of the phase volume, essentially. Therefore, (36.18) reads

$$-\beta A/N = \sup_e[(-\beta)e - I(e)] + S(\infty), \tag{36.19}$$

so $I(e) = \beta(A - E)/N - S_\infty = S_\infty - S$. The most probable e is the internal energy at $\beta = 0$. Thus, $I(e)$ is the information required to characterize the deviated energy distribution from uniform distribution: That is, the following KL entropy is

$$I(e) = \frac{1}{N}\sum_i f_i \log(Z_0 f_i) = S_\infty - S. \tag{36.20}$$

By the way, this can be obtained from Sanov's theorem + the contraction principle:

$$I(e) = \inf_{\nu:\int d\nu\, h = e} I^{(2)}(\nu). \tag{36.21}$$

Here $I^{(2)}$ is the level 2 large deviation functional with respect to the equal probability measure on the phase space. This relation is what Jaynes misunderstood as the principle to found statistical mechanics.

36.10 Perron-Frobenius eigenvalue problem

The Perron-Frobenius equation **31.4** reads

$$\varphi(x) = (\mathcal{L}_F\varphi)(x) = \int m(dy)\delta(x - F(y))\varphi(y) = \sum_{y\in F^{-1}(x)} \frac{\varphi(y)}{|F'(y)|}. \tag{36.22}$$

For reasonably chaotic systems ('(non-uniformly) hyperbolic systems'), the counterpart should read

$$\varphi(x) = (\mathcal{L}_F\varphi)(x) = \int m_+(dy)\delta(x - F(y)) = \sum_{y\in F^{-1}(x)} \frac{\varphi(y)}{L_+(y)}, \tag{36.23}$$

where m_+ is the Lebesgue measure (better, the Riemann volume of unstable manifolds; red curves in Lecture 39), L_+ is the expansion rate of the unstable manifold (the sum of all the positive Lyapunov characteristic numbers; cf. **33.6**), and δ must be defined wrt m_+.

Note the following formula:

$$(\mathcal{L}_{F^n}\varphi)(x) = \sum_{y\in F^{-n}(x)} \frac{\varphi(y)}{|(F^n)'(y)|} = (\mathcal{L}_F^n\varphi)(x). \tag{36.24}$$

Following the Fredholm integral equation, the corresponding eigenvalue problem reads

$$\varphi(x) = \lambda(\mathcal{L}_F\varphi)(x). \tag{36.25}$$

Note that $\mathcal{L}_F$ is a special case of the transfer operator **36.6** with $\phi = -\log|F'|$. The eigenvalue problem used in **36.7** is the reciprocal of λ in (36.25). The conventions in linear algebra and in integral equations are different.

36.11 Fredholm determinant for Perron-Frobenius operator[403]

(36.25) may be rewritten as

$$(1 - \lambda\mathcal{L}_F)\varphi = 0. \tag{36.26}$$

[403] Y Oono and Y Takahashi, "Chaos, external noise and Fredholm theory," Prog Theor Phys 63 1804 (1980).

Therefore, the eigenvalues should be the zeros of the 'determinant' $D(\lambda, F)$ of $1-\lambda\mathcal{L}_F$. To define this we use an identity $\det B = \exp(\mathrm{Tr}\,\log B)$:

$$\det(1-\lambda A) = \exp\left[\mathrm{Tr}\,\log(1-\lambda A)\right] = \exp\left[-\mathrm{Tr}\sum_{n=1}^{\infty}\frac{\lambda^n}{n}A^n\right]. \tag{36.27}$$

This implies that we have to define the trace of $\mathcal{L}_F^n$. Looking at (36.24) we define

$$\mathrm{Tr}\,\mathcal{L}_F^n = \sum_{z\in F^{-n}(z)}\frac{1}{|(F^n)'(z)|} \equiv Q_n. \tag{36.28}$$

Thus, we define

$$D(\lambda, F) \equiv \det(1-\lambda\mathcal{L}_F) = \exp\left[-\sum_{n=1}^{\infty}\frac{\lambda^n}{n}Q^n\right]. \tag{36.29}$$

Recall that the ζ-function (Artin-Mazur-Ruelle ζ-function) **26.9** is just the reciprocal of this quantity.

36.12 Significance of $D(\lambda, F)$

(1) The expansion of $D(\lambda, F)$ around $\lambda = 0$ is intimately related to the symbolic realization of the dynamical system.
(2) If $D(1, F) = 0$, then the system has an observable measure.[404]
(3) At criticality, $D(\omega, F) = 0$ for any ω such that $\omega^n = 1$. That is, the natural boundary of $D(\lambda, F)$ is a unit circle iff F is critical (under the condition that F' is bounded).

36.13 Free energy

Look at

$$-\log D(\lambda, F) = \sum_{n=1}^{\infty}\frac{\lambda^n}{n}Q^n. \tag{36.30}$$

The structure of Q_n is

$$Q_n = \mathrm{Tr}\,\mathcal{L}_F^n = \sum_{\text{fixed points of } F^n} e^{-\log|(F^n)'(y)|}. \tag{36.31}$$

[404]Precisely speaking, this is our conjecture.

Notice that the cain rule means

$$(F^n)'(y) = F'(F^{n-1}(x_0))F'(F^{n-2}(x_0)) \cdots F'(x_0) = \prod_i F'(x_i), \tag{36.32}$$

where $\{x_0, x_1, \cdots, x_{n-1}\}$ is a periodic orbit. $1/n$ in front of Q_n in (36.30) means that the actual sum is over the periodic trajectories. You could think that $\log|F'|$ is the energy (Hamiltonian) and that the trajectory positions correspond to 'microstates' of a statistical equilibrium system (see **36.7**), although there is no temperature (yet) β. Thus, (36.30) may be interpreted as the grand canonical partition function by setting the fugacity $\lambda = e^{\beta\mu}$. Q_n is the canonical partition function, so we may introduce the free energy A (per time = lattice point):[405]

$$A = -\limsup_{n\to\infty} \frac{1}{n} \log Q_n. \tag{36.33}$$

Notice that $\rho = e^A$ is the convergence radius of the zeta function = inverse of Perron-Frobenius eigenvalue.

If the nonwandering set is a stable periodic orbit, then $A < 0$.
If $A = 0$, there is an observable invariant measure.

36.14 Chaotic system under noise

Instead of $x \to F(x)$, let us add an additive noise

$$x_{n+1} = F(x_n) + \nu_n, \tag{36.34}$$

where we assume ν_n is a noise (at time n) which has a density distribution g. Then, the Perron-Frobenius equation is converted to

$$\varphi_\nu(x) = \int m(dy) g(x - F(y))\varphi_\nu(y) \equiv (\hat{\mathcal{L}}_F \varphi_\nu)(x). \tag{36.35}$$

We expect that in the $\nu \to 0$ limit (that is, the $g \to \delta$ limit), the system, if stable, should recover the noiseless system. Notice that, simply following the computational rule of the δ-function, we must conclude

$$\lim_{g\to\delta} \hat{\mathcal{L}}_F^n = \int m(dy)\delta(y - F_n(y)) = \sum_{z\in F^{-n}(z)} \frac{1}{|(F^n)'(z) - 1|} \equiv \hat{Q}_n. \tag{36.36}$$

[405]Mathematicians do not like '−' in front of the following definition, and from the convex analytical point of view mathematicians' convention is more rational than statistical-physicists', but here we stick to the physics tradition.

The difference between Q_n and $\hat{Q}_n$ is insignificant, if the system is sufficiently chaotic.

Thus, the statistical properties of a chaotic system is stable against noise. Thus, we may say that the macroscopic stability is warranted by microscopic instability. This is very suggestive of the stability of tropical rain forest systems.

36.15 Let us introduce temperature[406]

Instead of (36.31) let us introduce the canonical partition function

$$Q_n(\beta) = \sum_{\text{fixed points of } F^n} e^{-\beta \log |(F^n)'(y)|}. \tag{36.37}$$

Accordingly, we may introduce the temperature-dependent free energy

$$A(F, \beta) = -\beta^{-1} \limsup_{n\to\infty} \log Q_n(\beta). \tag{36.38}$$

36.16 Thermodynamics

The internal energy reads (use the Gibbs-Helmholtz relation)

$$E(\beta) = \frac{\partial \beta A}{\partial \beta} = \langle \log |F'| \rangle_\beta. \tag{36.39}$$

Entropy is

$$S(\beta) = \beta^2 \frac{\partial A}{\partial \beta} = \beta(E(\beta) - A(F, \beta)). \tag{36.40}$$

Actually, we know this is a Legendre transformation. If we compare this with the LD formalism, this entropy is just the Kolmogorov-Sinai entropy.

From **36.12** (2), if F allows an observable chaos, $A(1, F) = 0$, so we recover Rohlin's formula:

$$S(1) = \langle \log |F'| \rangle. \tag{36.41}$$

Note that $S(0)$ is given by

$$S(0) = \limsup_{n\to\infty} \frac{1}{n} [\#\mathrm{Fix}(F^n)] \tag{36.42}$$

[406] Y Takahashi and Y Oono, "Towards he statistical mechanics of chaos," Prog Theor Phys 71 851 (1984).

which is the topological entropy.[407] Entropy should be an increasing function of temperature: thus the KS entropy is bounded by topological entropy:

$$S(0) \geq S(1). \tag{36.43}$$

This is Dinaburg's theorem.[408]

36.17 What is β?

The conjecture is:
The Hausdorff dimension of the support of the observable measure if β_c such that $A(\beta_c, F) = 0$.

36.18 What is the outstanding conjecture theoretical physicists can make?

This is a summary of what I was pursuing.

A necessary and sufficient condition for a dynamical system to have an observable measure defined by the stability against noises is that the Fredholm determinant of the Perron-Frobenius (+-version) satisfies $D(1, F_+) = 0$.

$D(\lambda, F_+)$ may be factorized into holomorphic factors each of which has nondegenerate $\lambda = 1$ as its smallest zero and corresponds to the unique observable measure supported on an invariant set (= basic set). The observable measure can be described as a Gibbs measure with $|\log F_+|$ as the energy function.

[407] R. Bowen, TAMS 184 125 (1973).
[408] E. I. Dinaburg, Math USSR Izv 5 337 (1971).