

2 Large deviations, Gibbs measures

2a	Who needs ridiculously small probabilities? . . .	10
2b	Is the normal approximation helpful?	11
2c	A non-normal approximation	12
2d	Large deviations: upper bound	12
2e	Better bound via tilting	14
2f	Large deviations: lower bound	17
2g	Higher dimension: upper bound	18
2h	Higher dimension: lower bound	19
2i	Using conditions (1a1), (1a2)	20
2j	The function φ , at last	22
2k	Proving the theorem	23
2l	Equivalence of ensembles	24
2m	Hints to exercises	25

Theorem 1b4 is proved via the large deviations theory; a formula for $\varphi = [g|f]$ is given in terms of Gibbs measures.

2a Who needs ridiculously small probabilities?

2a1 Example. A fair coin is tossed 200 times. The probability of 10 “heads” is

$$2^{-200} \binom{200}{10} \approx 1.4 \cdot 10^{-44}.$$

We are pretty sure that this event will not occur in practice. Then, does it matter, is it 10^{-44} , or 10^{-40} , or 10^{-50} ?

For coin tossing it does not matter, but for statistical physics it does!

2a2 Example. Consider a system of 200 spins¹ $\omega_1, \dots, \omega_{200} = \pm 1$ with a one-particle Hamiltonian $h(\omega_1) = \omega_1$ and a given energy per particle

$$h^{(200)}(\omega_1, \dots, \omega_{200}) = -0.9 \in (-1, 1).$$

(Quite feasible.) Now, only 10 out of the 200 spins are +1, others are -1.

¹So-called spin- $\frac{1}{2}$ particles.

You may ask: so what? We still do not need 10^{-44} . Right; but see the next example.

2a3 Example. Consider a system of n spins,¹ each taking on three values $-1, 0, +1$, described by $\Omega^n = \{-1, 0, 1\}^n$ (with the counting measure) and the one-particle Hamiltonian $h(\omega_1) = \omega_1$. Introduce another macroscopic observable $f^{(n)}$ where $f(\omega_1) = \omega_1^2$. We want to know the conditional distribution (according to 1b1) of $f^{(n)}$ given $h^{(n)} \approx -0.9$. This question is physically meaningful for quite large n (much more than 200, in fact, such as 10^{23}). Probabilistically, we want to know the conditional distribution, given the condition of exponentially small probability (much smaller than 10^{-44}). Such conditional probabilities are ratios of ridiculously small unconditional probabilities. . .²

2b Is the normal approximation helpful?

Consider for now $\Omega^n = \{-1, +1\}^n$ with the uniform distribution (the counting measure normalized by dividing by 2^n). The random variable $(\omega_1 + \dots + \omega_n)/\sqrt{n}$ is approximately normal standard (γ^1),

$$\mathbb{P}\left(\frac{\omega_1 + \dots + \omega_n}{\sqrt{n}} = x\right) \approx \frac{2}{\sqrt{n}} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad \text{for } x = \frac{-n}{\sqrt{n}}, \frac{-n+2}{\sqrt{n}}, \dots, \frac{n}{\sqrt{n}}.$$

Taking for example $n = 200$ and $x = \frac{-200+20}{\sqrt{200}} \approx -12.7$ we get

$$\mathbb{P}\left(\frac{\omega_1 + \dots + \omega_{200}}{200} = -0.9\right) \approx 3.7 \cdot 10^{-37}$$

instead of $1.4 \cdot 10^{-44}$. Quite bad!

Replacing -0.9 with -0.6 we get the normal approximation $1.3 \cdot 10^{-17}$ ($x \approx -8.5$) to the probability $1.3 \cdot 10^{-18}$. For -0.3 : approximation $7.0 \cdot 10^{-6}$ ($x \approx -4.2$) to $6.3 \cdot 10^{-6}$. And for -0.15 : approximation 0.00595 ($x \approx -2.1$) to 0.00596 .

In fact, the normal approximation has a small *relative* error when³ $x^4 \ll n$. For the event $(\omega_1 + \dots + \omega_n)/n = a$ we have $x = a\sqrt{n}$, thus, $x^4 \ll n$ when $a^4 \ll 1/n$. Rather good for coin tossing, but far not enough for statistical physics.

¹So-called spin-1 particles.

²See 2j1 for the answer.

³Due to symmetry; for asymmetric distributions, $x^6 \ll n$ is required.

2c A non-normal approximation

For binomial probabilities, the normal approximation results from the Stirling formula

$$n! \sim \sqrt{2\pi n} n^n e^{-n} \quad \text{as } n \rightarrow \infty.$$

In fact, straightforward application of Stirling formula leads to

$$(2c1) \quad \mathbb{P}\left(\frac{\omega_1 + \cdots + \omega_n}{n} = a\right) \approx \\ \approx \frac{1}{\sqrt{1-a^2}} \frac{2}{\sqrt{n}} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{n}{2}((1-a)\ln(1-a) + (1+a)\ln(1+a))\right)$$

for $a = \frac{-n}{n}, \frac{-n+2}{n}, \dots, \frac{n}{n}$ (check it); the relative error is small when $(1-|a|)n$ is large. For example,

$$\mathbb{P}\left(\frac{\omega_1 + \cdots + \omega_{200}}{200} = -0.9\right) \approx 1.409 \cdot 10^{-44}$$

instead of $1.397 \cdot 10^{-44}$; quite good.

For small a we have

$$(1-a)\ln(1-a) + (1+a)\ln(1+a) = a^2 + O(a^4)$$

(check it), which gives the normal approximation if $na^4 \ll 1$ (check it). For larger a the non-normal approximation (2c1) works.

2d Large deviations: upper bound

Let Ω and μ be as in Sect. 1a,¹ and $f : \Omega \rightarrow \mathbb{R}$ a measurable function. For every $\lambda \in [0, \infty)$ and $a \in \mathbb{R}$,

$$\int e^{\lambda f} d\mu \geq e^{\lambda a} \mu\{f \geq a\}$$

(think, why); of course, $\{f \geq a\}$ means $\{\omega : f(\omega) \geq a\}$. Thus,

$$\mu\{f \geq a\} \leq \inf_{\lambda \geq 0} \frac{\int e^{\lambda f} d\mu}{e^{\lambda a}}.$$

Similarly,

$$\mu\{f \leq a\} \leq \inf_{\lambda \leq 0} \frac{\int e^{\lambda f} d\mu}{e^{\lambda a}}.$$

¹That is, μ is a finite or σ -finite positive measure on Ω .

We apply it to $f^{(n)}$, taking into account that

$$\int e^{\lambda n f^{(n)}} d\mu^n = \left(\int e^{\lambda f} d\mu \right)^n,$$

and get

$$\mu^n \{f^{(n)} \geq a\} \leq \left(\inf_{\lambda \geq 0} \frac{\int e^{\lambda f} d\mu}{e^{\lambda a}} \right)^n, \quad \mu^n \{f^{(n)} \leq a\} \leq \left(\inf_{\lambda \leq 0} \frac{\int e^{\lambda f} d\mu}{e^{\lambda a}} \right)^n.$$

2d1 Exercise. The function $\Lambda : \mathbb{R} \rightarrow (-\infty, +\infty]$ defined by

$$\Lambda(\lambda) = \ln \int e^{\lambda f} d\mu$$

is convex and lower semicontinuous.

Prove it.

2d2 Exercise. (a) The set $\{\Lambda < \infty\} = \{\lambda : \Lambda(\lambda) < \infty\}$ is an interval.

(b) Every interval can appear this way: (a, b) , $[a, b]$, $(a, b]$, (a, b) , $(-\infty, b)$, $(-\infty, b]$, (a, ∞) , $[a, \infty)$, $(-\infty, \infty)$, $\{a\}$ and \emptyset .

(c) The restriction of Λ to $\{\Lambda < \infty\}$ is continuous.

(d) The restriction of Λ to $\{\Lambda < \infty\}$ is strictly convex, unless $f = \text{const}$.

Prove it.

2d3 Exercise. If $\Lambda(\lambda - \varepsilon) < \infty$ and $\Lambda(\lambda + \varepsilon) < \infty$ then

$$e^{\Lambda(\lambda \pm \varepsilon)} = \sum_{n=0}^{\infty} \frac{(\pm \varepsilon)^n}{n!} \int f^n e^{-\lambda f} d\mu.$$

Prove it.

Thus, Λ is infinitely differentiable on $\text{Int}\{\Lambda < \infty\}$ (the interior of the interval), and

$$(2d4) \quad \frac{d^n}{d\lambda^n} e^{\Lambda(\lambda)} = \int f^n e^{\lambda f} d\mu \quad \text{for } \lambda \in \text{Int}\{\Lambda < \infty\}.$$

In terms of Λ we have

$$\mu^n \{f^{(n)} \geq a\} \leq \exp n \inf_{\lambda \geq 0} (\Lambda(\lambda) - a\lambda), \quad \mu^n \{f^{(n)} \leq a\} \leq \exp n \inf_{\lambda \leq 0} (\Lambda(\lambda) - a\lambda).$$

If $a = \Lambda'(\lambda)$ for some $\lambda \in \text{Int}\{\Lambda < \infty\}$ then $\inf_{\lambda_1 \in \mathbb{R}} (\Lambda(\lambda_1) - a\lambda_1) = \Lambda(\lambda) - a\lambda = \Lambda(\lambda) - \lambda\Lambda'(\lambda)$ (think, why); thus,

(2d5)

$$\begin{aligned} \mu^n \{f^{(n)} \geq \Lambda'(\lambda)\} &\leq \exp n (\Lambda(\lambda) - \lambda\Lambda'(\lambda)) \quad \text{for } \lambda \in [0, \infty) \cap \text{Int}\{\Lambda < \infty\}, \\ \mu^n \{f^{(n)} \leq \Lambda'(\lambda)\} &\leq \exp n (\Lambda(\lambda) - \lambda\Lambda'(\lambda)) \quad \text{for } \lambda \in (-\infty, 0] \cap \text{Int}\{\Lambda < \infty\}. \end{aligned}$$

2d6 Exercise. Consider again $\Omega = \{-1, 1\}$ with the counting measure, and $f(\omega_1) = \omega_1$. Calculate Λ and simplify the inequalities, getting

$$\mu^n\{f^{(n)} \geq a\} \leq 2^n \exp\left(-\frac{n}{2}((1-a)\ln(1-a) + (1+a)\ln(1+a))\right) \text{ for } a \in [0, 1),$$

$$\mu^n\{f^{(n)} \leq a\} \leq 2^n \exp\left(-\frac{n}{2}((1-a)\ln(1-a) + (1+a)\ln(1+a))\right) \text{ for } a \in (-1, 0].$$

Does it hold for $a = \pm 1$?

Compare it with (2c1).

2e Better bound via tilting

Let Ω, μ, f and Λ be as in Sect. 2d, $\text{Int}\{\Lambda < \infty\} \neq \emptyset$, and $f \neq \text{const}$.¹

Given $\lambda \in \text{Int}\{\Lambda < \infty\}$, we introduce a measure well-known in the large deviations theory as tilted measure, in mathematics and physics as Gibbs measure, and in statistical physics as canonical ensemble:

$$\nu = \exp(\lambda f - \Lambda(\lambda)) \cdot \mu.$$

2e1 Exercise. Check that

$$\int d\nu = 1, \quad \int f d\nu = \Lambda'(\lambda), \quad \int f^2 d\nu = \Lambda''(\lambda) + \Lambda'^2(\lambda),$$

$$\ln \int e^{\alpha f} d\nu = \Lambda(\lambda + \alpha) - \Lambda(\lambda) \quad \text{for } \alpha \in \mathbb{R}.$$

2e2 Exercise. If $\mu = \gamma^1$ (that is, $N(0, 1)$) and $f(x) = x$, then

- (a) $\Lambda(\lambda) = \lambda^2/2$;
- (b) ν is γ^1 shifted by λ (that is, $N(\lambda, 1)$);
- (c) $\int_0^\infty e^{\lambda x} \gamma^1(dx) = e^{\lambda^2/2} \gamma^1([-\lambda, \infty))$ for $\lambda \in \mathbb{R}$;
- (d) $\int_0^\infty e^{-\lambda x} \gamma^1(dx) \leq \min(\frac{1}{2}, \frac{1}{\sqrt{2\pi}\lambda})$ for $\lambda > 0$.

Prove it.

W.r.t. the probability measure ν the function f may be thought of as a random variable with $\mathbb{E} f = \Lambda'(\lambda)$ and $\text{Var} f = \Lambda''(\lambda) > 0$ (just because $f \neq \text{const}$). We note this fact also for subsequent use:

$$(2e3) \quad \Lambda''(\lambda) > 0 \quad \text{for all } \lambda \in \text{Int}\{\Lambda < \infty\} \quad \text{provided that } f \neq \text{const}.$$

2e4 Exercise. Check that

$$\nu^n = \exp n(\lambda f^{(n)} - \Lambda(\lambda)) \cdot \mu^n.$$

¹As before, it means $\text{ess inf } f \neq \text{ess sup } f$.

W.r.t. the probability measure ν^n the function $nf^{(n)}$ may be thought of as the sum of n independent copies of the random variable f ;

$$\mathbb{E} f^{(n)} = \Lambda'(\lambda), \quad \text{Var} f^{(n)} = \frac{\Lambda''(\lambda)}{n}.$$

2e5 Exercise. For every $\varepsilon > 0$ there exists $\delta > 0$ such that for all n ,

$$\nu^n \{|f^{(n)} - \Lambda'(\lambda)| > \varepsilon\} \leq e^{-\delta n}.$$

Prove it.

By the central limit theorem,

$$\nu^n \left\{ a \leq \frac{f^{(n)} - \Lambda'(\lambda)}{\sqrt{\Lambda''(\lambda)/n}} \leq b \right\} \rightarrow \gamma^1([a, b]) \quad \text{as } n \rightarrow \infty$$

whenever $-\infty \leq a < b \leq \infty$. In terms of μ^n ,

$$\int \mathbb{1}_{J_n}(f^{(n)}) e^{n(\lambda f^{(n)} - \Lambda(\lambda))} d\mu^n \rightarrow \gamma^1([a, b]),$$

where $J_n = [\Lambda'(\lambda) + a\sqrt{\Lambda''(\lambda)/n}, \Lambda'(\lambda) + b\sqrt{\Lambda''(\lambda)/n}]$. Also,

(2e6)

$$\begin{aligned} \mu^n \{f^{(n)} \in J_n\} &= \int \mathbb{1}_{J_n}(f^{(n)}) d\mu^n = \int \mathbb{1}_{J_n}(f^{(n)}) \exp n(\Lambda(\lambda) - \lambda f^{(n)}) d\nu^n = \\ &= e^{n\Lambda(\lambda)} \mathbb{E} e^{-\lambda n f^{(n)}} \mathbb{1}_{J_n}(f^{(n)}) = \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda)) \mathbb{E} e^{-\lambda n(f^{(n)} - \Lambda'(\lambda))} \mathbb{1}_{J_n}(f^{(n)}). \end{aligned}$$

In particular,

$$\begin{aligned} \mu^n \{f^{(n)} \geq \Lambda'(\lambda)\} &= \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda)) \mathbb{E} e^{-\lambda n(f^{(n)} - \Lambda'(\lambda))} \mathbb{1}_{[0, \infty)}(f^{(n)} - \Lambda'(\lambda)), \\ \mu^n \{f^{(n)} \leq \Lambda'(\lambda)\} &= \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda)) \mathbb{E} e^{-\lambda n(f^{(n)} - \Lambda'(\lambda))} \mathbb{1}_{(-\infty, 0]}(f^{(n)} - \Lambda'(\lambda)). \end{aligned}$$

We reduce the expectation to probabilities:

$$e^{-\lambda n x} \mathbb{1}_{[0, \infty)}(x) = \int_0^\infty \mathbb{1}_{[0, y]}(x) \lambda n e^{-\lambda n y} dy$$

(check it), therefore

$$\mathbb{E} e^{-\lambda n(f^{(n)} - \Lambda'(\lambda))} \mathbb{1}_{[0, \infty)}(f^{(n)} - \Lambda'(\lambda)) = \int_0^\infty \nu^n \{0 \leq f^{(n)} - \Lambda'(\lambda) \leq y\} \lambda n e^{-\lambda n y} dy$$

(check it). It follows that

$$\left| \mathbb{E} e^{-\lambda n(f^{(n)} - \Lambda'(\lambda))} \mathbb{1}_{[0, \infty)}(f^{(n)} - \Lambda'(\lambda)) - \int_0^\infty e^{-\lambda n \sqrt{\Lambda''(\lambda)/n} x} \gamma^1(dx) \right| \leq \varepsilon_n,$$

where

$$\varepsilon_n = \sup_{x \geq 0} \left| \nu^n \left\{ 0 \leq f^{(n)} - \Lambda'(\lambda) \leq \sqrt{\frac{\Lambda''(\lambda)}{n}} x \right\} - \gamma^1([0, x]) \right|.$$

Using 2e2(d), for $\lambda > 0$,

$$\mu^n \{f^{(n)} \geq \Lambda'(\lambda)\} \leq \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda)) \cdot \left(\varepsilon_n + \min \left(\frac{1}{2}, \frac{1}{\sqrt{2\pi\lambda\sqrt{n\Lambda''(\lambda)}}} \right) \right).$$

The central limit theorem ensures¹ that $\varepsilon_n \rightarrow 0$, which gives

$$\mu^n \{f^{(n)} \geq \Lambda'(\lambda)\} = \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda)) \cdot o(1) \quad \text{as } n \rightarrow \infty$$

for $\lambda \in (0, \infty) \cap \text{Int}\{\Lambda < \infty\}$; and similarly,

$$\mu^n \{f^{(n)} \leq \Lambda'(\lambda)\} = \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda)) \cdot o(1) \quad \text{as } n \rightarrow \infty$$

for $\lambda \in (-\infty, 0) \cap \text{Int}\{\Lambda < \infty\}$.

However, a stronger result,

$$\varepsilon_n \leq \frac{C}{\sqrt{n}}$$

is ensured by the Berry-Esseen theorem,² provided that

$$\int |f|^3 d\nu < \infty,$$

which is not a problem here, since $(\int |f|^3 d\nu)^{1/3} \leq (\int f^4 d\nu)^{1/4} < \infty$. The constant C depends on the distribution (thus, on λ) and does not depend on n . We get the following.

2e7 Theorem.³ For every $\lambda \in \text{Int}\{\Lambda < \infty\} \setminus \{0\}$ there exists $C < \infty$ such that for all n ,

$$\mu^n \{f^{(n)} \geq \Lambda'(\lambda)\} \leq \frac{C}{\sqrt{n}} \exp n(\Lambda(\lambda) - \lambda \Lambda'(\lambda))$$

¹In combination with a monotonicity argument.

²See W. Feller, An introduction to probability theory and its applications, vol. II, Sect. XVI.5.

³See A. Dembo and O. Zeitouni, Large deviations techniques and applications, Theorem 3.7.4 (Bahadur and Rao).

if $\lambda > 0$, and

$$\mu^n \left\{ f^{(n)} \leq \Lambda'(\lambda) \right\} \leq \frac{C}{\sqrt{n}} \exp n(\Lambda(\lambda) - \lambda\Lambda'(\lambda))$$

if $\lambda < 0$.

Compare it (again) with (2c1) (using 2d6).

2f Large deviations: lower bound

Let Ω, μ, f and Λ be as in Sect. 2e.

Consider intervals $J_n = [\Lambda'(\lambda) + a\sqrt{\Lambda''(\lambda)}/n, \Lambda'(\lambda) + b\sqrt{\Lambda''(\lambda)}/n]$ (of length $O(1/n)$, unlike Sect. 2e) for a given $\lambda \in \text{Int}\{\Lambda < \infty\}$. We have

$$\left| \nu^n \{f^{(n)} \in J_n\} - \gamma^1 \left(\left[\frac{a}{\sqrt{n}}, \frac{b}{\sqrt{n}} \right] \right) \right| \leq \varepsilon_n \leq \frac{C}{\sqrt{n}}$$

and $\gamma^1 \left(\left[\frac{a}{\sqrt{n}}, \frac{b}{\sqrt{n}} \right] \right) \sim \frac{1}{\sqrt{2\pi}} \frac{b-a}{\sqrt{n}}$ (think, why). Thus, for large n ,

$$\nu^n \{f^{(n)} \in J_n\} \geq \frac{c}{\sqrt{n}}$$

provided that $\frac{b-a}{\sqrt{2\pi}} - C > c > 0$. By (2e6),

$$\mu^n \{f^{(n)} \in J_n\} = \exp n(\Lambda(\lambda) - \lambda\Lambda'(\lambda)) \mathbb{E} e^{-\lambda n(f^{(n)} - \Lambda'(\lambda))} \mathbb{1}_{J_n}(f^{(n)}).$$

In particular, for $\lambda \geq 0$,

$$\begin{aligned} \mu^n \{0 \leq f^{(n)} - \Lambda'(\lambda) \leq b\sqrt{\Lambda''(\lambda)}/n\} &\geq \\ &\geq e^{n(\Lambda(\lambda) - \lambda\Lambda'(\lambda))} \cdot e^{-\lambda n b \sqrt{\Lambda''(\lambda)}/n} \nu^n \{f^{(n)} \in J_n\} \geq \\ &\geq e^{n(\Lambda(\lambda) - \lambda\Lambda'(\lambda))} \cdot e^{-\lambda b \sqrt{\Lambda''(\lambda)}} \cdot \frac{c}{\sqrt{n}} \end{aligned}$$

provided that $\frac{b}{\sqrt{2\pi}} - C > c > 0$. Having C (dependent on the distribution, thus, on λ) we take $b > C\sqrt{2\pi}$ and get the following (the case $\lambda \leq 0$ being similar).

2f1 Theorem. ¹ For every $\lambda \in \text{Int}\{\Lambda < \infty\}$ there exist $C < \infty$ and $c > 0$ such that for all n large enough,

$$\begin{aligned} \mu^n \left\{ \Lambda'(\lambda) \leq f^{(n)} \leq \Lambda'(\lambda) + \frac{C}{n} \right\} &\geq \frac{c}{\sqrt{n}} \exp n(\Lambda(\lambda) - \lambda\Lambda'(\lambda)) \quad \text{if } \lambda \geq 0, \\ \mu^n \left\{ \Lambda'(\lambda) - \frac{C}{n} \leq f^{(n)} \leq \Lambda'(\lambda) \right\} &\geq \frac{c}{\sqrt{n}} \exp n(\Lambda(\lambda) - \lambda\Lambda'(\lambda)) \quad \text{if } \lambda \leq 0. \end{aligned}$$

Compare it (once again) with (2c1) (using 2d6).

¹See again the Bahadur-Rao theorem (footnote 3 on page 16).

2g Higher dimension: upper bound

In most cases it is enough to know that a measure is $\exp(-nI + o(n))$ for some known I . Of course, $\frac{1}{\sqrt{n}} = \exp o(n)$, and $n^\alpha = \exp o(n)$ for every α , and even $e^{\pm\sqrt{n}} = \exp o(n)$.

Dimension 2 is treated here; other finite dimensions can be treated similarly.

Let Ω and μ be as before, and $f : \Omega \rightarrow \mathbb{R}^2$ a measurable function. We introduce $\Lambda : \mathbb{R}^2 \rightarrow (-\infty, \infty]$ by

$$\Lambda(\lambda) = \ln \int e^{\langle \lambda, f \rangle} d\mu$$

where $\langle \cdot, \cdot \rangle$ is the scalar product in \mathbb{R}^2 .

2g1 Exercise. ¹ Prove that Λ is convex and lower semicontinuous, and the set $\{\Lambda < \infty\} \subset \mathbb{R}^2$ is convex.

2g2 Exercise. Λ is infinitely differentiable on $\text{Int}\{\Lambda < \infty\}$, and

$$\frac{\partial^{k+l}}{\partial \lambda_1^k \partial \lambda_2^l} e^{\Lambda(\lambda)} = \int f_1^k f_2^l e^{\langle \lambda, f \rangle} d\mu$$

for $\lambda = (\lambda_1, \lambda_2) \in \text{Int}\{\Lambda < \infty\}$; here $f(\omega) = (f_1(\omega), f_2(\omega))$.

Prove it.

We assume that $\{\Lambda < \infty\} \neq \emptyset$.

We introduce the so-called Fenchel-Legendre transform $\Lambda^* : \mathbb{R}^2 \rightarrow (-\infty, \infty]$ of Λ by

$$\Lambda^*(a) = \sup_{\lambda \in \mathbb{R}^2} (\langle \lambda, a \rangle - \Lambda(\lambda)).$$

Being a supremum of linear functions, Λ^* is convex and lower semicontinuous.

Functions $f^{(n)} : \Omega^n \rightarrow \mathbb{R}^2$ are defined as before; and still,

$$\int \exp n \langle \lambda, f^{(n)} \rangle d\mu^n = \left(\int \exp \langle \lambda, f \rangle d\mu \right)^n = \exp n \Lambda(\lambda).$$

2g3 Exercise. Prove that $\mu^n \{f^{(n)} \in B\} \leq \exp n(\Lambda(\lambda) - \inf_{x \in B} \langle \lambda, x \rangle)$ for every n , Borel set $B \subset \mathbb{R}^2$, and $\lambda \in \mathbb{R}^2$.

Denote $B_\delta(a) = \{x \in \mathbb{R}^2 : \|x - a\| < \delta\}$.

¹Unlike 2d2(c), the restriction of Λ to $\{\Lambda < \infty\}$ need not be continuous. A sketch of a counterexample: it may happen that $\Lambda(\cos \varphi, \sin \varphi) = \sum_n \exp c_n(\cos(\varphi - \alpha_n) - 1)$; try $c_n = n^3$, $\alpha_n = 1/n$.

2g4 Exercise. Prove that for every $\lambda \in \mathbb{R}^2$, $\delta > 0$ and $a \in \mathbb{R}^2$,

$$\mu^n \{f^{(n)} \in B_\delta(a)\} \leq \exp n(\Lambda(\lambda) - \langle \lambda, a \rangle + \delta \|\lambda\|).$$

2g5 Exercise. For every $a \in \mathbb{R}^2$ and $C < \Lambda^*(a)$ there exists $\delta > 0$ such that for all n ,

$$\mu^n \{f^{(n)} \in B_\delta(a)\} \leq e^{-nC}.$$

2g6 Exercise. For every compact set $K \subset \mathbb{R}^2$,

$$\mu^n \{f^{(n)} \in K\} \leq \exp \left(-n \min_K \Lambda^* + o(n) \right).$$

Prove it.

2h Higher dimension: lower bound

Let Ω, μ, f and Λ be as in Sect. 2g, and $\text{Int}\{\Lambda < \infty\} \neq \emptyset$.

Given $\lambda \in \text{Int}\{\Lambda < \infty\}$, we introduce the tilted measure

$$\nu = \exp(\langle \lambda, f \rangle - \Lambda(\lambda)) \cdot \mu.$$

2h1 Exercise. Check that

$$\int d\nu = 1, \quad \int f d\nu = \text{grad } \Lambda(\lambda)$$

and

$$\nu^n = \exp n(\langle \lambda, f^{(n)} \rangle - \Lambda(\lambda)) \cdot \mu^n.$$

As before, $\mathbb{E} f^{(n)} = \text{grad } \Lambda(\lambda)$.

2h2 Exercise. Prove that for every $\delta > 0$,

$$\nu^n \{\|f^{(n)} - \text{grad } \Lambda(\lambda)\| < \delta\} \rightarrow 1 \quad \text{as } n \rightarrow \infty.$$

2h3 Exercise. Prove that

$$\mu^n \{f^{(n)} \in B\} \geq \exp n(\Lambda(\lambda) - \sup_{x \in B} \langle \lambda, x \rangle) \nu^n \{f^{(n)} \in B\}$$

for every n , Borel set $B \subset \mathbb{R}^2$, and $\lambda \in \mathbb{R}^2$.

2h4 Exercise. Prove that for every $\lambda \in \text{Int}\{\Lambda < \infty\}$ and $\delta > 0$,

$$\mu^n \{\|f^{(n)} - \text{grad } \Lambda(\lambda)\| < \delta\} \geq (1 - o(1)) \exp n(\Lambda(\lambda) - \langle \lambda, \text{grad } \Lambda(\lambda) \rangle - \delta \|\lambda\|).$$

2h5 Exercise. Let $G \subset \mathbb{R}^2$ be an open set. Prove that¹

$$\mu^n \{f^{(n)} \in G\} \geq \exp(n \sup(\Lambda(\lambda) - \langle \lambda, \text{grad } \Lambda(\lambda) \rangle) - o(n))$$

where the supremum is taken over all $\lambda \in \text{Int}\{\Lambda < \infty\}$ such that $\text{grad } \Lambda(\lambda) \in G$.

2h6 Exercise. Prove that

$$\Lambda^*(\text{grad } \Lambda(\lambda)) = \langle \lambda, \text{grad } \Lambda(\lambda) \rangle - \Lambda(\lambda)$$

for every $\lambda \in \text{Int}\{\Lambda < \infty\}$.

We define a set $T \subset \mathbb{R}^2$ by²

$$T = \{ \text{grad } \Lambda(\lambda) : \lambda \in \text{Int}\{\Lambda < \infty\} \}.$$

2h7 Exercise. Let $G \subset \mathbb{R}^2$ be an open set. Prove that

$$\mu^n \{f^{(n)} \in G\} \geq \exp\left(-n \inf_{G \cap T} \Lambda^* - o(n)\right).$$

The same holds in \mathbb{R}^n for all $n = 1, 2, 3, \dots$

2i Using conditions (1a1), (1a2)

We return to dimension one. Let Ω , μ , f and Λ be as in Sect. 2d, and $f \neq \text{const}$.

Assuming (1a1) or (1a2) we'll prove the so-called weak³ large deviations principle (LDP) with the rate function Λ^* . It means the upper bound

$$\mu^n \{f^{(n)} \in K\} \leq \exp\left(-n \min_K \Lambda^* + o(n)\right) \quad \text{for compact } K \subset \mathbb{R}$$

together with the lower bound

$$\mu^n \{f^{(n)} \in G\} \geq \exp\left(-n \inf_G \Lambda^* - o(n)\right) \quad \text{for open } G \subset \mathbb{R}.$$

To this end, by 2g6 and 2h7 (for dimension one) it suffices to show that

$$T = \text{Int}\{\Lambda^* < \infty\},$$

¹We admit that $o(n)$ may be infinite for a finite number of numbers n .

²“ T ” reminds of “tilting”.

³“Weak” since the upper bound is stated for compact sets rather than all closed sets.

where $T = \{\Lambda'(\lambda) : \lambda \in \text{Int}\{\Lambda < \infty\}\}$. The convex set $\{\Lambda^* < \infty\}$ need not be open, but anyway, the restriction of Λ^* to this set is continuous (due to convexity and lower semicontinuity); thus, $\inf_G \Lambda^* = \inf_{G \cap \{\Lambda^* < \infty\}} \Lambda^* = \inf_{G \cap \text{Int}\{\Lambda^* < \infty\}} \Lambda^* = \inf_{G \cap T} \Lambda^*$.

Assume (1a1): $\mu(\Omega) < \infty$ and $\int e^{\lambda f} d\mu < \infty$ for all $\lambda \in \mathbb{R}$. Thus, $\text{Int}\{\Lambda < \infty\} = \mathbb{R}$, and Λ' is strictly increasing (recall (2e3)), which implies existence of limits,

$$-\infty \leq \Lambda'(-\infty) < \Lambda'(+\infty) \leq +\infty.$$

2i1 Exercise. Prove that

$$T = (\Lambda'(-\infty), \Lambda'(+\infty)) \subset \{\Lambda^* < \infty\} \subset [\Lambda'(-\infty), \Lambda'(+\infty)].$$

Thus, $T = \text{Int}\{\Lambda^* < \infty\}$, and the LDP under (1a1) is verified. In addition, a relation to the bounds of f is shown below.

2i2 Exercise. Prove that

$$\frac{\Lambda(\lambda)}{\lambda} \rightarrow \Lambda'(-\infty) \text{ as } \lambda \rightarrow -\infty, \quad \text{and} \quad \frac{\Lambda(\lambda)}{\lambda} \rightarrow \Lambda'(+\infty) \text{ as } \lambda \rightarrow +\infty.$$

2i3 Exercise. Prove that

$$\text{ess inf } f \leq \Lambda'(-\infty) < \Lambda'(+\infty) \leq \text{ess sup } f.$$

If $a < \text{ess sup } f$ then $\mu\{f \geq a\} > 0$; we have $\int e^{\lambda f} d\mu \geq e^{\lambda a} \mu\{f \geq a\}$ for $\lambda > 0$, thus $\Lambda(\lambda) \geq \lambda a + \ln \mu\{f \geq a\}$ and $\Lambda'(+\infty) \geq a$, which shows that $\Lambda'(+\infty) \geq \text{ess sup } f$. Similarly, $\Lambda'(-\infty) \leq \text{ess inf } f$. We get under (1a1)

$$-\infty \leq \text{ess inf } f = \Lambda'(-\infty) < \Lambda'(+\infty) = \text{ess sup } f \leq +\infty.$$

Assume now (1a2): $\mu(\Omega) = \infty$ and $\int e^{\lambda f} d\mu < \infty$ for all $\lambda \in (-\infty, 0)$. Then $\{\Lambda < \infty\} = (-\infty, 0)$, since this convex set does not contain 0. We have

$$-\infty \leq \Lambda'(-\infty) < \Lambda'(0-) = +\infty$$

(since $\Lambda'(0-) < \infty$ would imply $\Lambda(0) < \infty$).

2i4 Exercise. Prove that

$$T = (\Lambda'(-\infty), +\infty) \subset \{\Lambda^* < \infty\} \subset [\Lambda'(-\infty), +\infty).$$

Also $\text{ess sup } f = +\infty$ (since $\int e^{-\text{ess sup } f} d\mu \leq \int e^{-f} d\mu < \infty$).

2i5 Exercise. Prove that

$$\Lambda'(-\infty) \geq \text{ess inf } f.$$

2i6 Exercise. Prove that

$$\Lambda'(-\infty) \leq \text{ess inf } f.$$

We get under (1a2)

$$-\infty \leq \text{ess inf } f = \Lambda'(-\infty) < \Lambda'(0-) = \text{ess sup } f = +\infty.$$

In both cases,

$$T = \text{Int}\{\Lambda^* < \infty\} = (\text{ess inf } f, \text{ess sup } f).$$

2j The function φ , at last

Let $f, g : \Omega \rightarrow \mathbb{R}$ and $\varepsilon > 0$ be such that $f - \varepsilon g$ and $f + \varepsilon g$ satisfy (1a1) or (1a2), and $f \neq \text{const}$ (as required in Theorem 1b4). We combine them into $h : \Omega \rightarrow \mathbb{R}^2$, $h(\cdot) = (f(\cdot), g(\cdot))$ and consider the corresponding $\Lambda_h : \mathbb{R}^2 \rightarrow (-\infty, +\infty]$ as in Sect. 2g.

Case $\mu(\Omega) < \infty$: the convex set $\{\Lambda_h < \infty\}$ contains two lines $\{(\lambda, \pm\varepsilon\lambda) : \lambda \in \mathbb{R}\}$, therefore it is the whole \mathbb{R}^2 , and surely, $\mathbb{R} = \{(\lambda, 0) : \lambda \in \mathbb{R}\} \subset \text{Int}\{\Lambda_h < \infty\} \subset \mathbb{R}^2$.

Case $\mu(\Omega) = \infty$: the convex set $\{\Lambda_h < \infty\}$ contains two rays $\{(\lambda, \pm\varepsilon\lambda) : \lambda \in (-\infty, 0)\}$, therefore it contains the sector $\{(\lambda_1, \lambda_2) : \lambda_1 < 0, |\lambda_2| \leq \varepsilon|\lambda_1|\}$, and does not contain the origin; and surely, $\{(\lambda, 0) : \lambda \in (-\infty, 0)\} \subset \text{Int}\{\Lambda_h < \infty\}$.

We have also the function $\Lambda_f : \mathbb{R} \rightarrow (-\infty, +\infty]$ corresponding to f as in 2i, and we know that

$$T_f = \{\Lambda'_f(\lambda) : \lambda \in \text{Int}\{\Lambda_f < \infty\}\} = (\text{ess inf } f, \text{ess sup } f),$$

since f satisfies (1a1) or (1a2). And clearly, Λ_f is the restriction of Λ_h to the line $\mathbb{R} = \{(\lambda, 0) : \lambda \in \mathbb{R}\} \subset \mathbb{R}^2$. Of course, $\text{Int}\{\Lambda_f < \infty\}$ is either \mathbb{R} (if $\mu(\Omega) < \infty$) or $(-\infty, 0)$ (if $\mu(\Omega) = \infty$). In both cases $\text{Int}\{\Lambda_f < \infty\} \subset \text{Int}\{\Lambda_h < \infty\}$ under the embedding $\mathbb{R} \rightarrow \mathbb{R}^2$, $\lambda \mapsto (\lambda, 0)$.

The function Λ'_f is strictly increasing by (2e3) and maps $\text{Int}\{\Lambda_f < \infty\}$ onto $T_f = (\text{ess inf } f, \text{ess sup } f)$. For every $a \in (\text{ess inf } f, \text{ess sup } f)$ there exists one and only one $\lambda \in \text{Int}\{\Lambda_f < \infty\}$ such that $\Lambda'_f(\lambda) = a$. We have

$$\text{grad } \Lambda_h(\lambda, 0) = (a, \varphi(a))$$

for a continuous $\varphi : (\text{ess inf } f, \text{ess sup } f) \rightarrow \mathbb{R}$, namely,

$$\varphi(a) = \left. \frac{d}{d\lambda_2} \right|_{\lambda_2=0} \Lambda((\Lambda'_f)^{-1}(a), \lambda_2),$$

not only a continuous function, but also an infinitely differentiable function. In terms of the tilted measure

$$\nu = \exp(\lambda f - \Lambda_f(\lambda)) \cdot \mu$$

we have (by 2h1) $\int h d\nu = \text{grad } \Lambda_h(\lambda, 0)$, that is,

$$a = \int f d\nu \quad \text{and} \quad \varphi(a) = \int g d\nu;$$

an equivalent definition of φ .

2j1 Example. Continuing Example 2a3, consider $\Omega = \{-1, 0, 1\}$, $h(\omega) = \omega$, $f(\omega) = \omega^2$. The function $\varphi = [f|h]$ can be written out implicitly:

$$\varphi\left(\frac{x^2 - 1}{x^2 + x + 1}\right) = \frac{x^2 + 1}{x^2 + x + 1} \quad \text{for } x \in (0, \infty);$$

the tilted measure is

$$\nu(\{-1\}) = \frac{1}{x^2 + x + 1}, \quad \nu(\{0\}) = \frac{x}{x^2 + x + 1}, \quad \nu(\{1\}) = \frac{x^2}{x^2 + x + 1}.$$

In particular, $x \approx 0.09289$ gives $\varphi(-0.9) \approx 0.9157$. Thus, the conditional distribution of $f^{(n)}$ given $h^{(n)} \approx -0.9$ is concentrated near 0.9157.

2k Proving the theorem

Let f , g and φ be as in Sect. 2j. In order to prove Theorem 1b4 we have to prove that $\mathbb{P}(g^{(n)} \in (c, d) | f^{(n)} \in [a, b]) \rightarrow 1$ whenever $[a, b] \subset (\text{ess inf } f, \text{ess sup } f)$ and $(c, d) \subset \mathbb{R}$ satisfy $\varphi([a, b]) \subset (c, d)$. We'll prove a bit stronger statement:

$$\frac{\mu^n\{f^{(n)} \in [a, b] \text{ and } g^{(n)} \notin (c, d)\}}{\mu^n\{f^{(n)} \in (a, b)\}} \rightarrow 0$$

(the denominator being non-zero for large n).

2k1 Exercise. If $\frac{\mu^n\{f^{(n)} \in [a_1, b_1] \text{ and } g^{(n)} \notin (c, d)\}}{\mu^n\{f^{(n)} \in (a_1, b_1)\}} \rightarrow 0$, $\frac{\mu^n\{f^{(n)} \in [a_2, b_2] \text{ and } g^{(n)} \notin (c, d)\}}{\mu^n\{f^{(n)} \in (a_2, b_2)\}} \rightarrow 0$ and $b_1 = a_2$ then $\frac{\mu^n\{f^{(n)} \in [a_1, b_2] \text{ and } g^{(n)} \notin (c, d)\}}{\mu^n\{f^{(n)} \in (a_1, b_2)\}} \rightarrow 0$.

Prove it.

We use h , Λ_h , Λ_f introduced in Sect. 2j.

It may happen that $(\Lambda'_f)^{-1}(a) < 0 < (\Lambda'_f)^{-1}(b)$. In this case we split the interval $[a, b]$ in two and use 2k1. Thus, we restrict ourselves to the case $(\Lambda'_f)^{-1}(a) \geq 0$. (The other case, $(\Lambda'_f)^{-1}(b) \leq 0$, is similar.)

We have $\lambda \in [0, \infty) \cap \text{Int}\{\Lambda_f < \infty\}$ such that $\Lambda'_f(\lambda) = a$. Denote $r = \lambda a - \Lambda_f(\lambda)$, then $\Lambda_f^*(a) = r$. By the lower bound of the LDP (Sect. 2i),

$$\mu^n \{f^{(n)} \in (a, b)\} \geq \exp\left(-n \inf_{(a,b)} \Lambda_f^* - o(n)\right) \geq \exp(-nr - o(n)),$$

since¹ $\inf_{(a,b)} \Lambda_f^* \leq \Lambda_f^*(a) = r$. It is sufficient to prove that for some $\delta > 0$,

$$\mu^n \{f^{(n)} \in [a, b] \text{ and } g^{(n)} \notin (c, d)\} \leq \exp(-n(r + \delta)).$$

We have $(c, d) \ni \varphi(a) = \int g \, d\nu$ where $\nu = \exp(\lambda f - \Lambda_f(\lambda)) \cdot \mu$ is the tilted measure. Also, $\int e^{\alpha g} \, d\nu < \infty$ for all α small enough (positive or negative), since $(\lambda, 0) \in \text{Int}\{\Lambda_h < \infty\}$. By (2e5) (adapted a bit), for some $\delta > 0$,

$$\nu^n \{g^{(n)} \notin (c, d)\} \leq e^{-\delta n} \quad \text{for all } n.$$

Thus (using 2e4),

$$\begin{aligned} \mu^n \{f^{(n)} \in [a, b] \text{ and } g^{(n)} \notin (c, d)\} &= \\ &= \int \mathbb{1}_{[a,b]}(f^{(n)}) (1 - \mathbb{1}_{(c,d)}(g^{(n)})) \exp n(\Lambda_f(\lambda) - \lambda f^{(n)}) \, d\nu_n \leq \\ &\leq \exp n(\Lambda_f(\lambda) - \lambda a) \int (1 - \mathbb{1}_{(c,d)}(g^{(n)})) \, d\nu_n \leq e^{-rn} e^{-\delta n}, \end{aligned}$$

which completes the proof.

2l Equivalence of ensembles

The probability measure

$$B \mapsto \mathbb{P}(B \mid h^{(n)} \in [E, E + \Delta E]) = \frac{\mu^n(B \cap \{h^{(n)} \in [E, E + \Delta E]\})}{\mu^n\{h^{(n)} \in [E, E + \Delta E]\}}$$

for a large n and small ΔE is well-known in statistical physics as the microcanonical ensemble,² provided that h is the Hamiltonian.

¹In fact, $\inf_{(a,b)} \Lambda_f^* = \Lambda_f^*(a)$, since Λ_f^* is increasing on $[a, b]$.

²“... the *basic postulate of equilibrium statistical mechanics* ... expresses the fact that we know very little about the microscopic state of the system: we only assume that its energy lies in a narrow interval $(E, E + \Delta E)$ each of these states is equally probable ... This is the famous principle of equal *a priori* probabilities. ... The microcanonical ensemble is of prime theoretical importance ... however ... proves to be a mathematically difficult and unflexible tool.” R. Balescu, “Equilibrium and nonequilibrium statistical mechanics”, 1975, Sect. 4.2 “The microcanonical ensemble”.

The tilted measure

$$\nu^n = \exp n(\lambda h^{(n)} - \Lambda(\lambda)) \cdot \mu^n,$$

where λ is chosen so that $\Lambda'(\lambda) = E$, is well-known in statistical physics as the canonical ensemble,¹ traditionally written as²

$$\nu^n(d\omega_1 \dots d\omega_n) = \frac{1}{Z(\beta)} e^{-\beta h(\omega_1) - \dots - \beta h(\omega_n)} \mu(d\omega_1) \dots \mu(d\omega_n)$$

where $\beta = -\lambda$ is called the inverse temperature, and $Z(\beta) = e^{n\Lambda(\lambda)} = \int e^{-\beta h(\omega_1) - \dots - \beta h(\omega_n)} \mu(d\omega_1) \dots \mu(d\omega_n)$ is called the partition function.³

Let h and g satisfy the conditions of Theorem 1b4.

For every $\varepsilon > 0$ there exists $\Delta E > 0$ such that

$$\mathbb{P}(g^{(n)} \in (\varphi(E) - \varepsilon, \varphi(E) + \varepsilon) \mid h^{(n)} \in [E, E + \Delta E]) \rightarrow 1$$

as $n \rightarrow \infty$. On the other hand, for every $\varepsilon > 0$ there exists $\delta > 0$ such that for all n ,

$$\nu^n\{g^{(n)} \in (\varphi(E) - \varepsilon, \varphi(E) + \varepsilon)\} \geq 1 - e^{-\delta n}.$$

Thus, a macroscopic observable $g^{(n)}$ concentrates around the same value $\varphi(E)$ in both ensembles, microcanonical and canonical. This phenomenon is well-known in statistical physics as equivalence of ensembles.⁴

2m Hints to exercises

2d1: (a) Hölder inequality; (b) Fatou's lemma.

2d2 (b): try $\Omega = \mathbb{R}$, $f(x) = x$, $\mu(dx) = p(x) dx$, $p(x) \sim x^\alpha e^{-\gamma x}$ and $p(-x) \sim x^\beta e^{-\delta x}$ for $x \rightarrow +\infty$. (c): use 2d1. (d): strict Hölder inequality.

2d3: $|\sum_{n=0}^N e^{\lambda f} \frac{(\pm \varepsilon f)^n}{n!}| \leq e^{\lambda f} e^{\varepsilon |f|} \leq e^{(\lambda - \varepsilon)f} + e^{(\lambda + \varepsilon)f}$; use the dominated convergence theorem.

2d6: Transform $\frac{e^\lambda - e^{-\lambda}}{e^\lambda + e^{-\lambda}} = a$ into $e^\lambda = \sqrt{\frac{1+a}{1-a}}$.

¹“It was introduced for the first time by J.W. Gibbs (in the classical case) around 1900.” Balescu, Sect. 4.3 “The canonical ensemble”, page 119.

²We restrict ourselves to ideal systems (recall Sect. 1a).

³“It is one of the most important quantities of equilibrium statistical mechanics.” Balescu, Sect. 4.3, page 118.

⁴“This result is very important in practice. It allows us, in many cases, to use in a given problem interchangeably one or the other ensemble, the choice being motivated by practical convenience in the calculations.” Balescu, Sect. 4.6 “Equivalence of the equilibrium ensembles: fluctuations.”

2e5: Use (2d5) and 2e1: $\nu^n\{f^{(n)} \geq \Lambda'(\lambda + \alpha)\} \leq \exp n(\Lambda(\lambda + \alpha) - \Lambda(\lambda) - \alpha\Lambda'(\lambda + \alpha))$ for small $\alpha > 0$.

2g1: similar to 2d1.

2g2: similar to 2d4.

2g3: recall Sect. 2d.

2g6: show that $\limsup \frac{1}{n} \ln \mu^n\{f^{(n)} \in K\} \leq -\min_K \Lambda^*$; to this end, given $C < \min_K \Lambda^*$, cover K by a finite number of disks $B_\delta(a)$ as in 2g5.

2i1: consider $\lambda a - \Lambda(\lambda)$ as $\lambda \rightarrow \pm\infty$.

2i5: $\int e^{\lambda f} d\mu \leq e^{(\lambda+1) \text{ess inf } f} \int e^{-f} d\mu$ for $\lambda < -1$.

2i6: Similarly to the case of (1a1).

Index

Berry-Esseen theorem, 16	random variable, 14
central limit theorem, 15	sum of random variables, 15
ensemble	tilted measure, 14
canonical, 14, 25	$\{f \geq a\}$, 12
microcanonical, 24	Int, 13
Fenchel-Legendre transform, 18	Λ^* , 18
Gibbs measure, 14	Λ_f , 22
inverse temperature, 25	Λ_h , 22
large deviations principle, 20	Λ , 13
LDP, 20	Λ', Λ'' , 14
partition function, 25	ν , 14
	ν^n , 14
	T , 20
	T_f , 22