## Lecture 5. Limit theorems

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## Table of Contents

Law of Large Numbers

## Central Limit Theorem

Laplace asymptotics

## Cramér's Theorem for Large Deviations

## Law of Large Numbers

- Let $\left\{X_{j}\right\}_{j=1}^{\infty}$ be a sequence of independently and identically distributed (abbreviated as i.i.d. in the later text) random variables. Let $\eta=\mathbb{E} X_{1}$ and $S_{n}$ the partial sum of $X_{j}$ from 1 to $n$.


## Law of Large Numbers

- Let $\left\{X_{j}\right\}_{j=1}^{\infty}$ be a sequence of independently and identically distributed (abbreviated as i.i.d. in the later text) random variables. Let $\eta=\mathbb{E} X_{1}$ and $S_{n}$ the partial sum of $X_{j}$ from 1 to $n$.
- The well-known law of large numbers validates the intuitive characterization of the mathematical expectation: it is the limit of empirical average when the sample size $n$ goes to infinity. It is also the theoretical basis of the Monte Carlo methods.


## Weak Law of Large Numbers

Theorem (Weak law of large numbers (WLLN))
For i.i.d. random variables $\left\{X_{j}\right\}_{j=1}^{\infty}$ with $\mathbb{E}\left|X_{j}\right|<\infty$, we have

$$
\frac{S_{n}}{n} \rightarrow \eta \quad \text { in probability. }
$$

Proving the result under the stated assumption is quite involved. We will give a proof of the WLLN under the stronger assumption that $\mathbb{E}\left|X_{j}\right|^{2}<\infty$.

## Weak Law of Large Numbers: Proof

## Proof.

Without loss of generality, we can assume $\eta=0$. Using
Chebyshev's inequality, we have

$$
\mathbb{P}\left\{\left|\frac{S_{n}}{n}\right|>\epsilon\right\} \leq \frac{1}{\epsilon^{2}} \mathbb{E}\left|\frac{S_{n}}{n}\right|^{2}
$$

for any $\epsilon>0$. Using independence, we have

$$
\mathbb{E}\left|S_{n}\right|^{2}=\sum_{i, j=1}^{n} \mathbb{E}\left(X_{i} X_{j}\right)=n \mathbb{E}\left|X_{1}\right|^{2}
$$

Hence

$$
\mathbb{P}\left\{\left|\frac{S_{n}}{n}\right|>\epsilon\right\} \leq \frac{1}{n \epsilon^{2}} \mathbb{E}\left|X_{1}\right|^{2} \rightarrow 0
$$

as $n \rightarrow \infty$.

## Strong Law of Large Numbers

Theorem (Strong law of large numbers (SLLN))
For i.i.d. random variables $\left\{X_{j}\right\}_{j=1}^{\infty}$ we have

$$
\frac{S_{n}}{n} \rightarrow \eta \quad \text { a.s. }
$$

if and only if $\mathbb{E}\left|X_{j}\right|<\infty$.

## Strong Law of Large Numbers: Proof

## Proof.

We will only prove SLLN under the stronger assumption that $\mathbb{E}\left|X_{j}\right|^{4}<\infty$. More general case may be referred to ${ }^{1}$.
Without loss of generality, we can assume $\eta=0$. Using
Chebyshev's inequality, we obtain

$$
\mathbb{P}\left\{\left|\frac{S_{n}}{n}\right|>\epsilon\right\} \leq \frac{1}{\epsilon^{4}} \mathbb{E}\left|\frac{S_{n}}{n}\right|^{4}
$$

Using independence, we get

$$
\mathbb{E}\left|S_{n}\right|^{4}=\sum_{i, j, k, l=1}^{n} \mathbb{E}\left(X_{i} X_{j} X_{k} X_{l}\right)=n \mathbb{E}\left|X_{j}\right|^{4}+3 n(n-1)\left(\mathbb{E}\left|X_{j}\right|^{2}\right)^{2}
$$

${ }^{1}$ K.L. Chung. A course in probability theory. Academic Press, third edition, 2001.

## Strong Law of Large Numbers: Proof

We have $\left(\mathbb{E}\left|X_{j}\right|^{2}\right)^{2} \leq \mathbb{E}\left|X_{j}\right|^{4}<\infty$ by Hölder inequality. Hence

$$
\mathbb{P}\left\{\left|\frac{S_{n}}{n}\right|>\epsilon\right\} \leq \frac{C}{n^{2} \epsilon^{4}}
$$

Since the series $1 / n^{2}$ is summable we get

$$
\mathbb{P}\left\{\left|\frac{S_{n}}{n}\right|>\epsilon, \text { i.o. }\right\}=0
$$

by Borel-Cantelli lemma. This implies that

$$
\frac{S_{n}}{n} \rightarrow 0 \quad \text { a.s. }
$$

and we are done.

## Law of Large Numbers: Counter Example

## Example (Cauchy distribution)

The following example shows that the law of large numbers does not hold if the assumed condition is not satisfied. Consider the i.i.d. random variables $\left\{X_{j}\right\}_{j=1}^{\infty}$ with Cauchy distribution having probability density function

$$
\frac{1}{\pi\left(1+x^{2}\right)}, \quad x \in \mathbb{R} .
$$

We have $\mathbb{E} X_{j}=0$ by symmetry and $\mathbb{E}\left|X_{j}\right|=\infty, \mathbb{E}\left|X_{j}\right|^{2}=\infty$. In this case, we can prove $S_{n} / n$ always has the same distribution as $X_{1}$. Thus the weak and strong law of large numbers are both violated.

## Table of Contents

## Law of Large Numbers

Central Limit Theorem

Laplace asymptotics

## Cramér's Theorem for Large Deviations

## Central Limit Theorem

The following central limit theorem explains why the normal or normal-like distributions are so widely observed in the nature. Theorem (Lindeberg-Lévy central limit theorem (CLT))
Let $\left\{X_{j}\right\}_{j=1}^{\infty}$ be a sequence of i.i.d. random variables. Assume that $\mathbb{E} X_{j}^{2}<\infty$ and let $\sigma^{2}=\operatorname{var}\left(X_{j}\right)$. Then

$$
\frac{S_{n}-n \eta}{\sqrt{n \sigma^{2}}} \rightarrow N(0,1)
$$

in the sense of distribution.

## Central Limit Theorem: Proof

## Proof.

Assume without loss of generality $\eta=0$ and $\sigma=1$, otherwise we can shift and rescale $X_{j}$. Let $f$ be the characteristic function of $X_{1}$ and let $g_{n}$ be the characteristic function of $S_{n} / \sqrt{n}$. Then

$$
g_{n}(\xi)=\mathbb{E} e^{i \xi S_{n} / \sqrt{n}}=\prod_{j=1}^{n} \mathbb{E} e^{i \xi X_{j} / \sqrt{n \sigma^{2}}}=\prod_{j=1}^{n} f\left(\frac{\xi}{\sqrt{n}}\right)=f^{n}\left(\frac{\xi}{\sqrt{n}}\right) .
$$

Using Taylor expansion and the properties of characteristic functions we obtain

$$
\begin{aligned}
f\left(\frac{\xi}{\sqrt{n}}\right) & =f(0)+\frac{\xi}{\sqrt{n}} f^{\prime}(0)+\frac{1}{2}\left(\frac{\xi}{\sqrt{n}}\right)^{2} f^{\prime \prime}(0)+o\left(\frac{1}{n}\right) \\
& =1-\frac{\xi^{2}}{2 n}+o\left(\frac{1}{n}\right)
\end{aligned}
$$

## Central Limit Theorem: Proof

Hence
$g_{n}(\xi)=f(\xi / \sqrt{n})^{n}=\left(1-\frac{\xi^{2}}{2 n}+o\left(\frac{1}{n}\right)\right)^{n} \rightarrow e^{-\frac{1}{2} \xi^{2}} \quad$ as $n \rightarrow \infty$
for every $\xi \in \mathbb{R}^{1}$. This completes the proof by using Levy's continuity theorem.

## CLT: Implication on MC

The central limit theorem is the theoretical basis for the assumption that additive noise can be modeled by Gaussian noises. It also gives an estimate for the rate of convergence in the law of large numbers. Since by CLT we have

$$
\frac{S_{n}}{n}-\eta \sim \frac{\sigma}{\sqrt{n}}
$$

The rate of convergence of $S_{n} / n$ to $\eta$ is $O\left(n^{-\frac{1}{2}}\right)$. This is the reason why most Monte Carlo methods has a rate of convergence of $O\left(n^{-\frac{1}{2}}\right)$ where $n$ is the sample size.

## CLT: Application in polymer physics

The central limit theorem is fundamental to understand the end-to-end statistics for a polymer. The simplest model for flexible polymers is called the freely jointed chain, in which a polymer consists of $K$ units, each of length $b_{0}$ and able to point in any direction independently of each other.


Figure: Schematics of the freely jointed chain.

## CLT: Application in polymer physics

Denote the bond vectors as $\boldsymbol{r}_{k}(k=1, \ldots, K)$, which has i.i.d. distribution density

$$
p(\boldsymbol{r})=\frac{1}{4 \pi b_{0}^{2}} \delta\left(\boldsymbol{r}-b_{0}\right) .
$$

The end-to-end vector

$$
\boldsymbol{R}=\sum_{k=1}^{K} \boldsymbol{r}_{k}
$$

From the central limit theorem, we have asymptotically

$$
\boldsymbol{R} \sim N\left(0, K b_{0}^{2} \boldsymbol{I}\right), \quad K \gg 1
$$

Note that this Gaussian type approximation as $K \gg 1$ is independent of the choice of the bond vector distribution. This model is called Gaussian chain in polymer physics.

## Table of Contents

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## Central Limit Theorem

Laplace asymptotics

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## Laplace asymptotics

- Laplace method is the basis of large deviation theory. It is widely used in many fields of applied mathematics. We will only introduce the one-dimensional version of Laplace asymptotics in this section. For more details, see ${ }^{2}$.

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## Laplace asymptotics

- Laplace method is the basis of large deviation theory. It is widely used in many fields of applied mathematics. We will only introduce the one-dimensional version of Laplace asymptotics in this section. For more details, see ${ }^{2}$.
- Let us consider the Laplace integral

$$
F(t)=\int_{\mathbb{R}} e^{t h(x)} d x, \quad t \gg 1
$$

where $h(x) \in C^{2}(\mathbb{R}), h(0)=0$ is the only global maximum such that

$$
h(x) \leq-b \quad \text { if } \quad|x| \geq c
$$

for positive reals $b, c$. Suppose $h(x) \rightarrow-\infty$ fast enough as $x \rightarrow \infty$ to ensure the convergence of $F$ for $t=1$ and assume $h^{\prime \prime}(0)<0$, then the Laplace Lemma holds.

[^1]
## Laplace asymptotics

Lemma (Laplace Lemma)
As $t \rightarrow \infty$, to leading order

$$
F(t) \sim \sqrt{2 \pi}\left(-t h^{\prime \prime}(0)\right)^{-\frac{1}{2}} .
$$

## Laplace asymptotics

Lemma (Laplace Lemma)
As $t \rightarrow \infty$, to leading order

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$$

Proof.
If $h(x)=h^{\prime \prime}(0) x^{2} / 2, h^{\prime \prime}(0)<0$, then

$$
\int_{\mathbb{R}} e^{t h(x)} d x=\sqrt{2 \pi}\left(-t h^{\prime \prime}(0)\right)^{-\frac{1}{2}}
$$

In general, for any $\epsilon>0$, there exists $\delta>0$ such that for any $|x| \leq \delta$,

$$
\left|h(x)-\frac{h^{\prime \prime}(0)}{2} x^{2}\right| \leq \epsilon x^{2}
$$

## Laplace asymptotics: Proof

It follows that

$$
\begin{aligned}
\int_{[-\delta, \delta]} \exp \left(\frac{t x^{2}}{2}\left(h^{\prime \prime}(0)-2 \epsilon\right)\right) d x & \leq \int_{[-\delta, \delta]} \exp (t h(x)) d x \\
& \leq \int_{[-\delta, \delta]} \exp \left(\frac{t x^{2}}{2}\left(h^{\prime \prime}(0)+2 \epsilon\right)\right) d x
\end{aligned}
$$

For this $\delta>0$, there exists $\eta>0$ by assumptions such that

$$
h(x) \leq-\eta \quad \text { if } \quad|x| \geq \delta
$$

thus

$$
\int_{|x| \geq \delta} \exp (\operatorname{th}(x)) d x \leq e^{-(t-1) \eta} \int_{\mathbb{R}} e^{h(x)} d x \sim \mathcal{O}\left(e^{-\alpha t}\right), \alpha>0, \quad \text { for } \quad t>1
$$

## Laplace asymptotics: Proof

First consider the upper bound, we have

$$
\begin{aligned}
& \int_{\mathbb{R}} \exp (t h(x)) d x \\
& \leq \int_{\mathbb{R}} \exp \left(\frac{t x^{2}}{2}\left(h^{\prime \prime}(0)+2 \epsilon\right)\right) d x-\int_{|x| \geq \delta} \exp \left(\frac{t x^{2}}{2}\left(h^{\prime \prime}(0)+2 \epsilon\right)\right) d x+\mathcal{O}\left(e^{-\alpha t}\right) \\
&= \sqrt{2 \pi}\left[t\left(-h^{\prime \prime}(0)-2 \epsilon\right)\right]^{-\frac{1}{2}}+\mathcal{O}\left(e^{-\beta t}\right) \\
& \text { where } \beta>0 . \text { In fact, we ask } \epsilon<-h^{\prime \prime}(0) / 2 \text { here. }
\end{aligned}
$$

The proof of lower bound is similar. By the arbitrary smallness of $\epsilon$, we have

$$
\lim _{t \rightarrow \infty} F(t) / \sqrt{2 \pi}\left(-t h^{\prime \prime}(0)\right)^{-\frac{1}{2}}=1
$$

which completes the proof.

## Laplace asymptotics: LDT form

The result is easily extended to the case where $h(0) \neq 0$. The term $e^{t h(0)}$ will appear in the leading order and another commonly used form ignoring the prefactor is the so-called saddle point approximation

$$
\lim _{t \rightarrow \infty} \frac{1}{t} \log F(t)=\sup _{x \in \mathbb{R}} h(x)
$$

which is the typical form in large deviation theory and widely used in physics literature.

## Table of Contents

## Law of Large Numbers

## Central Limit Theorem

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- The laws of large numbers says that for any $\epsilon>0$, with probability close to $1,\left|S_{n} / n-\eta\right|<\epsilon$ for large enough $n$; conversely if $y \neq \eta$, then the probability that $S_{n} / n$ is close to $y$ goes to zero as $n \rightarrow \infty$.


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- Events of this type, i.e. $\left\{\left|S_{n} / n-y\right|<\epsilon\right\}$, are called large deviation events compared with the small deviation events from the mean like the set $\left\{\left|S_{n} / n-\eta\right| \leq c / \sqrt{n}\right\}$ in central limit theorem.


## Rate function

To estimate the precise rate at which $\mathbb{P}\left\{\left|S_{n} / n-y\right|<\epsilon\right\}$ goes to zero, we assume here that the distribution $\mu$ of the $X_{j}$ 's have finite exponential moments. Let us define the moment generating function

$$
M(\lambda)=\mathbb{E} e^{\lambda X_{j}}=\int_{\mathbb{R}} e^{\lambda x} d \mu(x)<\infty, \quad \lambda \in \mathbb{R}
$$

the cumulant generating function

$$
\Lambda(\lambda)=\log M(\lambda)
$$

and the Legendre-Fenchel transform of $\Lambda(\lambda)$ as

$$
I(x)=\sup _{\lambda}\{x \lambda-\Lambda(\lambda)\} .
$$

Then we have the large deviation type theorem for the i.i.d. sums.

## Cramér's Theorem

Theorem (Cramér's Theorem)
The distribution of the empirical average $\mu_{n}$ defined by

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(i) For any closed set $F \in \mathcal{B}$

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(ii) For any open set $G \in \mathcal{B}$

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\varliminf_{n \rightarrow \infty} \frac{1}{n} \log \mu_{n}(G) \geq-\inf _{x \in G} I(x)
$$

$I(x)$ is called the rate function.

## Cramér's Theorem: Intuition

For the so-called $I$-continuity set $\Gamma$, i.e. $\inf _{x \in \Gamma^{\circ}} I(x)=\inf _{x \in \bar{\Gamma}} I(x)$, this theorem suggests that roughly

$$
\mu_{n}(\Gamma) \asymp \exp \left(-n \inf _{x \in \Gamma} I(x)\right)
$$

Here we use the notation " $\nearrow$ " instead of " $\approx$ " since the equivalence is in the logarithmic scale, i.e. $a_{n} \asymp b_{n}$ if $\log a_{n} \sim \log b_{n}$.

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Before the proof, we need some results on the Legendre-Fenchel transform and some elementary properties of $I(x)$.

## Legendre-Fenchel Transform

## Lemma (Legendre-Fenchel Transform)

Suppose $f(x): \mathbb{R}^{d} \rightarrow \overline{\mathbb{R}}=\mathbb{R} \cup\{ \pm \infty\}$ is a lower semicontinuous convex function. The conjugate function $F(y)$ of $f(x)$ (Legendre-Fenchel transform) defined as

$$
F(y)=\sup _{x}\{(x, y)-f(x)\}
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has the following properties:

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$$

(iii) The conjugacy relation holds:

$$
f(x)=\sup _{y}\{(x, y)-F(y)\} .
$$

## Legendre-Fenchel Transform

where we utilize the rule

$$
\begin{aligned}
& \alpha+\infty=\infty, \alpha-\infty=-\infty \quad \text { for } \alpha \text { finite } \\
& \alpha \cdot \infty=\infty, \alpha \cdot(-\infty)=-\infty, \quad \text { for } \alpha>0 \\
& 0 \cdot \infty=0 \cdot(-\infty)=0, \quad \inf \emptyset=\infty, \sup \emptyset=-\infty
\end{aligned}
$$

The readers may be referred to ${ }^{34}$ for proof details.

[^2]
## Heuristic derivation of the rate function

Now we apply the Laplace asymptotics to explain heuristically why the rate function takes the interesting form

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$$

Suppose the Cramér's theorem is already correct, then roughly we have

$$
\mu_{n}(d x) \propto \exp (-n I(x)) d x
$$

and thus by Laplace asymptotics

$$
\begin{aligned}
\lim _{n \rightarrow \infty} \frac{1}{n} \log \mathbb{E}^{\mu_{n}}(\exp (n \Phi(x))) & :=\lim _{n \rightarrow \infty} \frac{1}{n} \log \int_{\mathbb{R}} \exp (n \Phi(x)) \mu_{n}(d x) \\
& =\sup _{x}\{\Phi(x)-I(x)\}
\end{aligned}
$$

## Heuristic derivation of the rate function

Now we take $\Phi(x)=\lambda x$ then

$$
\mathbb{E}^{\mu_{n}}(\exp (n \lambda x))=\mathbb{E} \exp \left(\lambda \sum_{j=1}^{n} X_{j}\right)=\left[\mathbb{E} \exp \left(\lambda X_{j}\right]^{n}=(M(\lambda))^{n}\right.
$$

The equation leads to

$$
\Lambda(\lambda)=\sup _{x}\{\lambda x-I(x)\}
$$

By the conjugacy relation of Legendre-Fenchel transform, we obtain the rate function $I(x)$.

## Properties of Rate Function

Lemma (Properties of rate function)
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(iii) $I(x)$ is non-decreasing in $[\eta, \infty)$ and non-increasing in $(-\infty, \eta]$.

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(ii) $I(x)$ is non-negative and $I(\eta)=0$.
(iii) $I(x)$ is non-decreasing in $[\eta, \infty)$ and non-increasing in $(-\infty, \eta]$.
(iv) If $x>\eta, I(x)=\sup \{\lambda x-\Lambda(\lambda)\}$; If $x<\eta$, $I(x)=\sup _{\lambda<0}\{\lambda x-\Lambda(\lambda)\}$.

## Properties of Rate Function: Proof

## Proof.

(i) The convexity of $\Lambda(\lambda)$ follows by Hölder's inequality. For any
$0 \leq \theta \leq 1$,

$$
\begin{aligned}
\Lambda\left(\theta \lambda_{1}+(1-\theta) \lambda_{2}\right) & =\log \mathbb{E}\left(\exp \left(\theta \lambda_{1} X_{j}\right) \exp \left((1-\theta) \lambda_{2} X_{j}\right)\right) \\
& \leq \log \left(\left(\mathbb{E} \exp \left(\lambda_{1} X_{j}\right)\right)^{\theta}\left(\mathbb{E} \exp \left(\lambda_{2} X_{j}\right)\right)^{(1-\theta)}\right) \\
& =\theta \Lambda\left(\lambda_{1}\right)+(1-\theta) \Lambda\left(\lambda_{2}\right)
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$$

Thus $\Lambda(\lambda)$ is a convex function. The rest is a direct application of Lemma.

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& \leq \log \left(\left(\mathbb{E} \exp \left(\lambda_{1} X_{j}\right)\right)^{\theta}\left(\mathbb{E} \exp \left(\lambda_{2} X_{j}\right)\right)^{(1-\theta)}\right) \\
& =\theta \Lambda\left(\lambda_{1}\right)+(1-\theta) \Lambda\left(\lambda_{2}\right)
\end{aligned}
$$

Thus $\Lambda(\lambda)$ is a convex function. The rest is a direct application of Lemma.
(ii) Taking $\lambda=0$, we obtain $x \cdot 0-\Lambda(0)=0$. Thus $I(x) \geq 0$. On the other hand, we have

$$
\Lambda(\lambda)=\log \mathbb{E} \exp \left(\lambda X_{j}\right) \geq \log \exp (\lambda \eta)=\lambda \eta
$$

by Jensen's inequality. This gives $I(\eta) \leq 0$. Combing with $I(x) \geq 0$ we get the result.

## Properties of Rate Function: Proof

(iii) From the convexity of $I(x)$ and it achieves minimum at $x=\eta$, we immediately obtain the desired monotone property in $(-\infty, \eta]$ and $[\eta, \infty)$.

## Properties of Rate Function: Proof

(iii) From the convexity of $I(x)$ and it achieves minimum at $x=\eta$, we immediately obtain the desired monotone property in $(-\infty, \eta$ ] and $[\eta, \infty)$.
(iv) If $x>\eta$, then when $\lambda \leq 0$

$$
\lambda x-\Lambda(\lambda) \leq \lambda \eta-\Lambda(\lambda) \leq 0
$$

Thus the supremum is only achieved when $\lambda>0$ by the non-negativity of $I(x)$. Similar proof can be applied to the case $x<\eta$.

## Proof of Cramér's Theorem: Upper Bound

Proof of Cramér's Theorem. Without loss of generality, we assume $\eta=0$. (i) Upper bound. Suppose $x>0, J_{x}:=[x, \infty)$. For $\lambda>0$,

$$
\begin{aligned}
\mu_{n}\left(J_{x}\right) & =\int_{x}^{\infty} \mu_{n}(d y) \leq e^{-\lambda x} \int_{x}^{\infty} e^{\lambda y} \mu_{n}(d y) \\
& \leq e^{-\lambda x} \int_{-\infty}^{\infty} e^{\lambda y} \mu_{n}(d y)=e^{-\lambda x}\left[M\left(\frac{\lambda}{n}\right)\right]^{n}
\end{aligned}
$$

Taking $n \lambda$ instead of $\lambda$ in the above equation, we obtain

$$
\frac{1}{n} \log \mu_{n}\left(J_{x}\right) \leq-(\lambda x-\Lambda(\lambda))
$$

and accordingly

$$
\frac{1}{n} \log \mu_{n}\left(J_{x}\right) \leq-\sup _{\lambda>0}\{\lambda x-\Lambda(\lambda)\}=-I(x)
$$

## Proof of Cramér's Theorem: Upper Bound

If $x<0$, we can define $\tilde{J}_{x}=(-\infty, x]$. Similarly as above we get

$$
\frac{1}{n} \log \mu_{n}\left(\tilde{J}_{x}\right) \leq-I(x)
$$

For a closed set $F \in \mathcal{B}$, if $0 \in F, \inf _{x \in F} I(x)=0$. Then the upper bound holds obviously. Otherwise, let $\left(x_{1}, x_{2}\right)$ is the maximal interval satisfying the condition $\left(x_{1}, x_{2}\right) \cap F=\emptyset$ and $0 \in\left(x_{1}, x_{2}\right)$. So $x_{1}, x_{2} \in F, F \subset \tilde{J}_{x_{1}} \cup J_{x_{2}}$. From monotonicity of $I(x)$ in $(-\infty, 0]$ and $[0, \infty)$, we obtain

$$
\begin{aligned}
\varlimsup_{n \rightarrow \infty} \frac{1}{n} \log \mu_{n}(F) & \leq \max \left(\varlimsup_{n \rightarrow \infty} \frac{1}{n} \log \mu_{n}\left(\tilde{J}_{x_{1}}\right), \varlimsup_{n \rightarrow \infty} \frac{1}{n} \log \mu_{n}\left(J_{x_{2}}\right)\right) \\
& \leq-\min \left(I\left(x_{1}\right), I\left(x_{2}\right)\right)=-\inf _{x \in F} I(x)
\end{aligned}
$$

## Proof of Cramér's Theorem: Lower Bound

(ii) Lower bound. For any nonempty open set $G$, it is sufficient to prove that for any $x \in G$

$$
\underline{\lim }_{n \rightarrow \infty} \frac{1}{n} \log \mu_{n}(G) \geq-I(x)
$$

Now fix $x$ and assume $I(x)<\infty$.

## Proof of Cramér's Theorem: Lower Bound

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$$

Now fix $x$ and assume $I(x)<\infty$.
Case 1. If the supremum

$$
I(x)=\sup _{\lambda}\{\lambda x-\Lambda(\lambda)\}
$$

can not be achieved, then $x \neq 0$. Suppose $x>0$ and there exists $\lambda_{n} \rightarrow \infty$ such that

$$
I(x)=\lim _{n \rightarrow \infty}\left(\lambda_{n} x-\Lambda\left(\lambda_{n}\right)\right)
$$

## Proof of Cramér's Theorem: Lower Bound

We have

$$
\int_{-\infty}^{x-0} \exp \left(\lambda_{n}(y-x) \mu(d y) \rightarrow 0 \text { as } n \rightarrow \infty\right.
$$

by dominated convergence theorem. On the other hand

$$
\begin{aligned}
\lim _{n \rightarrow \infty} \int_{x}^{\infty} \exp \left(\lambda_{n}(y-x) \mu(d y)\right. & =\lim _{n \rightarrow \infty} \int_{-\infty}^{\infty} \exp \left(\lambda_{n}(y-x) \mu(d y)\right. \\
& =\exp (-I(x))<\infty
\end{aligned}
$$

Thus $\mu((x, \infty))=0$ and

$$
\exp (-I(x))=\lim _{n \rightarrow \infty} \int_{x}^{\infty} \exp \left(\lambda_{n}(y-x) \mu(d y)=\mu(\{x\})\right.
$$

## Proof of Cramér's Theorem: Lower Bound

We have

$$
\mu_{n}(G) \geq \mu_{n}(\{x\}) \geq(\mu(\{x\}))^{n}=\exp (-n I(x))
$$

and thus

$$
\frac{1}{n} \log \mu_{n}(G) \geq-I(x)
$$

Similar proof can be applied to the case $x<a$.

## Proof of Cramér's Theorem: Lower Bound

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and thus

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\frac{1}{n} \log \mu_{n}(G) \geq-I(x)
$$

Similar proof can be applied to the case $x<a$.
Case 2. Suppose that the supremum is attained at $\lambda_{0}$ such that

$$
I(x)=\lambda_{0} x-\Lambda\left(\lambda_{0}\right)
$$

Then $x=\Lambda^{\prime}\left(\lambda_{0}\right)=M^{\prime}\left(\lambda_{0}\right) / M\left(\lambda_{0}\right)$. Define a new probability measure as

$$
\tilde{\mu}(d y)=\frac{1}{M\left(\lambda_{0}\right)} \exp \left(\lambda_{0} y\right) \mu(d y)
$$

## Proof of Cramér's Theorem: Lower Bound

It has the expectation

$$
\int_{\mathbb{R}} y \tilde{\mu}(d y)=\frac{1}{M\left(\lambda_{0}\right)} \int_{\mathbb{R}} y \exp \left(\lambda_{0} y\right) \mu(d y)=\frac{M^{\prime}\left(\lambda_{0}\right)}{M\left(\lambda_{0}\right)}=x .
$$

If $x \geq 0$, then $\lambda_{0} \geq 0$. For sufficiently small $\delta>0$, we have $(x-\delta, x+\delta) \subset \bar{G}$,

$$
\begin{aligned}
\mu_{n}(G) & \geq \mu_{n}(x-\delta, x+\delta) \\
& =\int_{\left\{\left|\frac{1}{n} \sum_{j=1}^{n} y_{j}-x\right|<\delta\right\}} \mu\left(d y_{1}\right) \cdots \mu\left(d y_{n}\right) \\
& \left.\left.\geq \exp \left(-n \lambda_{0}(x+\delta)\right) \int_{\left\{\left\lvert\, \frac{1}{n}\right.\right.} \sum_{j=1}^{n} y_{j}-x \right\rvert\,<\delta\right\} \\
& =\exp \left(-n \lambda_{0}(x+\delta)\right) M\left(\lambda_{0}\right)^{n} \int_{\left\{\left|\frac{1}{n} \sum_{j=1}^{n} y_{j}-x\right|<\delta\right\}} \tilde{\mu}\left(d y_{1}\right) \cdots \tilde{\mu}\left(d y_{n}\right) .
\end{aligned}
$$

## Proof of Cramér's Theorem

By the WLLN, we have

$$
\int_{\left\{\left|\frac{1}{n} \sum_{j=1}^{n} y_{j}-x\right|<\delta\right\}} \tilde{\mu}\left(d y_{1}\right) \cdots \tilde{\mu}\left(d y_{n}\right) \rightarrow 1 \text { as } n \rightarrow \infty .
$$

Thus
$\underline{\lim }_{n \rightarrow \infty} \frac{1}{n} \log \mu_{n}(G) \geq-\lambda_{0}(x+\delta)+\Lambda\left(\lambda_{0}\right)=-I(x)-\lambda_{0} \delta$ for all $0<\delta \ll 1$.
Similar proof can be applied to the case $x<a$.

## Example of Cramér's Theorem

Example (Cramér's theorem applied to $\operatorname{Ber}(\mathrm{p})$ )
We have $\Lambda(\lambda)=\ln \left(p e^{\lambda}+q\right)$ where $q=1-p$. The rate function

$$
I(x)= \begin{cases}x \log \frac{x}{p}+(1-x) \ln \frac{1-x}{q}, & x \in[0,1] \\ \infty, & \text { otherwise }\end{cases}
$$

Here we take the convention $0 \log 0=0$. It is obvious that $I(x) \geq 0$, and $I(x)$ achieves its global minimum 0 at $x^{*}=p$.

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Here we take the convention $0 \log 0=0$. It is obvious that $I(x) \geq 0$, and $I(x)$ achieves its global minimum 0 at $x^{*}=p$.

- $I(x)$ has important background in information theory. It is called relative entropy, or Kullback-Leibler distance between two distributions $\mu$ and $\nu$ defined as follows

$$
D(\mu \| \nu)=\sum_{i=1}^{r} \mu_{i} \log \frac{\mu_{i}}{\nu_{i}}
$$

where $\mu=\left(\mu_{1}, \mu_{2}, \ldots, \mu_{r}\right), \nu=\left(\nu_{1}, \nu_{2}, \ldots, \nu_{r}\right)$. In the previous case, we have $r=2, \mu=(x, 1-x)$ and $\nu=(p, q)$, the underlying Bernoulli distribution.

## Connections with statistical mechanics

There are intimate relations between the large deviation theory and equilibrium statistical mechanics ${ }^{5}$. Now let us only consider the simplest case here. For the Bernoulli trials with parameter $p$, we can obtain the rate function as

$$
I(x)=x \ln \frac{x}{p}+(1-x) \ln \frac{1-x}{q}, x \in[0,1]
$$

which is also called the relative entropy. When $p=1 / 2$ we have

$$
I(x)=x \ln x+(1-x) \ln (1-x)+\ln 2, x \in[0,1] .
$$

In this case, the rate function is exactly the negative Shannon entropy up to a constant $\ln 2$. Below we will show that it has direct connection to Boltzmann entropy in statistical mechanics.

[^3]
## Connections with statistical mechanics: Entropy

- Consider a system with $n$ independent spins being up or down with equal probability $1 / 2$. If it is up, we label it as 1 , and 0 otherwise. We define the set of microstates as

$$
\Omega=\left\{\omega: \omega=\left(s_{1}, s_{2}, \ldots, s_{n}\right), s_{i}=1 \text { or } 0\right\} .
$$

For each microstate $\omega$, we define its mean energy as

$$
h_{n}(\omega)=\frac{1}{n} \sum_{i=1}^{n} s_{i} .
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## Connections with statistical mechanics: Entropy

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- In thermodynamics, the entropy is a function of the macrostate energy. In statistical mechanics, Boltzmann gives a clear mathematical definition of the entropy

$$
S=k_{B} \ln W
$$

in the micro-canonical ensemble (the number of spins $n$ and total energy $h_{n}=E$ are fixed in this set-up), where $k_{B}$ is the Boltzmann constant, $W$ is the number of the microstates corresponding to the fixed energy $E$. Actually this formula is carved in Boltzmann's tombstone.

## Connections with statistical mechanics: LDT

- From large deviation theory we have

$$
I(E)=\lim _{n \rightarrow \infty}-\frac{1}{n} \ln \mathbb{P}\left(h_{n} \in[E, E+d E]\right),
$$

where $d E$ is an infinitesimal quantity and

$$
\begin{aligned}
I(E) & =\lim _{n \rightarrow \infty}-\frac{1}{n} \ln \frac{W\left(h_{n} \in[E, E+d E]\right)}{2^{n}} \\
& =\ln 2-\frac{1}{k_{B}} \lim _{n \rightarrow \infty} \frac{1}{n} S_{n}(E) .
\end{aligned}
$$

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\end{aligned}
$$

- Taking the normalization of $S$ with $1 / n$ in the $n \rightarrow \infty$ limit, we obtain

$$
k_{B} I(E)=k_{B} \ln 2-S(E),
$$

where $S(E)$ is the Boltzmann entropy in statistical mechanics. So we have that the rate function is the negative entropy (with factor $1 / k_{B}$ ) up to an additive constant. This is a general statement.

## Connections with statistical mechanics: Free Energy

In the canonical ensemble in statistical mechanics (the number of spins $n$ and the temperature $T$ are fixed in this set-up), let us investigate the physical meaning of $\Lambda$. The logarithmic moment generating function of $H_{n}(\omega)=n h_{n}(\omega)$ with normalization $1 / n$ is

$$
\Lambda(\lambda)=\lim _{n \rightarrow \infty} \frac{1}{n} \ln \mathbb{E} e^{\lambda H_{n}}
$$

where we take $H_{n}$ instead of a single R.V. $s_{i}$ since it admits more general interpretation. Take $\lambda=-\beta=-\left(k_{B} T\right)^{-1}$, we have

$$
\Lambda(-\beta)=\lim _{n \rightarrow \infty} \frac{1}{n} \ln \left(\sum_{\omega} e^{-\beta H_{n}(\omega)}\right)-\ln 2
$$

Thus the free energy $F(\beta)$ is the negative logarithmic moment generating function up to a constant.

## Connections with statistical mechanics

Define the partition function

$$
Z_{n}(\beta)=\sum_{\omega} e^{-\beta H_{n}(\omega)}
$$

and free energy

$$
F_{n}(\beta)=-\beta^{-1} \ln Z_{n}(\beta),
$$

we have

$$
\Lambda(-\beta)=-\beta \lim _{n \rightarrow \infty} \frac{1}{n} F_{n}(\beta)-\ln 2=-\beta F(\beta)-\ln 2 .
$$

## Connections with statistical mechanics

According to the large deviation theory we have

$$
-\beta F(\beta)-\ln 2=\sup _{E}\left\{-\beta E-\ln 2+k_{B}^{-1} S(E)\right\}
$$

i.e.

$$
F(\beta)=\inf _{E}\{E-T S(E)\} .
$$

The infimum is achieved at the critical point $E^{*}$ such that

$$
\left.\frac{\partial S(E)}{\partial E}\right|_{E=E^{*}}=\frac{1}{T}
$$

which is exactly a thermodynamic relation between $S$ and $T$. Here $E^{*}$ is essentially the internal energy $U$.


[^0]:    ${ }^{2}$ C.M. Bender and S.A. Orszag. Advanced Mathematical Methods for Scientists and Engineers: Asymptotic Methods and Perturbation Theory=

[^1]:    ${ }^{2}$ C.M. Bender and S.A. Orszag. Advanced Mathematical Methods for Scientists and Engineers: Asymptotic Methods and Perturbation Theory=

[^2]:    ${ }^{3}$ R.T. Rockafellar. Convex analysis. Princeton University Press, Princeton, 1970.
    ${ }^{4}$ R.T. Rockafellar and R. J-B Wets. Variational Analysis. Springer-Verlag, Berlin and Heidelberg, 2009.

[^3]:    ${ }^{5}$ R.S. Ellis. Entropy, Large deviations, and statistical mechanics. Springer-Verlag, 1st edition edition, 1985.

