

# Stochastic Simulation

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# Chapter VI

## Rare-Event Simulation

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This is why we look at importance sampling.

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- ▶ An algorithm is defined as a family  $Z(x)$  of such estimators.

Q: find algorithm  $s$  such that the required  $R$  does not explode.

Different flavors: *bounded relative error, logarithmic efficiency, ...*

## Two generic examples

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Example 1: **partial sums**. We wish to estimate

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for  $n$  large and  $a > \mathbb{E}X_1$ .



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Example 2: **hitting probabilities**. We wish to estimate

$$\alpha(B) := \mathbb{P}(\exists n \in \mathbb{N} : S_n \geq B),$$

for  $B$  large and  $\mathbb{E}X_1 < 0$ .

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These examples were dealt with by Jan-Pieter last week.

As they are the most important examples, I'll say a bit more about them, and explain at an intuitive level why exponential twisting works so nicely.

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As they are the most important examples, I'll say a bit more about them, and explain at an intuitive level why exponential twisting works so nicely.

(It can be seen as my personal view on Section VI.6.)

## Standard example 1: partial sums

Consider, with  $S_n := \sum_{i=1}^n X_i$ , the probability

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for  $n$  large and  $a > \mathbb{E}X_1$ .

This probability tends to 0 by virtue of the law of large numbers.

## Standard example 1: partial sums

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Assume moment generating function  $\hat{F}(\theta) := \mathbb{E}e^{\theta X} < \infty$  for some  $\theta > 0$  ( $\sim$  light tails!)

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Bahadur & Rao:

Assume moment generating function  $\hat{F}(\theta) := \mathbb{E}e^{\theta X} < \infty$  for some  $\theta > 0$  ( $\sim$  light tails!)

Define Legendre transform

$$I(a) = \sup_{\theta} (\theta a - \log \hat{F}(\theta)).$$

Then

$$\pi_n / \left( \frac{C_a}{\sqrt{n}} e^{-nI(a)} \right) = \mathbb{P} \left( \frac{S_n}{n} > a \right) / \left( \frac{C_a}{\sqrt{n}} e^{-nI(a)} \right) \rightarrow 1$$

(if  $X$  non-lattice; if  $X$  lattice similar formula applies).



## Standard example 1: partial sums

This formula only holds for  $n \rightarrow \infty$ , so there is still a need to estimate  $\pi_n$ !

How can that be efficiently done?

Naive simulation: as we have seen, # runs  $\sim 400/\pi_n$ , that is, grows exponentially in  $n$ ...

Idea: *mimic conditional distribution*.

## Intermezzo: conditional distribution

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Of course, we would like to pick  $\mathbb{Q}$  such that variance of new estimator is minimal. Say  $p$  is rare-event probability we wish to estimate.

Proposal: let  $\mathbb{Q}$  coincide with the distribution *conditional on* the event  $A$ :

$$\mathbb{Q}(\omega) = \mathbb{P}(\omega \mid \omega \in A) = \frac{\mathbb{P}(\omega)}{p}$$

if  $\omega \in A$  and 0 else.

## Intermezzo: conditional distribution

Then,

$$\text{Var}_{\mathbb{Q}}(LI) = \mathbb{E}_{\mathbb{Q}}(L^2I) - p^2 = \int_{\omega \in A} L^2 d\mathbb{Q}(\omega) - p^2.$$

But

$$\int_{\omega \in A} L^2 d\mathbb{Q}(\omega) = \int_{\omega \in A} p^2 \frac{d\mathbb{P}(\omega)}{p} = p^2,$$

so that  $\text{Var}_{\mathbb{Q}}(LI) = 0$ .

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But we could try to **mimic** the conditional distribution!

## Standard example 1: partial sums

Consider distribution of some  $X_i$ , and condition on  $S_n \geq na$ :

$$g(x) := \mathbb{P}(X_i \in [x, x + dx) \mid S_n \geq na) = \frac{f(x) \mathbb{P}(S_{n-1} \geq na - x)}{\mathbb{P}(S_n \geq na)},$$

with  $f(x)$  density of  $X_i$  under  $\mathbb{P}$ .



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Bahadur-Rao:

$$\mathbb{P}(S_n \geq na) \sim \frac{C_a}{\sqrt{n}} e^{-nl(a)},$$

whereas

$$\mathbb{P}(S_{n-1} \geq na - x) \sim \frac{C_a}{\sqrt{n}} \exp\left(- (n-1) \cdot I\left(\frac{na-x}{n-1}\right)\right).$$

(Use that  $\sqrt{n} \sim \sqrt{n-1}$ .)

## Standard example 1: partial sums

Let us consider, for  $n \rightarrow \infty$ ,

$$\exp\left(- (n-1) \cdot I\left(\frac{na-x}{n-1}\right)\right).$$

Well, it equals

$$\exp\left(- (n-1) \cdot I\left(\frac{(n-1)a + a - x}{n-1}\right)\right) \approx - (n-1)I(a) - (a-x)I'(a).$$

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As a consequence,

$$g(x) = \frac{f(x) \mathbb{P}(S_{n-1} \geq na - x)}{\mathbb{P}(S_n \geq na)} \approx f(x) \cdot \exp(I(a) + (x-a)I'(a)).$$

## Standard example 1: partial sums

Now we verify that

$$g(x) = \frac{f(x) \mathbb{P}(S_{n-1} \geq na - x)}{\mathbb{P}(S_n \geq na)} \approx f(x) \cdot \exp(I(a) + (x - a)I'(a))$$

is a genuine density.

To this end, we need some basic convex analysis.

## Standard example 1: partial sums

Now we verify that  $f(x) \cdot \exp(I(a) + (x - a)I'(a))$  is a genuine density.

Define by  $\theta(a)$  the optimizer in the definition of  $I(a)$ :

$$I(a) = \sup_{\theta} (\theta a - \log \hat{F}(\theta)) = \theta(a)a - \log \hat{F}(\theta(a)).$$

Hence  $\theta(a)$  satisfies

$$a = \frac{\hat{F}'(\theta(a))}{\hat{F}(\theta(a))}.$$

This entails that

$$I'(a) = \theta(a) + \theta'(a) \left( a - \frac{\hat{F}'(\theta(a))}{\hat{F}(\theta(a))} \right) = \theta(a).$$

## Standard example 1: partial sums

We conclude that we have to consider

$$f(x) \cdot \exp(I(a) + (x - a)\theta(a)).$$

Notice that this expression is non-negative, and in addition

$$\begin{aligned} & \int f(x) \cdot \exp(I(a) + (x - a)\theta(a)) dx \\ &= \exp(I(a) - \theta(a)a) \cdot \int e^{\theta(a)x} f(x) dx \\ &= \exp(I(a) - \theta(a)a) \hat{F}(\theta(a)) = e^{I(a) - I(a)} = \end{aligned}$$

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Hence

$$f(x) \cdot \exp(I(a) + (x - a)\theta(a)) = f(x) \frac{e^{\theta(a)x}}{\hat{F}(\theta(a))}$$

is a density.

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We determined a proxy for the distribution of the increments, conditional on  $S_n \geq na$ .

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Now we analyze the performance of the resulting estimator.  
Recall that under the original measure

$$\text{Var}(I) = \pi_n(1 - \pi_n) \approx \pi_n \approx (C_a/\sqrt{n}) \cdot e^{-nI(a)}.$$

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So we have to analyze  $\mathbb{E}_{\mathbb{Q}}(L^2 I)$  for large  $n$ .

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So we have to analyze  $\mathbb{E}_{\mathbb{Q}}(L^2 I)$  for large  $n$ .

Observe:

$$L = \prod_{i=1}^n \frac{f(X_i)}{g(X_i)} = \prod_{i=1}^n \frac{\hat{F}(\theta(a))}{e^{\theta(a)X_i}} = (\hat{F}(\theta(a)))^n \cdot e^{-\theta(a)S_n}.$$

## Standard example 1: partial sums

If  $l = 1$  (that is,  $S_n \geq na$ ),

$$L = (\hat{F}(\theta(a)))^n \cdot e^{-\theta(a)S_n} \leq (\hat{F}(\theta(a)))^n \cdot e^{-\theta(a)a} = e^{-2nl(a)}.$$

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In other words,

$$\text{Var}_{\mathbb{Q}}(LI) = \mathbb{E}_{\mathbb{Q}}(L^2I) - \pi_n^2 \leq \mathbb{E}_{\mathbb{Q}}(L^2I) \leq e^{-2nl(a)}.$$

Recall that under  $\mathbb{P}$  we had

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$$\text{Var}(I) = \pi_n(1 - \pi_n) \approx \pi_n \approx (C_a/\sqrt{n}) \cdot e^{-nl(a)}.$$

$\implies$  Substantial variance reduction!

## Standard example 1: partial sums

As an aside: more refined analysis is possible:

$$\text{Var}_{\mathbb{Q}}(LI) \sim \frac{\tilde{C}_a}{\sqrt{n}} e^{-2nl(a)}.$$

Straightforward computation: number of runs  $R$  required grows roughly proportional to  $\sqrt{n}$  (rather than  $1/\pi_n$ , that is proportional to  $\sqrt{n}e^{nl(a)}$ ).



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$\implies$  Procedure is logarithmically efficient

## Standard example II: hitting probabilities

Focus now on

$$\alpha(B) := \mathbb{P}(\exists n \in \mathbb{N} : S_n \geq B),$$

where it is assumed that  $\mathbb{E}X_1 < 0$ .

Again *light-tailed* regime, that is,  $\hat{F}(\theta) = \mathbb{E}e^{\theta X} = 1$  has a positive solution, say  $\theta^*$ .

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Cramér-Lundberg:  $\alpha(B) \sim Ce^{-\theta^*B}$ .

Consider distribution of some  $X_i$ , and condition on  $\{\exists n \in \mathbb{N} : S_n \geq B\}$ : informally,

$$g(x) := \mathbb{P}(X_i \in [x, x + dx) \mid \exists n \in \mathbb{N} : S_n \geq B) = \frac{f(x)\alpha(B-x)}{\alpha(B)},$$

with  $f(x)$  density of  $X_i$  under  $\mathbb{P}$ .

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with  $f(x)$  density of  $X_i$  under  $\mathbb{P}$ .

With Cramér-Lundberg:

$$g(x) \approx f(x) \cdot e^{\theta^*x}.$$

This is a density as  $\theta^*$  solves  $\hat{F}(\theta^*) = 1$ .

## Standard example II: hitting probabilities

It can be proven that  $\mathbb{E}_{\mathbb{Q}} X_1 > 0$ , so event is not rare anymore.  
Hence, the hitting time  $T$  is finite a.s., so  $I = 1$  a.s.

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Also,

$$L = e^{-\theta^* S_T}.$$

Thus

$$\alpha(B) = \mathbb{E}_{\mathbb{Q}}(L) = e^{-\theta^* B} \mathbb{E}_{\mathbb{Q}} e^{\theta^*(B-S_T)} \approx C e^{-\theta^* B}.$$

## Standard example II: hitting probabilities

This entails

$$\alpha(B) = \mathbb{E}_{\mathbb{Q}}(L) = e^{-\theta^* B} \mathbb{E}_{\mathbb{Q}} e^{\theta^*(B-S_T)} \approx C e^{-\theta^* B}.$$

In addition

$$\text{Var}_{\mathbb{Q}}(L) \sim \tilde{C} e^{-2\theta^* B},$$

so that number of runs needed remains bounded when  $B$  grows!



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⇒ Procedure has bounded relative error

Markov modulation

(Cf. Section VI.7.)

## Markov modulation

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Idea: often  $X_i$  are affected by external (background) process. Let background process be a discrete-time Markov chain on  $\{1, \dots, d\}$ .

For instance,  $X_i$  is distributed as a sample from the random variable  $Y_j$  (with density  $f_j(\cdot)$ ) when  $J_i = j$ .

Transition probabilities of Markov chain  $J$  are given by  $p_{ij}$ ; equilibrium probabilities are  $\pi_j$ .

## Markov modulation

We again focus on

$$\alpha(B) := \mathbb{P}(\exists n \in \mathbb{N} : S_n \geq B),$$

where it is assumed that

$$\sum_{j=1}^d \pi_j \mathbb{E} Y_j < 0.$$

## Markov modulation

Idea: solve eigensystem

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$$x_j = \mathbb{E} e^{\theta Y_j} \sum_{k=1}^d p_{jk} x_k.$$

Perron-Frobenius: there is a positive eigenvalue such that  $x$  is positive componentwise and  $\theta > 0$ .

## Markov modulation

With  $(x, \theta)$  solving the eigensystem

$$x_j = \mathbb{E} e^{\theta Y_j} \sum_{k=1}^d p_{jk} x_k,$$

clearly

$$q_{jk} = p_{jk} \frac{x_k}{x_j} \mathbb{E} e^{\theta Y_j}$$

form a transition probability matrix.



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form a transition probability matrix.

In addition, define the twisted increments by

$$g_j(y) = f_j(y) \frac{e^{\theta y}}{\mathbb{E} e^{\theta Y_j}}.$$

## Markov modulation

Observe

$$\alpha(B) := \mathbb{P}(\exists n \in \mathbb{N} : S_n \geq B) = \mathbb{P}(T_B < \infty),$$

with  $T_B$  the first hitting time of  $[B, \infty)$ .

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with  $T_B$  the first hitting time of  $[B, \infty)$ .

Can we evaluate likelihood ratio?

Observe that  $T_B < \infty$  with probability 1 under  $\mathbb{Q}$ .

## Markov modulation

By definition,

$$L = \prod_{i=1}^{T_B} \left( \frac{p_{J_i J_{i+1}}}{q_{J_i J_{i+1}}} \right) \left( \frac{f_{J_i}(X_i)}{g_{J_i}(X_i)} \right).$$

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This can be simplified to

$$L = \prod_{i=1}^{T_B} \left( \frac{x_{J_i}}{x_{J_{i+1}}} \frac{1}{\mathbb{E} e^{\theta Y_{J_i}}} \right) \left( \frac{\mathbb{E} e^{\theta Y_{J_i}}}{e^{\theta Y_{J_i}}} \right),$$

which equals

$$\frac{x_{J_0}}{x_{J_{T_B+1}}} e^{-\theta S_{T_B}}.$$

## Markov modulation

From

$$L = \frac{X_{J_0}}{X_{J_{T_B+1}}} e^{-\theta S_{T_B}},$$

we conclude that, for a finite constant  $C$ ,

$$\alpha(B) = \mathbb{E}_{\mathbb{Q}}(LI) = \mathbb{E}_{\mathbb{Q}}(L) \leq Ce^{-\theta S_{T_B}}.$$

Actually it can be proven that, as  $B \rightarrow \infty$ ,

$$\alpha(B) \sim \tilde{C}e^{-\theta S_{T_B}},$$

and that the procedure has bounded relative error.

## Caveats

Slight variations to the 'leading examples' model may already cause serious problems... For  $a_- < \mu := \mathbb{E}X_1 < a_+$ ,

$$\pi_n := \mathbb{P} \left( \frac{S_n}{n} \notin (a_-, a_+) \right).$$

Assume w.l.o.g.  $I(a_+) < I(a_-)$ .



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Slight variations to the 'leading examples' model may already cause serious problems... For  $a_- < \mu := \mathbb{E}X_1 < a_+$ ,

$$\pi_n := \mathbb{P} \left( \frac{S_n}{n} \notin (a_-, a_+) \right).$$

Assume w.l.o.g.  $I(a_+) < I(a_-)$ . This intuitively means that most likely point in set is  $a_+$ .

Define, as before,

$$\theta(a) := \arg \sup_{\theta} (\theta a - \log \hat{F}(\theta)).$$

## Caveats

Naïvely, one would use

$$g(x) = f(x) \frac{e^{\theta(a_+)x}}{\hat{F}(\theta(a_+))}.$$

To check how this change of measure performs, we analyze

$$\begin{aligned} \mathbb{E}_{\mathbb{Q}}(L^2 I) &= \left( \mathbb{E}_{\mathbb{Q}}(e^{-2\theta(a_+)S_n} \mathbf{1}_{\{S_n \geq na_+\}}) \right. \\ &\quad \left. + \mathbb{E}_{\mathbb{Q}}(e^{-2\theta(a_+)S_n} \mathbf{1}_{\{S_n \leq na_-\}}) \right) \times (\hat{F}(\theta(a_+)))^{2n}. \end{aligned}$$

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First term:

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Second term is more difficult. Observe: undershoot below level  $na_-$  will be modest. Hence

$$\begin{aligned} & \lim_{n \rightarrow \infty} \frac{1}{n} \log \left( \mathbb{E}_{\mathbb{Q}} \left( e^{-2\theta(a_+) S_n} \mathbf{1}_{\{S_n \leq na_-\}} \right) \times (\hat{F}(\theta(a_+)))^{2n} \right) \\ &= -2\theta(a_+)a_- + \lim_{n \rightarrow \infty} \frac{1}{n} \log \mathbb{Q} \left( \frac{S_n}{n} \leq a_- \right) + 2 \log \hat{F}(\theta(a_+)). \end{aligned}$$

## Caveats

To find decay rate of  $\mathbb{Q}(S_n/n \leq a_-)$ , let  $J(\cdot)$  be the Legendre-Fenchel transform under  $\mathbb{Q}$ , that is

$$\begin{aligned} J(a_-) &= \sup_{\theta} \left[ \theta a_- - \log \mathbb{E}_{\mathbb{Q}} e^{\theta X_1} \right] \\ &= \sup_{\theta} \left[ \theta a_- - \log \phi(\theta + \theta(a_+)) + \log \hat{F}(\theta(a_+)) \right] \\ &= -\theta(a_+)a_- + \sup_{\theta} \left[ (\theta + \theta(a_+))a_- - \log \hat{F}(\theta + \theta(a_+)) \right] \\ &\quad + \log \hat{F}(\theta(a_+)) \\ &= -\theta(a_+)a_- + I(a_-) + \log \hat{F}(\theta(a_+)). \end{aligned}$$

We obtain that

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{1}{n} \log \left( \mathbb{E}_{\mathbb{Q}} \left( e^{-2\theta(a_+)S_n} \mathbf{1}_{\{S_n \leq na_-\}} \right) \times (\hat{F}(\theta(a_+)))^{2n} \right) \\ = -\theta(a_+)a_- - I(a_-) + \log \hat{F}(\theta(a_+)). \end{aligned}$$

## Caveats

Hence logarithmic efficiency if

$$-2I(a_+) \geq -\theta(a_+)a_- - I(a_-) + \log \hat{F}(\theta(a_+)),$$

or

$$I(a_+) + \theta(a_+)a_+ \leq I(a_-) + \theta(a_+)a_-.$$

This condition is not always met!

## Caveats

**Example.** Let the  $X_i$  be i.i.d. samples from an exponential distribution with mean 1. We take  $a_+ = 2$  and  $a_- < 1$ . We have that  $\theta(a_+) = 1 - 1/a_+$  and  $I(a_+) = a_+ - 1 - \log a_+$ . The inequality to be verified is therefore

$$3 - \log 2 \leq \frac{3}{2}a_- - \log a_-, \quad \text{or} \quad \log a_- \leq \frac{3}{2}a_- - 3 + \log 2.$$

Numerical search: condition is met when  $0 < a_- < 0.119$ .



## Caveats & remedies

This type of problems arises often when 'overflow set' has 'unfavorable' shape.

**Remedy 1:** Split rare event of interest in disjoint parts:

$$\alpha(n) = \mathbb{P}(\bar{X}_n \notin (a_-, a_+)) = \mathbb{P}\left(\frac{S_n}{n} \geq a_+\right) + \mathbb{P}\left(\frac{S_n}{n} \leq a_-\right),$$

and estimate each separately.

## Caveats & remedies

**Remedy 2:** Adaptive change-of-measure. Main problem: rare event can be reached through path that is 'far away' from most-likely path, leading to large likelihood ratio. Can be avoided by updating the change-of-measure during simulation run, depending on current position.

## Caveats & remedies

**Remedy 3:** Random change-of-measure. In this approach, one flips a coin, and the outcome decides from which twisted distribution one samples. Assume  $p \in (0, 1)$ ; measure  $\mathbb{Q}$ : tilt with parameter  $\theta(a_+) > 0$  ( $\theta(a_-) < 0$ ) with probability  $p$  ( $1 - p$ , respectively). Likelihood equals

$$L = \left( p e^{\theta(a_+) S_n} \hat{F}(\theta(a_+))^n + (1 - p) e^{\theta(a_-) S_n} \hat{F}(\theta(a_-))^n \right)^{-1}.$$

## Caveats & remedies

Then  $\mathbb{E}_{\mathbb{Q}}(L^2I)$  is smaller than

$$\begin{aligned} & \mathbb{E}_{\mathbb{Q}} \left( \left( \frac{1\{S_n \geq na_+\}}{pe^{\theta(a_+)S_n} \hat{F}(\theta(a_+))} \right)^2 + \right. \\ & \quad \left. \left( \frac{1\{S_n \leq na_-\}}{(1-p)e^{\theta(a_-)S_n} \hat{F}(\theta(a_-))} \right)^2 \right) \\ & \leq \frac{1}{p^2} e^{-2nl(a_+)} + \frac{1}{(1-p)^2} e^{-2nl(a_-)}, \end{aligned}$$

which has decay rate  $-2l(a_+)$ . Hence procedure is logarithmically efficient.

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- ... and we wish you all the best in preparing the exam!