Large deviation principle for a random continuous variable A_n

rate function

$$p(A_n = a) \underset{n\to\infty}{\approx} \exp(-n\, I(a))$$

$$P(A_n \in da) \underset{n\to\infty}{\approx} p(A_n = a)\, da$$

- Gärtner-Ellis theorem:

scaled cumulant generating function

$$\lambda(k) = \lim_{n\to\infty} \frac{1}{n} \ln\left[\langle \exp(n A_n k)\rangle\right]$$

if $\lambda(k)$ exists and is differentiable $\forall k$

$\Rightarrow$ 1) Large deviation principle for A_n

2) $I(a) = \sup_k \left[k a - \lambda(k)\right] \rightarrow I = \lambda^*$

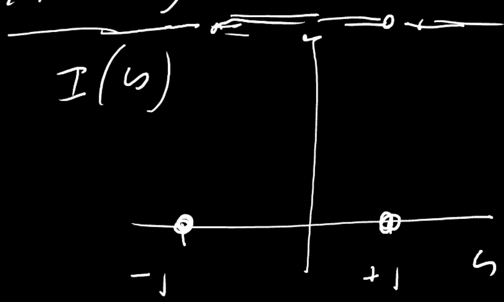
- Varadhan theorem (ALWAYS)

$I^* = \lambda \qquad \lambda(k) = \sup_a \left[a k - I(a)\right]$

Example in which G-E th does not work:

$$p(Y_n = y) = \frac{1}{2}\left[\delta(y-1) + \delta(y+1)\right] \quad \forall n$$

$$I(y) = -\lim_{n\to\infty}\frac{1}{n}\ln p(Y_n = y)$$

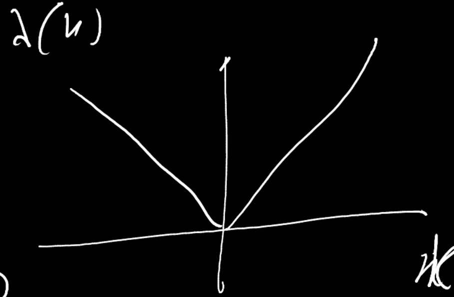


$$= \begin{cases} 0 & \text{if } y = \pm 1 \\ \infty & \text{otherwise} \end{cases}$$

$$\lambda(k) = \lim_{n\to\infty}\frac{1}{n}\ln\left[\langle \exp(n Y_n k)\rangle\right]$$

$$= \lim_{n\to\infty}\frac{1}{n}\ln\left[\frac{\exp(kn) + \exp(-kn)}{2}\right]$$

$$= \mathrm{sgn}(k)\, k = |k|$$

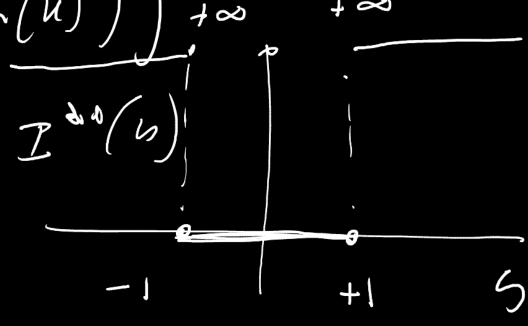


$\lambda(k)$ not differentiable for $k=0$

$\lambda = I^*$ — compute $\lambda^* = I^{**}$

$$I^{**}(y) = \sup_k\left[ky - \lambda(k)\right] = \begin{cases} 0 & \text{if } y\in[-1,1] \\ +\infty & \text{otherwise}\end{cases}$$

$$= \sup_k\left[k(y - \mathrm{sgn}(k))\right]$$



$I^{**} \neq I \longrightarrow$

I^{**} is the convex envelope of I

(1) $I^* = \lambda$ ALWAYS (Varadhan th.)

(2) I non convex $\Rightarrow \lambda^* = I^{**} \neq I$

I^{**} is the convex envelope of I

$(I^{**} \leq I)$

(3) $(I^{**})^* = I^* = \lambda$

Different rate functions can share the same $\lambda(k)$

($\Rightarrow$ all have the same convex envelope)

(4) I non strictly convex $\Rightarrow \lambda(k)$ non differentiable

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Large deviation theory and statistical mechanics (equilibrium)

- entropy $\longrightarrow$ rate function
  free energy $\longrightarrow$ generating function
- variational principles (max entropy principle / minimum free energy principle)

n particles

- $\omega = (\omega_1, \dots, \omega_n)$ ω_i = state of the ith particle
  $\hookrightarrow$ state of n particles $\longrightarrow$ microstates

$\omega_i \in \Lambda$ $\omega \in \Lambda_n$

- $H_n(\omega)$ = total energy (extensive)

$h_n(\omega) = H_n(\omega)/n$ energy density

- prior probability measure = uniform measure (in Λ^n) $P(d\omega) = d\omega/|\Lambda|^n$

(Boltzmann hypoth. of equiprobable microstates)

- External conditions / constraints $\Rightarrow$ statistical mechanics ensemble

- Macrostates (thermodynamic observables)

any function $M_n(\omega)$ ("coarse-graining")

* $n \to \infty$ $\Rightarrow$ Thermodynamic Limit

Entropy is the rate function for h_n

(microcanonical)

$$P(h_n \in du) = \int_{\{\omega \in \Lambda_n : h_n(\omega) \in du\}} P(d\omega) = \frac{\Omega(h_n \in du)}{|\Lambda|^n}$$

$$P(d\omega) = d\omega/|\Lambda|^n, \quad \Omega(h_n \in du) = \int_{\{\omega \in \Lambda_n : h_n(\omega) \in du\}} d\omega$$

$$I(u) = \lim_{n\to\infty} -\frac{1}{n} \ln P(h_n \in du)$$

$$\boxed{I(u) \stackrel{!}{=} \ln|\Lambda| - s(u)}$$

$$s(u) = \lim_{n\to\infty} \frac{1}{n} \ln\left[\mathcal{N}(h_n \in du) \right]$$

microcanonical entropy density

$$\lambda(k) = \lim_{n\to\infty} \frac{1}{n} \ln\left[\langle \exp(n k h_n) \rangle \right] \qquad \beta = -k$$

$$\langle \exp(n k h_n) \rangle = \int_{\Lambda_n} \overbrace{\exp(k n h_n)}^{\exp(-\beta H_n)} \, d\omega \big/ |\Lambda|^n$$

$$= Z_n(\beta) \big/ |\Lambda|^n \qquad \beta = -k$$

$$\boxed{\lambda(k) = -\varphi(\beta)\big|_{\beta=-k} - \ln|\Lambda|}$$

canonical free energy (Helmholtz)

$$\varphi(\beta) = \lim_{n\to\infty} -\frac{1}{n} \ln Z_n(\beta) \to \text{adimensional free energy}$$

(Massieu potential)

proper free energy $f(\beta) = \varphi(\beta)/\beta$

$$\varphi(\beta) = \inf_u \left[\beta u - s(u) \right] \qquad \text{V. th.}$$

$$s(u) = \inf_\beta \left[u\beta - \varphi(\beta) \right] \qquad \text{G.E. th}$$

Variational principles:

- Microcanonical ensemble (max ent principle)

$$P^u(d\omega) \equiv P(d\omega / h_n \in du) = \begin{cases} \frac{P(d\omega)}{P(h_n \in du)} & \text{if } h_n(\omega) \in du \\ 0 & \text{otherwise} \end{cases}$$

macrostate $M_n(\omega)$

$$\underline{\underline{P^u(M_n \in dm)}} = P(M_n \in dm / h_n \in du)$$

$$= \frac{P(h_n \in du, M_n \in dm)}{P(h_n \in du)}$$

joint probability $\tilde{S}(m)$

$S(u)$

we assume a large deviation principle for M_n

($\Rightarrow M_n$ thermodynamic observable)

$$P(M_n \in dm) \underset{n \to \infty}{\approx} \exp(n \tilde{S}(m))\, dm$$

(rate function $-\tilde{S}(m)$)

it can be proved that if $\underline{h_n(\omega) = \tilde{h}(M_n(\omega))}$

("contraction principle") ("contraction")

different $m \to$ same u

$$\Rightarrow P^u(M_n \in dm) \underset{n \gg 1}{\overset{\wedge}{\sim}} \exp(-n I^u(m))\, dm$$

(Large dev. principle for M_n in the microcan. ensemble)

$$I^u(m) = \begin{cases} S(u) - \tilde{S}(m) & \text{if } \underbrace{\tilde{h}(m) = u} \\ \infty & \text{otherwise} \end{cases}$$

Most probable values for M_n:

$$m : I^u(m) = 0 \longrightarrow \underbrace{\tilde{S}(m) = S(u)}$$

m : m globally maximizes $\tilde{S}(m)$ with $\tilde{h}(m) = u$ (constraint)

(in general $I^u(m) \geq 0$)

$$\underbrace{S(u) = \sup_{m : \tilde{h}(m) = u} \tilde{S}(m)}$$

max entropy principle (constrained energy value $\tilde{h}(m) = u$)

similarly:

minimum free energy principle

$$\underbrace{\varphi(\beta) = \inf_m \big(\underbrace{\beta \tilde{h}(m) - \tilde{S}(m)}\big)}$$

(effective free energy $\tilde{\varphi}(m)$)

<u>contraction $\tilde{h}(m)$</u>