Estimation of the probability of the union of rare events

Mathis Le Bail

August 19, 2022

Introduction

 $X \in \mathbb{R}^d$ a random variable of distribution F_X . We want to estimate $\pi = \mathbb{P}(X \in A)$ where A is the event of interest.

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Sample size $\it N$ needed to acquire a 10% relative precision for the half-width of the 95% confidence interval

$$\begin{split} &\frac{1.96\,\sqrt{\pi(1-\pi)}}{\pi\sqrt{N}}\approx 0.1\\ &N\approx \frac{100\times 1.96^2\pi(1-\pi)}{\pi^2}\sim \frac{100\times 1.96^2}{\pi}\\ &\pi\sim 10^{-8}\Rightarrow N\sim 10^{10} \end{split} \tag{3}$$

Efficiency properties in rare-event simulation

Family of rare events $\{R(\tau)\}$, $\pi(\tau) = \mathbb{P}(R(\tau)) \to 0$ when $\tau \to \infty$.

$$R(\tau) = (X > \tau)$$
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 Π_{τ} is asymptotically optimal or weakly efficient if

$$\frac{\log(\mathbb{E}(\Pi_{\tau}^{2}))}{2\log(\pi(\tau))} \underset{\tau \to \infty}{\to} 1 \tag{5}$$



 $\widehat{\Pi_n(\tau)} = \frac{1}{n} \sum_{i=1}^n \Pi_{\tau}^i$ the average of the i.i.d n random variables $\Pi_{\tau}^1,...,\Pi_{\tau}^n$ to estimate $\pi(\tau)$.

$$\mathbb{P}\left(\left|\frac{\widehat{\Pi_n(\tau)} - \pi(\tau)}{\pi(\tau)}\right| > \epsilon\right) < \delta \tag{6}$$

· Chebyshev's inequality gives us

$$\mathbb{P}\left(\left|\frac{\widehat{\Pi_n(\tau)} - \pi(\tau)}{\pi(\tau)}\right| > \epsilon\right) \le \frac{Var(\frac{\Pi_n(\tau)}{\pi(\tau)})}{\epsilon^2} = \frac{Var(\Pi_\tau)}{n\pi(\tau)^2\epsilon^2} \tag{7}$$

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CMC estimator :

$$\frac{\textit{Var}(\Pi_{\tau})}{\textit{n}\pi(\tau)^{2}\epsilon^{2}} = \frac{1 - \pi(\tau)}{\textit{n}\pi(\tau)\epsilon^{2}} \approx \frac{1}{\textit{n}\pi(\tau)\epsilon^{2}} \Rightarrow \textit{n} \approx \mathcal{O}(\frac{1}{\pi(\tau)})$$

$$\pi = \int \mathbb{1}_{A}(x) f(x) dx = \int \mathbb{1}_{A}(x) \frac{f(x)}{q(x)} q(x) dx = \mathbb{E}_{q} \left[\mathbb{1}_{A}(X) \frac{f(X)}{q(X)} \right]$$
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• q must be such that q(x) > 0 for all x where $\mathbb{1}_A(x)f(x) \neq 0$

$$\Pi_n^{IS} = \frac{1}{n} \sum_{i=1}^n \frac{f(X_i)}{q(X_i)} \mathbb{1}_A(X_i)$$
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 $Var(\hat{\Pi_n^{S}}) = \frac{1}{n} \int \frac{(\mathbb{1}_A(x) f(x) - \pi q(x))^2}{q(x)} dx$ (10)

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• We note $\mathbb P$ the probability associated to the pdf f and $\mathbb P^*$ the probability associated to the pdf q^* , we have $\mathbb P^*(.) = \mathbb P(.|A)$ and $\mathbb P^*(dx) = \frac{\mathbb I_A(x)}{\mathbb P(A)}\mathbb P(dx)$



Estimating the probability of the union of rare events

- X a d-dimensional random vector and J fixed integer
- fixed unit vector $\omega_j \in \mathbb{R}^d$ and $\tau_j \in \mathbb{R}$ for $j \in \{1,...,J\}$
- Rare events : $H_j = \{x : x^\top \omega_j \geqslant \tau_j\}$
- $\bullet \ \ H = \cup_{j=1}^J H_j$

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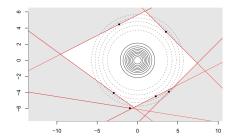


Figure: Graphical representation of a standard bivariate Gaussian distribution with J=6 half-spaces which are the rare events

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$$\max_{1 \leqslant j \leqslant J} P_j =: \underline{\mu} \leqslant \mu \leqslant \bar{\mu} := \sum_{j=1}^J P_j$$

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Some notations :

- $H_j(x) = \mathbb{1}_{H_i}(x)$
- $S(x) = \sum_{j=1}^{J} H_j(x)$ counts the number of rare events
- $T_s = \Pr(S = s)$ gives the distribution of S.

The mixture components are the conditional distributions $q_j = (X \mid \omega_j^\top X \geqslant \tau_j)$. We have $q_j(x) = p(x)H_j(x)/P_j$. And the mixture distribution resulting is :

$$q_{\alpha}^* = \sum_{j=1}^{J} \alpha_j^* q_j \tag{12}$$

with
$$\alpha_j^* \equiv \frac{P_j}{\sum P_j}$$

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Theorem

If $1 \le J < \infty$ and $\min_{j} P_{j} > 0$ and $n \ge 1$, then

$$\hat{\mu}_{\alpha^*} = \frac{\bar{\mu}}{n} \sum_{i=1}^n \frac{1}{S(X_i)} \tag{13}$$

where $X_i \sim q_{lpha}^*$, satisfies $\mathbb{P}(rac{ar{\mu}}{J} \leq \hat{\mu}_{lpha^*} \leq ar{\mu}) = 1$,

$$\mathbb{E}\left(\hat{\mu}_{\alpha^*}\right) = \mu \tag{14}$$

and

$$\operatorname{Var}(\hat{\mu}_{\alpha^*}) \leq \frac{1}{n} \left(\bar{\mu} \sum_{s=1}^{J} \frac{T_s}{s} - \mu^2 \right) \leqslant \frac{\mu(\bar{\mu} - \mu)}{n} \tag{15}$$

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• We take
$$\omega_j^{\top} = \frac{\gamma_j^{\top} \Sigma^{\frac{1}{2}}}{\sqrt{\gamma_j^{\top} \Sigma \gamma_j}}$$
 and $\tau_j = \frac{\kappa_j - \gamma_j^{\top} \eta}{\sqrt{\gamma_j^{\top} \Sigma \gamma_j}}$.
$$\gamma_j^{\top} y \ge \kappa_j$$

 $\Leftrightarrow \omega_i^\top x > \tau_i$

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Sampling method : To sample $X_i = x_i$ from the q_α^* distribution, we have to be able to sample $X \sim \mathcal{N}(0, I)$ conditionally on $X^\top \omega \geqslant \tau$ for a unit vector ω and scalar τ

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In practice, $Y = \Phi^{-1}(U\Phi(-\tau))$ and we deliver X = -X. We get better numerical stability in sampling $Z \sim \mathcal{N}(0, I)$ conditionally on $X^{\top}\omega \leq -\tau$



Efficiency of the ALOE algorithm

Corollary

Let $\hat{\mu}_{\alpha^*} = \frac{\bar{\mu}}{n} \sum_{i=1}^n \frac{1}{S(X_i)}$ where $X_i \sim q_{\alpha}^*$ with q_{α}^* defined in (12).

Then $Var(\hat{\mu}_{\alpha^*}) \leq \frac{\bar{\mu}^2}{4n}$. If $\underline{\mu} \geq \frac{\bar{\mu}}{2}$ then also $Var(\hat{\mu}_{\alpha^*}) \leq \frac{\underline{\mu}(\bar{\mu} - \underline{\mu})}{n}$. Similarly,

$$\frac{Var(\hat{\mu}_{\alpha^*})}{\mu^2} \le \frac{1}{n} \min \left\{ \frac{\bar{\mu}}{\underline{\mu}} - 1, J - 1 \right\} \le \frac{J - 1}{n} \tag{18}$$

This corollary gives us the property of strong efficiency for (13) since it implies in particular for J fixed :

$$\lim_{\mu \to 0} \frac{Var(\hat{\mu}_{\alpha^*})}{\mu^2} < \infty \tag{19}$$



$$au_j = au$$
 $P_j = \Phi(- au)$ $\bar{\mu} = \sum P_j = J\Phi(- au)$ $r(au) = rac{Var(\hat{\mu}_{lpha^*})}{\mu^2}$

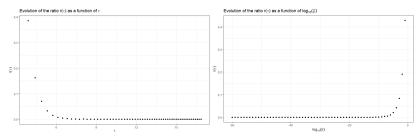


Figure: Results of the computation of the ratios $r(\tau)$ where the first and the second moments have been estimated from 1000 samples

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$$-\infty = L_0 < L_1 < ... < L_m = \tau$$

$$p = \mathbb{P}(h(X) \ge \tau) = \prod_{k=1}^{m} \mathbb{P}(h(X) > L_k | h(X) > L_{k-1})$$
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• i.i.d. sample $(X_1,...,X_N)$ from the distribution π , $X_1^1=X_1,...,X_N^1=X_N$. For each k,

$$L_k = \min(h(X_1^k), ..., h(X_N^k))$$
 (21)

$$X_{i}^{k+1} = \begin{cases} X_{i}^{k} & \text{if } h(X_{i}^{k}) > L_{k} \\ X^{*} \sim (X|h(X) > L_{k}) & \text{if } h(X_{i}^{k}) = L_{k} \end{cases}$$
 (22)

A new i.i.d sample $(X_1^{k+1},...,X_N^{k+1})$ from the distribution $\pi_k:(X|h(X)>L_k)$



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 (20)

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$$L_{k} = \min(h(X_{1}^{k}), ..., h(X_{N}^{k}))$$
 (21)

$$X_{i}^{k+1} = \begin{cases} X_{i}^{k} & \text{if } h(X_{i}^{k}) > L_{k} \\ X^{*} \sim (X|h(X) > L_{k}) & \text{if } h(X_{i}^{k}) = L_{k} \end{cases}$$
 (22)

A new i.i.d sample $(X_1^{k+1},...,X_N^{k+1})$ from the distribution $\pi_k:(X|h(X)>L_k)$

• Computation cost : $\mathcal{O}(-N\log(N)\log(p))$



Properties

$$\hat{\rho} = \left(1 - \frac{1}{N}\right)^M \text{ with } M = \max\{k : L_k \le \tau\}$$
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Proposition

The estimator \hat{p} is a discrete random variable taking values in

$$\left\{1, \left(1 - \frac{1}{N}\right), \left(1 - \frac{1}{N}\right)^2, \ldots\right\}$$

with probability

$$\mathbb{P}\left(\hat{p} = \left(1 - \frac{1}{N}\right)^{k}\right) = \frac{p^{N}(-N\log(p))^{k}}{k!}, \quad k = 0, 1, 2, \dots$$
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It follows that

$$\mathbb{E}[\hat{p}] = p \quad and \quad Var(\hat{p}) = p^2(p^{-\frac{1}{N}} - 1)$$
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$$CV_{CMC}^2 = \frac{1}{Np}$$
 versus $CV^2 = \frac{Var(\hat{p})}{p^2} = (p^{-\frac{1}{N}} - 1) \approx \frac{-\log(p)}{N}$ (26)

New estimator ALOE

$$\hat{q}_{\alpha^*|\hat{P}_1,...,\hat{P}_J}(x) \approx \sum_{j=1}^J \frac{\hat{P}_j}{\sum_k \hat{P}_k} q_j(x) = \sum_{j=1}^J \frac{\hat{P}_j}{\sum_k \hat{P}_k} \frac{p(x)H_j(x)}{P_j}$$
(27)

New estimator ALOE

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$$\hat{\mu}_{\alpha^*} = \frac{1}{n} \sum_{i=1}^{n} \frac{p(x_i) H_{1:J}(x_i)}{\sum_{j=1}^{J} \frac{\hat{P}_j}{\sum_{k}^{j} \hat{P}_k} \frac{p(x_i) H_j(x_i)}{P_j}} = \frac{\sum_{k}^{j} \hat{P}_k}{n} \sum_{i=1}^{n} \frac{1}{\sum_{j=1}^{J} \frac{\hat{P}_j}{P_j} H_j(x_i)}$$
(28)

New estimator ALOE

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Proposition

Let $\hat{\mu}_{\alpha^*}$ given by (28). Then

$$\mathbb{E}[\hat{\mu}_{\alpha^*}] \approx \mu \tag{29}$$

and

$$Var(\hat{\mu}_{\alpha^*}) \approx \frac{1}{n} \mathbb{E} \left[\sum_{k} \hat{P}_k \int_{H} \frac{1}{\sum_{j=1}^{J} \frac{\hat{P}_j}{\hat{P}_j} H_j(x)} p(x) \, \mathrm{d}x \right] - \frac{\mu^2}{n}$$
(30)



 $\bullet \ \ \text{If there is a ϵ such that } \frac{\hat{\rho_j}}{P_j} \geq \epsilon \ \text{for all } j \Rightarrow \textit{Var}(\hat{\mu}_{\alpha^*}) \leq \frac{\mu}{n} \left(\frac{\bar{\mu}}{\epsilon} - \mu\right)$

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$$\hat{P}_{j} = (1 - \frac{1}{N})^{M_{j}} \text{ with } M_{j} = \min(\{k : L_{k} \le \tau_{j}\}, I_{\max}^{j})$$
 (31)

$$\frac{\hat{P}_j}{P_j} \ge \frac{\left(1 - \frac{1}{N}\right)^{l_{max}^j}}{P_j} \ge \min_j \frac{\left(1 - \frac{1}{N}\right)^{l_{max}^j}}{P_j} = \epsilon \tag{32}$$

$$\Psi(x) = \max_{j} \frac{h_{j}(x)}{\tau_{j}} \Rightarrow \mathbb{P}(\Psi(X) \ge 1) = \mu$$
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Variance ratio :

$$\frac{\frac{\mu}{n}\left(\frac{\bar{\mu}}{\epsilon} - \mu\right)}{\mu^{2}\left(\mu^{-\frac{1}{kN}} - 1\right)} = \frac{1}{n} \frac{\frac{1}{\epsilon}\frac{\bar{\mu}}{\mu} - 1}{\mu^{-\frac{1}{kN}} - 1} \underset{N\gg_{1}}{\approx} \frac{1}{n} \frac{\frac{1}{\epsilon}\frac{\bar{\mu}}{\mu} - 1}{\frac{-\log(\mu)}{kN}} = \frac{kN}{n} \frac{\frac{1}{\epsilon}\frac{\bar{\mu}}{\mu} - 1}{-\log(\mu)}$$
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Computation cost :

$$\frac{-N\log(N)\log(P)J}{-kN\log(kN)\log(\mu)J} = \frac{\log(N)\log(P)}{k\log(kN)\log(JP)} = \frac{1}{k} \frac{1}{1 + \frac{\log(k)}{\log(N)}} \frac{1}{1 + \frac{\log(J)}{\log(P)}}$$
(35)



Numerical examples - Circumscribed Polygon

 $\mathcal{P}(J,\tau)\subset\mathbb{R}^2$ a regular polygon of $J\geq 3$ sides circumscribed around the circle of radius $\tau>0$

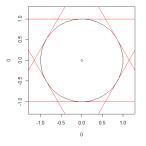


Figure: Circumscribed polygon for J = 6

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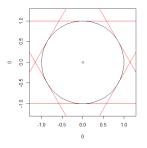
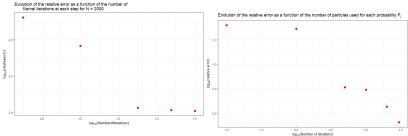


Figure: Circumscribed polygon for J = 6

$$\bullet \ 1 \geq \frac{\mathbb{P}(X \in H)}{\exp(\frac{-\tau^2}{2})} \geq 1 - \frac{\pi^2 \tau^2}{6J^2}$$

• For $J = 360, \tau = 6$, we have $\mu \approx 1.52 \times 10^{-8}$





(a) Relative error on the estimate $\hat{\mu}$ of the ALOE algorithm for different numbers of kernel iterations at each step in the multilevel splitting part of the algorithm

(b) Relative error on the estimate $\hat{\mu}$ of the ALOE algorithm in logarithmic scale for different numbers N of particles

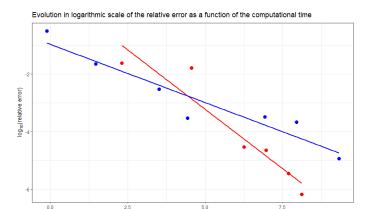
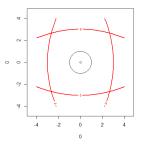


Figure: Relative error as a function of the computational time. The red dots are obtained from the new ALOE estimator and the blue ones from the more intuitive one. The lines are the linear regressions performed on these sets of points

log₁₀(computation time)

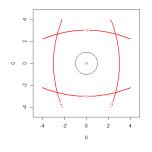
Numerical examples - Rare events with quadratic curves boundaries

• $H_j = \{(x, y) : c(x \sin(\theta_j) + y \cos(\theta_j))^2 + (x \cos(\theta_j) - y \sin(\theta_j)) \ge \tau_j\}$ where c a constant and $0 \le \theta_j \le 2\pi$



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We run our numerical example with :

- θ_j goes from 0 to 2π by step of $\frac{\pi}{8}$, J=16
- $\tau_i = \tau = 4$

For N=3000, the new ALOE estimator gives $\hat{\mu}=2.854815\times 10^{-7}$



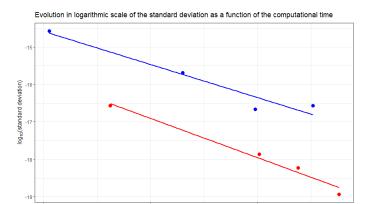


Figure: Standard deviation of $\hat{\mu}$ as a function of the computation time. The red dots are obtained from the new ALOE estimator and the blue ones from the more intuitive one. The lines are the linear regressions performed on these sets of points

log₁₀(computation time)