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#### Large Deviations for i.i.d. Random Variables

**Content.** Chernoff bound using exponential moment generating functions. Properties of a moment generating functions. Legendre transforms.

### **1** Preliminary notes

The Weak Law of Large Numbers tells us that if  $X_1, X_2, \ldots$ , is an i.i.d. sequence of random variables with mean  $\mu \triangleq \mathbb{E}[X_1] < \infty$  then for every  $\epsilon > 0$ 

$$\mathbb{P}(|\frac{X_1 + \ldots + X_n}{n} - \mu| > \epsilon) \to 0,$$

as  $n \to \infty$ .

But how quickly does this convergence to zero occur? We can try to use Chebyshev inequality which says

$$\mathbb{P}(|\frac{X_1 + \ldots + X_n}{n} - \mu| > \epsilon) \le \frac{\operatorname{Var}(X_1)}{n\epsilon^2}.$$

This suggest a "decay rate" of order  $\frac{1}{n}$  if we treat  $Var(X_1)$  and  $\epsilon$  as a constant. Is this an accurate rate? Far from so ...

In fact if the higher moment of  $X_1$  was finite, for example,  $\mathbb{E}[X_1^{2m}] < \infty$ , then using a similar bound, we could show that the decay rate is at least  $\frac{1}{n^m}$  (exercise).

The goal of the large deviation theory is to show that in many interesting cases the decay rate is in fact *exponential*:  $e^{-cn}$ . The exponent c > 0 is called the *large deviations rate*, and in many cases it can be computed explicitly or numerically.

### 2 Large deviations upper bound (Chernoff bound)

Consider an i.i.d. sequence with a common probability distribution function  $F(x) = \mathbb{P}(X \le x), x \in \mathbb{R}$ . Fix a value  $a > \mu$ , where  $\mu$  is again an expectation corresponding to the distribution F. We consider probability that the average of  $X_1, \ldots, X_n$  exceeds a. The WLLN tells us that this happens with probability converging to zero as n increases, and now we obtain an estimate on this probability. Fix a positive parameter  $\theta > 0$ . We have

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) = \mathbb{P}(\sum_{1 \le i \le n} X_i > na)$$
$$= \mathbb{P}(e^{\theta \sum_{1 \le i \le n} X_i} > e^{\theta na})$$
$$\leq \frac{\mathbb{E}[e^{\theta \sum_{1 \le i \le n} X_i}]}{e^{\theta na}} \quad \text{Markov inequality}$$
$$= \frac{\mathbb{E}[\prod_i e^{\theta X_i}]}{(e^{\theta a})^n},$$

But recall that  $X_i$ 's are i.i.d. Therefore  $\mathbb{E}[\prod_i e^{\theta X_i}] = (\mathbb{E}[e^{\theta X_1}])^n$ . Thus we obtain an upper bound

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) \le \left(\frac{\mathbb{E}[e^{\theta X_1}]}{e^{\theta a}}\right)^n.$$
(1)

Of course this bound is meaningful only if the ratio  $\mathbb{E}[e^{\theta X_1}]/e^{\theta a}$  is less than unity. We recognize  $\mathbb{E}[e^{\theta X_1}]$  as the moment generating function of  $X_1$  and denote it by  $M(\theta)$ . For the bound to be useful, we need  $\mathbb{E}[e^{\theta X_1}]$  to be at least finite. If we could show that this ratio is less than unity, we would be done – exponentially fast decay of the probability would be established.

Similarly, suppose we want to estimate

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} < a),$$

for some  $a < \mu$ . Fixing now a negative  $\theta < 0$ , we obtain

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} < a) = \mathbb{P}(e^{\theta \sum_{1 \le i \le n} X_i} > e^{\theta n a})$$
$$\leq \left(\frac{M(\theta)}{e^{\theta a}}\right)^n,$$

and now we need to find a negative  $\theta$  such that  $M(\theta) < e^{\theta a}$ . In particular, we need to focus on  $\theta$  for which the moment generating function is finite. For this purpose let  $\mathcal{D}(M) \triangleq \{\theta : M(\theta) < \infty\}$ . Namely  $\mathcal{D}(M)$  is the set of values  $\theta$  for which the moment generating function is finite. Thus we call  $\mathcal{D}$  the domain of M.

## 3 Moment generating function. Examples and properties

Let us consider some examples of computing the moment generating functions.

• Exponential distribution. Consider an exponentially distributed random variable X with parameter  $\lambda$ . Then

$$M(\theta) = \int_0^\infty e^{\theta x} \lambda e^{-\lambda x} dx$$
$$= \lambda \int_0^\infty e^{-(\lambda - \theta)x} dx$$

When  $\theta < \lambda$  this integral is equal to  $\frac{-1}{\lambda-\theta}e^{-(\lambda-\theta)x}\Big|_0^\infty = 1/(\lambda-\theta)$ . But when  $\theta \ge \lambda$ , the integral is infinite. Thus the exp. moment generating function is finite iff  $\theta < \lambda$  and is  $M(\theta) = \lambda/(\lambda-\theta)$ . In this case the domain of the moment generating function is  $\mathcal{D}(M) = (-\infty, \lambda)$ .

**Standard Normal distribution.** When X has standard Normal distribution, we obtain

$$M(\theta) = \mathbb{E}[e^{\theta X}] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\theta x} e^{-\frac{x^2}{2}} dx$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{x^2 - 2\theta x + \theta^2 - \theta^2}{2}} dx$$
$$= e^{\frac{\theta^2}{2}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{(x-\theta)^2}{2}} dx$$

Introducing change of variables  $y = x - \theta$  we obtain that the integral is equal to  $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{2}} dy = 1$  (integral of the density of the standard Normal distribution). Therefore  $M(\theta) = e^{\frac{\theta^2}{2}}$ . We see that it is always finite and  $\mathcal{D}(M) = \mathbb{R}$ .

In a retrospect it is not surprising that in this case  $M(\theta)$  is finite for all  $\theta$ . The density of the standard Normal distribution "decays like"  $\approx e^{-x^2}$  and this is faster than just exponential growth  $\approx e^{\theta x}$ . So no matter how large is  $\theta$  the overall product is finite.

• **Poisson distribution.** Suppose *X* has a Poisson distribution with parameter *λ*. Then

$$M(\theta) = \mathbb{E}[e^{\theta X}] = \sum_{m=0}^{\infty} e^{\theta m} \frac{\lambda^m}{m!} e^{-\lambda}$$
$$= \sum_{m=0}^{\infty} \frac{(e^{\theta} \lambda)^m}{m!} e^{-\lambda}$$
$$= e^{e^{\theta} \lambda - \lambda},$$

(where we use the formula  $\sum_{m\geq 0} \frac{t^m}{m!} = e^t$ ). Thus again  $\mathcal{D}(M) = \mathbb{R}$ . This again has to do with the fact that  $\lambda^m/m!$  decays at the rate similar to 1/m! which is faster then any exponential growth rate  $e^{\theta m}$ .

We now establish several properties of the moment generating functions.

**Proposition 1.** The moment generating function  $M(\theta)$  of a random variable X satisfies the following properties:

- (a) M(0) = 1. If  $M(\theta) < \infty$  for some  $\theta > 0$  then  $M(\theta') < \infty$  for all  $\theta' \in [0, \theta]$ . Similarly, if  $M(\theta) < \infty$  for some  $\theta < 0$  then  $M(\theta') < \infty$  for all  $\theta' \in [\theta, 0]$ . In particular, the domain  $\mathcal{D}(M)$  is an interval containing zero.
- (b) Suppose  $(\theta_1, \theta_2) \subset \mathcal{D}(M)$ . Then  $M(\theta)$  as a function of  $\theta$  is differentiable in  $\theta$  for every  $\theta_0 \in (\theta_1, \theta_2)$ , and furthermore,

$$\frac{d}{d\theta}M(\theta)\Big|_{\theta=\theta_0} = \mathbb{E}[Xe^{\theta_0 X}] < \infty.$$

Namely, the order of differentiation and expectation operators can be changed.

*Proof.* Part (a) is left as an exercise. We now establish part (b). Fix any  $\theta_0 \in (\theta_1, \theta_2)$  and consider a  $\theta$ -indexed sequence of random variables

$$Y_{\theta} \triangleq \frac{\exp(\theta X) - \exp(\theta_0 X)}{\theta - \theta_0}.$$

Since  $\frac{d}{d\theta} \exp(\theta x) = x \exp(\theta x)$ , then almost surely  $Y_{\theta} \to X \exp(\theta_0 X)$ , as  $\theta \to \theta_0$ . Thus to establish the claim it suffices to show that convergence of expectations holds as well, namely  $\lim_{\theta\to\theta_0} \mathbb{E}[Y_{\theta}] = \mathbb{E}[X \exp(\theta_0 X)]$ , and  $\mathbb{E}[X \exp(\theta_0 X)] < \infty$ . For this purpose we will use the Dominated Convergence Theorem. Namely, we will identify a random variable Z such that  $|Y_{\theta}| \le Z$  almost surely in some interval  $(\theta_0 - \epsilon, \theta_0 + \epsilon)$ , and  $\mathbb{E}[Z] < \infty$ .

Fix  $\epsilon > 0$  small enough so that  $(\theta_0 - \epsilon, \theta_0 + \epsilon) \subset (\theta_1, \theta_2)$ . Let  $Z = \epsilon^{-1} \exp(\theta_0 X + \epsilon |X|)$ . Using the Taylor expansion of  $\exp(\cdot)$  function, for every  $\theta \in (\theta_0 - \epsilon, \theta_0 + \epsilon)$ , we have

$$Y_{\theta} = \exp(\theta_0 X) \left( X + \frac{1}{2!} (\theta - \theta_0) X^2 + \frac{1}{3!} (\theta - \theta_0)^2 X^3 + \dots + \frac{1}{n!} (\theta - \theta_0)^{n-1} X^n + \dots \right),$$

which gives

$$\begin{aligned} |Y_{\theta}| &\leq \exp(\theta_0 X) \left( |X| + \frac{1}{2!} (\theta - \theta_0) |X|^2 + \dots + \frac{1}{n!} (\theta - \theta_0)^{n-1} |X|^n + \dots \right) \\ &\leq \exp(\theta_0 X) \left( |X| + \frac{1}{2!} \epsilon |X|^2 + \dots + \frac{1}{n!} \epsilon^{n-1} |X|^n + \dots \right) \\ &= \exp(\theta_0 X) \epsilon^{-1} \left( \exp(\epsilon |X|) - 1 \right) \\ &\leq \exp(\theta_0 X) \epsilon^{-1} \exp(\epsilon |X|) \\ &= Z. \end{aligned}$$

It remains to show that  $\mathbb{E}[Z] < \infty$ . We have

$$\mathbb{E}[Z] = \epsilon^{-1} \mathbb{E}[\exp(\theta_0 X + \epsilon X) \mathbf{1}\{X \ge 0\}] + \epsilon^{-1} \mathbb{E}[\exp(\theta_0 X - \epsilon X) \mathbf{1}\{X < 0\}]$$
  
$$\leq \epsilon^{-1} \mathbb{E}[\exp(\theta_0 X + \epsilon X)] + \epsilon^{-1} \mathbb{E}[\exp(\theta_0 X - \epsilon X)]$$
  
$$= \epsilon^{-1} M(\theta_0 + \epsilon) + \epsilon^{-1} M(\theta_0 - \epsilon)$$
  
$$< \infty,$$

since  $\epsilon$  was chosen so that  $(\theta_0 - \epsilon, \theta_0 + \epsilon) \subset (\theta_1, \theta_2) \subset \mathcal{D}(M)$ . This completes the proof of the proposition.

# Problem 1.

- (a) Establish part (a) of Proposition 1.
- (b) Construct an example of a random variable for which the corresponding interval is trivial  $\{0\}$ . Namely,  $M(\theta) = \infty$  for every  $\theta > 0$ .

(c) Construct an example of a random variable X such that  $\mathcal{D}(M) = [\theta_1, \theta_2]$ for some  $\theta_1 < 0 < \theta_2$ . Namely, the the domain  $\mathcal{D}$  is a non-zero length closed interval containing zero.

Now suppose the i.i.d. sequence  $X_i, i \ge 1$  is such that  $0 \in (\theta_1, \theta_2) \subset \mathcal{D}(M)$ , where M is the moment generating function of  $X_1$ . Namely, M is finite in a neighborhood of 0. Let  $a > \mu = \mathbb{E}[X_1]$ . Applying Proposition 1, let us differentiate this ratio with respect to  $\theta$  at  $\theta = 0$ :

$$\frac{d}{d\theta}\frac{M(\theta)}{e^{\theta a}} = \frac{\mathbb{E}[X_1 e^{\theta X_1}]e^{\theta a} - ae^{\theta a}\mathbb{E}[e^{\theta X_1}]}{e^{2\theta a}} = \mu - a < 0.$$

Note that  $M(\theta)/e^{\theta a} = 1$  when  $\theta = 0$ . Therefore, for sufficiently small positive  $\theta$ , the ratio  $M(\theta)/e^{\theta a}$  is smaller than unity, and (1) provides an exponential bound on the tail probability for the average of  $X_1, \ldots, X_n$ .

Similarly, if  $a < \mu$ , the ratio  $M(\theta)/e^{\theta a} < 1$  for sufficiently small negative  $\theta$ .

We now summarize our findings.

**Theorem 1** (Chernoff bound). Given an i.i.d. sequence  $X_1, \ldots, X_n$  suppose the moment generating function  $M(\theta)$  is finite in some interval  $(\theta_1, \theta_2) \ni 0$ . Let  $a > \mu = \mathbb{E}[X_1]$ . Then there exists  $\theta > 0$ , such that  $M(\theta)/e^{\theta a} < 1$  and

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) \le \left(\frac{M(\theta)}{e^{\theta a}}\right)^n.$$

Similarly, if  $a < \mu$ , then there exists  $\theta < 0$ , such that  $M(\theta)/e^{\theta a} < 1$  and

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} < a) \le \left(\frac{M(\theta)}{e^{\theta a}}\right)^n.$$

How small can we make the ratio  $M(\theta)/\exp(\theta a)$ ? We have some freedom in choosing  $\theta$  as long as  $\mathbb{E}[e^{\theta X_1}]$  is finite. So we could try to find  $\theta$  which minimizes the ratio  $M(\theta)/e^{\theta a}$ . This is what we will do in the rest of the lecture. The surprising conclusion of the large deviations theory is very often that such a minimizing value  $\theta^*$  exists and is tight. Namely it provides *the correct decay rate*! In this case we will be able to say

$$\mathbb{P}(\frac{\sum_{1 \leq i \leq n} X_i}{n} > a) \approx \exp(-I(a, \theta^*)n)$$
  
where  $I(a, \theta^*) = -\log\left(M(\theta^*)/e^{\theta^*a}\right)$ .

### 4 Legendre transforms

Theorem 1 gave us a large deviations bound  $(M(\theta)/e^{\theta a})^n$  which we rewrite as  $e^{-n(\theta a - \log M(\theta))}$ . We now study in more detail the exponent  $\theta a - \log M(\theta)$ .

**Definition 1.** A Legendre transform of a random variable X is the function  $I(a) \triangleq \sup_{\theta \in \mathbb{R}} (\theta a - \log M(\theta)).$ 

Let us go over the examples of some distributions and compute their corresponding Legendre transforms.

• Exponential distribution with parameter  $\lambda$ . Recall that  $M(\theta) = \lambda/(\lambda - \theta)$  when  $\theta < \lambda$  and  $M(\theta) = \infty$  otherwise. Therefore when  $\theta < \lambda$ 

$$I(a) = \sup_{\theta} (a\theta - \log \frac{\lambda}{\lambda - \theta})$$
  
= 
$$\sup_{\theta} (a\theta - \log \lambda + \log(\lambda - \theta)),$$

and  $I(a) = -\infty$  otherwise. Setting the derivative of  $g(\theta) = a\theta - \log \lambda + \log(\lambda - \theta)$  equal to zero we obtain the equation  $a - 1/(\lambda - \theta) = 0$  which has the unique solution  $\theta^* = \lambda - 1/a$ . For the boundary cases, we have  $a\theta - \log \lambda + \log(\lambda - \theta)) \to -\infty$  when either  $\theta \uparrow \lambda$  or  $\theta \to -\infty$  (check). Therefore

$$I(a) = a(\lambda - 1/a) - \log \lambda + \log(\lambda - \lambda + 1/a)$$
  
=  $a\lambda - 1 - \log \lambda + \log(1/a)$   
=  $a\lambda - 1 - \log \lambda - \log a$ .

The large deviations bound then tells us that when  $a > 1/\lambda$ 

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) \approx e^{-(a\lambda - 1 - \log \lambda - \log a)n}.$$

Say  $\lambda = 1$  and a = 1.2. Then the approximation gives us  $\approx e^{-(.2 - \log 1.2)n}$ .

Note that we can obtain an exact expression for this tail probability. Indeed,  $X_1, X_1 + X_2, \ldots, X_1 + X_2 \cdots + X_n, \ldots$  are the events of a Poisson process with parameter  $\lambda = 1$ . Therefore we can compute the probability  $\mathbb{P}(\sum_{1 \le i \le n} X_i > 1.2n)$  exactly: it is the probability that the Poisson

process has at most n-1 events before time 1.2n. Thus

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > 1.2) = \mathbb{P}(\sum_{1 \le i \le n} X_i > 1.2n)$$
$$= \sum_{0 \le k \le n-1} \frac{(1.2n)^k}{k!} e^{-1.2n}$$

It is not at all clear how revealing this expression is. In hindsight, we know that it is approximately  $e^{-(.2-\log 1.2)n}$ , obtained via large deviations theory.

• Standard Normal distribution. Recall that  $M(\theta) = e^{\frac{\theta^2}{2}}$  when  $X_1$  has the standard Normal distribution. The expected value  $\mu = 0$ . Thus we fix a > 0 and obtain

$$I(a) = \sup_{\theta} (a\theta - \frac{\theta^2}{2})$$
$$= \frac{a^2}{2},$$

achieved at  $\theta^* = a$ . Thus for a > 0, the large deviations theory predicts that

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) \approx e^{-\frac{a^2}{2}n}.$$

Again we could compute this probability directly. We know that  $\frac{\sum_{1 \le i \le n} X_i}{n}$  is distributed as a Normal random variable with mean zero and variance 1/n. Thus

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) = \frac{\sqrt{n}}{\sqrt{2\pi}} \int_a^\infty e^{-\frac{t^2 n}{2}} dt.$$

After a little bit of technical work one could show that this integral is "dominated" by its part around *a*, namely,  $\int_{a}^{a+\epsilon} \cdot$ , which is further approximated by the value of the function itself at *a*, namely  $\frac{\sqrt{n}}{\sqrt{2\pi}}e^{-\frac{a^2}{2}n}$ . This is consistent with the value given by the large deviations theory. Simply the lower order magnitude term  $\frac{\sqrt{n}}{\sqrt{2\pi}}$  disappears in the approximation on the log scale.

• **Poisson distribution.** Suppose X has a Poisson distribution with parameter  $\lambda$ . Recall that in this case  $M(\theta) = e^{e^{\theta}\lambda - \lambda}$ . Then

$$I(a) = \sup_{\theta} (a\theta - (e^{\theta}\lambda - \lambda)).$$

Setting derivative to zero we obtain  $\theta^* = \log(a/\lambda)$  and  $I(a) = a \log(a/\lambda) - (a - \lambda)$ . Thus for  $a > \lambda$ , the large deviations theory predicts that

$$\mathbb{P}(\frac{\sum_{1 \le i \le n} X_i}{n} > a) \approx e^{-(a \log(a/\lambda) - a + \lambda)n}.$$

In this case as well we can compute the large deviations probability explicitly. The sum  $X_1 + \cdots + X_n$  of Poisson random variables is also a Poisson random variable with parameter  $\lambda n$ . Therefore

$$\mathbb{P}(\sum_{1 \le i \le n} X_i > an) = \sum_{m > an} \frac{(\lambda n)^m}{m!} e^{-\lambda n}.$$

But again it is hard to infer a more explicit rate of decay using this expression

### 5 Additional reading materials

- Chapter 0 of [2]. This is non-technical introduction to the field which describes motivation and various applications of the large deviations theory. Soft reading.
- Chapter 2.2 of [1].

## References

- [1] A. Dembo and O. Zeitouni, *Large deviations techniques and applications*, Springer, 1998.
- [2] A. Shwartz and A. Weiss, *Large deviations for performance analysis*, Chapman and Hall, 1995.

15.070J / 6.265J Advanced Stochastic Processes Fall 2013

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