RARE EVENT SIMULATION

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Abstract : This paper deals with estimations of probabilities of rare events using fast simulation based on the splitting method. In this technique, the sample paths are split into multiple copies at various stages in the simulation. Our aim is to optimize the algorithm and to obtain a precise confidence interval of the estimator using branching processes. The numerical results presented suggest that the method is reasonably efficient.

Key words : rare event, simulation, RESTART, splitting method, variance, Laplace transform, Galton-Watson, branching process.

1 Introduction

The analysis of rare events is of great importance in many fields because of the risk associated to the event. Their probabilities are often about 10^{-9} to 10^{-12}. One can use many ways to study them : the first is statistical analysis, based on the standard extreme value distributions but this needs a long observation period (see Aldous [1]), the second is modelling which leads to estimating the rare event probability either by analytical approach (see Sadowsky [10]), or by simulation.

In this paper we focus on the simulation approach based on Monte-Carlo method. Nevertheless crude simulation is impracticable for estimating such small probabilities : to estimate probabilities of order 10^{-10} with acceptable confidence would require the simulation of at least 10^{12} events (which corresponds to the occurrence of one hundred rare events).

To overcome these limits, fast simulation techniques are applied. In particular, importance sampling (IS) is a refinement of Monte-Carlo methods. The main idea of IS is to make the occurrence of the rare event more frequent. More precisely IS consists in selecting a change of measure that minimizes

the variance of the estimator. Using another method based on particles systems, Cerou et al. [3] give theoretical results on the convergence of this kind of algorithm. In this paper, we deal with the RESTART (REpetitive Simulation Trials After Reaching Thresholds) algorithm presented by Villen-Altamirano in [11] and based on splitting. The basic idea of splitting is to partition the space-state of the system into a series of nested subsets and to consider the rare event as the intersection of a nested sequence of events. When a given subset is entered by a sample trajectory, random retrials are generated from the initial state corresponding to the state of the system at the entry point. Thus the system trajectory has been split into a number of new sub-trajectories. However the analysis of the RESTART model arises numerous difficulties lying on the lack of hypothesis and the complexity of formulae.

In this paper, we build a simple model of splitting for which we are able to derive precise conclusions. It is based on the same idea : before entering the rare event A there exists intermediate states visited more often than A by the trajectory : $A = B_{M+1} \subset B_M \subset .. \subset B_1$. Let $P_i = \mathbb{P}(B_i|B_{i-1})$ $i = 2, .., M+1$ and $P_1 = \mathbb{P}(B_1)$. The fact that a sample trajectory enters B_i is represented by a Bernoulli trial. Every time a sample trajectory enters a subset B_i, $i = 1, .., M$ it is divided in a number R_i of sub-trajectories starting from level i. More precisely we generate N random variables with common law Bernoulli $Ber(P_1)$ and check whether the subset B_1 is reached or not. If so, we duplicate the trials in R_1 retrials of $Ber(P_2)$ and check whether the subset B_2 is reached or not... Thus

$$P = \mathbb{P}(A) = P_1..P_{M+1} \tag{1}$$

and an unbiased estimator of P is

$$\hat{P} := \frac{1}{N}\sum_{i=1}^{N} \hat{P}_i = \frac{N_A}{NR_1..R_M} \tag{2}$$

where $\hat{P}_i$ are i.i.d., N_A is the number of trials that reach A during the simulation and N the number of particles initially generated. An optimal algorithm is chosen via the minimization of the variance of $\hat{P}$ for a given budget. For this, we have to describe the cost of a given simulation : each time a particle is launched, it generates an average cost which is supposed here to be a function h of the transition probability. Therefore, the (average) cost is

$$C = N\sum_{i=0}^{M} r_i h(P_{i+1}) P_{i|0} \tag{3}$$

where $r_i = R_1..R_i$, $i = 1, .., M$, $r_0 = 1$ and $P_{i|0} = P_1..P_i$, $i = 1, .., M+1$,

$P_{0|0} = 1$. Then, the optimal algorithm is described by

$$\begin{cases} P_i = P^{\frac{1}{M+1}} & i = 1, .., M+1 \\ R_i = \frac{1}{P_i} & i = 1, .., M \\ N = \frac{C}{(M+1)h(P^{1/M+1})}. \end{cases} \tag{4}$$

and M is given by $M = [\frac{\ln P}{y_0}] - 1$ or $M = [\frac{\ln P}{y_0}]$ where y_0 is the solution of an equation described below (see Eq.(30)). The optimal sampling number is independent of the budget and this former only determines the optimal number of independent particles firstly generated. In the special case of $h = 1$,

$$M = [-0.6275 \ln P] - 1 \ \text{ or } \ [-0.6275 \ln P], \qquad R_i \approx 5 \ \text{ and } \ P_i \approx \frac{1}{5} \tag{5}$$

Thus the optimal sampling number and the optimal transition probabilities are independent of the rare event probability. For example, if $P = 10^{-12}$ and $C = 10^3$, $M = 16$, $P_i \approx 0.2$, $R_i = 5$ and $N = 59$.

Example 1.1 *To analyse the behavior of the different implementations described above, we perform a simulation experiment using these methods. We consider a queuing network and we want to estimate the occupancy of finite buffer queuing system $M/M/1/C_0$. The results are presented in Figure 1. As*

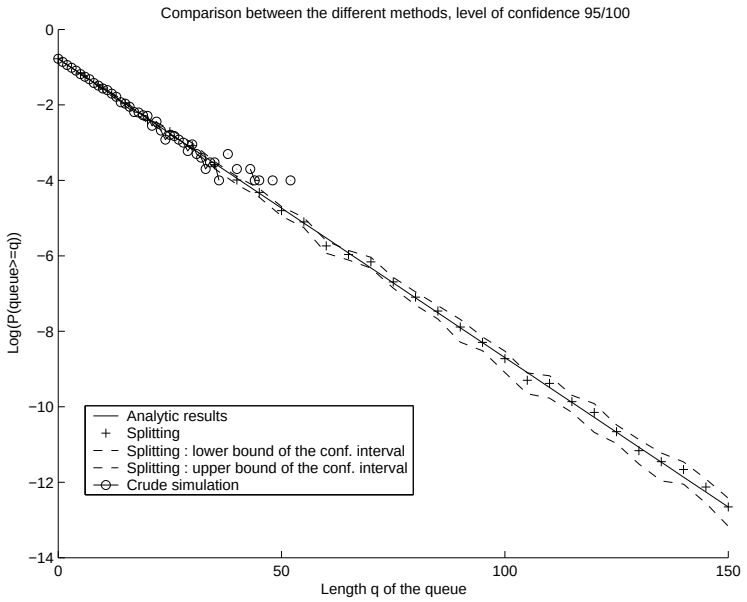


FIG. 1 – Comparison between the different methods-Queuing theory model

expected and since we proceed for a given cost C ($C = 10^4$), crude simulation stops after a few iterations, the number of samples run at the beginning being not sufficient. However note that splitting simulation and theoretical analysis give very close results.

Example 1.2 *This model can be applied to approximate counting, see Jerrum and Sinclair [7] and Diaconis and Holmes [5]. Given a positive real vector $\mathbf{a} = (a_i)_{i=1}^n$ and a real number b, we want to estimate the number of $0-1$ vectors $\mathbf{x} = (x_i)_{i=1}^n$ s.t.*

$$\mathbf{a}.\mathbf{x} := \sum_{i=1}^{n} a_i x_i \leq b \tag{6}$$

For more details see 3.2.

Remark 1.1 *Hereafter we shall take all the R_i equal to R and all the P_i equal to $P_0 = \frac{1}{R}$. Thus $RP_0 = 1$.*

The aim of the paper is to give a precise confidence interval of $\hat{P}$. The bound involving the variance of $\hat{P}$ and given by the Markov inequality is not precise enough. Therefore, as done in the theory of large deviations, we introduce the Laplace transform of $\hat{P}_1$ which can be rewritten as $\mathbb{E}(e^{\lambda \hat{P}_1}) = P_0 f_M(e^{\lambda/R^M}) + 1 - P_0$ where f_M is the M-th functional iterate of a $Bin(R, P_0)$ generating function (g.f.). The elementary theory of branching processes leads to precise bounds of f_M and to a precise confidence interval that we may compare to the confidence interval if we only use the variance. For example, for $P = 10^{-9}$, $C = 10^8$ and $\alpha = 0.02$, the variance gives a bound about 10^{-2} and the Laplace transform gives a bound approximatively 10^{-12}.

The paper is organized as follows. Section 2 describes the importance splitting model, presents our model and goals : the analysis of the behavior of the probability P of a rare event and introduces an estimator $\hat{P}$ of P. Section 3 is dedicated to the optimization of the algorithm. In section 4, we obtain a precise confidence interval of the estimator via branching processes. Finally in section 5, we conclude and discuss the merits of this approach and potential directions for further researches.

2 Importance splitting model

Our goal is to estimate the probability of a rare event A corresponding for example to the hit of a certain level L by a process $X(t)$. The main hypothesis is to suppose that before entering the target event there exists intermediate states visited more frequently than A by the trajectory : thus define a sequence of sets of states B_i such as $A = B_{M+1} \subset B_M \subset .. \subset B_1$,

which determines a partition of the state space into regions $B_i - B_{i+1}$ called *importance regions*. In general, these sets are defined through a function Φ called *importance function* from the state space to $\mathbb{R}$ such that for all i, $B_i = \{\Phi \leq T_i\}$ for some value T_i called *thresholds* with $T_1 \leq T_2 \leq .. \leq T_M \leq L$.

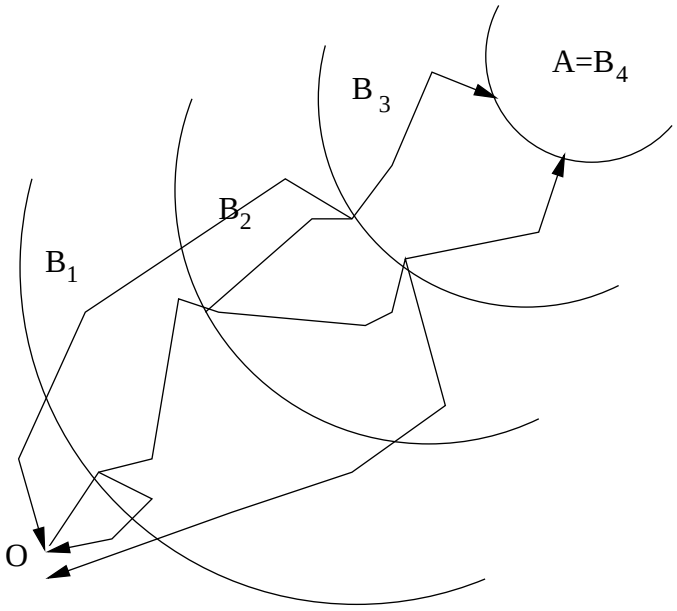


FIG. 2 – Splitting model

In this model a more frequent occurrence of the rare event is achieved by performing a number of simulation retrials when the process enters regions where the chance of occurrence of the rare event is higher. The fundamental idea consists in generating N Bernoulli $Ber(P_1)$ and check whether the subset B_1 is reached or not. If so, we duplicate the trials in R_1 retrials of Bernoulli $Ber(P_2)$ and check whether the subset B_2 is reached or not... If none of the higher levels are reached, the simulation stops.

Thus by the Bayes formula,

$$\begin{aligned} \mathbb{P}(A) &= \mathbb{P}(A|B_M)\mathbb{P}(B_M|B_{M-1})..\mathbb{P}(B_2|B_1)\mathbb{P}(B_1) \quad (7) \\ &:= P_{M+1}P_M..P_2P_1. \quad (8) \end{aligned}$$

Then P is the product of $M+1$ quantities (conditional probabilities) that are easier to estimate and with more accuracy than the probability P of the rare event itself, for a given simulation effort.

The estimator $\hat{P}$ of P defined in (2) can be rewritten as

$$\hat{P} = \frac{1}{NR_1..R_M} \sum_{i_0=1}^{N} \sum_{i_1=1}^{R_1} .. \sum_{i_M=1}^{R_M} \mathbf{1}_{i_0} \mathbf{1}_{i_0 i_1} .. \mathbf{1}_{i_0 i_1 .. i_M} \quad (9)$$

where $\mathbf{1}_{i_0 i_1..i_j}$ represents the result of the j-th trial. In that case,

$$\hat{P}_{i_0} = \frac{1}{R_1..R_M} \sum_{i_1=1}^{R_1} .. \sum_{i_M=1}^{R_M} \mathbf{1}_{i_0} \mathbf{1}_{i_0 i_1} .. \mathbf{1}_{i_0 i_1..i_M} \tag{10}$$

Moreover, we define $\mathbb{P}(A)$ as the probability of reaching A and we suppose that the process forget the past after reaching a level ; this happens as soon as the process is Markov.

3 Study of the variance and optimization

3.1 Variance of the estimator

Firstly, note that $\hat{P}$ is unbiased since

$$E(\hat{P}) = \mathbb{E}(\frac{N_A}{NR_1..R_M}) = \frac{1}{NR_1.R_M} \sum_{i_0=1}^{N} \sum_{i_1=1}^{R_1} .. \sum_{i_M=1}^{R_M} \mathbb{E}(\mathbf{1}_{i_0} \mathbf{1}_{i_0 i_1} .. \mathbf{1}_{i_0 i_1..i_M}) = P \tag{11}$$

As done in [11], the variance of the estimator $\hat{P}$ is derived by induction and the variance for k thresholds is given by

$$\mathrm{var}(\hat{P}^{(k)}) = \frac{(P_1..P_{k+1})^2}{N} \Big[\sum_{i=0}^{k} \frac{1}{r_i} (\frac{1}{P_{i+1|0}} - \frac{1}{P_{i|0}}) \Big] \tag{12}$$

where $\hat{P}^{(k)}$ represents the estimator of P in a simulation with k thresholds.

Clearly the formula holds in straightforward simulation i.e. when $k = 0$, since $\hat{P}$ is a renormalized sum of i.i.d. Bernoulli variables with parameter P.

To go from k to $k+1$, assume (12) thus we have to prove that this formula holds for $k + 1$ thresholds. First of all note that for all X and Y random variables which are independent given the set B and X $\sigma(B)$-measurable we have

$$\mathrm{var}(XY) = \ \mathrm{var}(X)\ \mathrm{var}(Y) + \ \mathrm{var}(X)\mathbb{E}(Y)^2 + \ \mathrm{var}(Y)\mathbb{E}(X)^2 \tag{13}$$

Now let

$$X_{i_0} = \mathbf{1}_{i_0}, \qquad Z_{i_0} = \frac{1}{R_1..R_{k+1}} \sum_{i_1=1}^{R_1} .. \sum_{i_{k+1}=1}^{R_{k+1}} \mathbf{1}_{i_0 i_1} .. \mathbf{1}_{i_0 i_1..i_{k+1}} \tag{14}$$

The random variables X_{i_0} are i.i.d. with common law $Ber(P_1)$ and conditionally at the event B_1, X_{i_0} and Z_{i_0} are independent. Note that each Z_{i_0} is the estimator of P in a model with k thresholds, T_2 to T_{k+1} for the trajectory issued from the success of X_{i_0}. Thus

$$\mathbb{E}(Z) = P_2..P_{k+2} \tag{15}$$

and by the induction's hypothesis,

$$\mathrm{var}(Z) = (P_2..P_{k+2})^2[\sum_{i=1}^{k+1} \frac{1}{R_1..R_i}(\frac{1}{P_{i+1|1}} - \frac{1}{P_{i|1}})] \tag{16}$$

So applying (13) with $X \sim Ber(P_1)$ and $Z \sim Z_{i_0}$, we have

$$\mathrm{var}(\hat{P}^{(k+1)}) := \frac{1}{N^2}\ \mathrm{var}(\sum_{i_0=1}^{N} X_{i_0} Z_{i_0}) \tag{17}$$

$$= \frac{P_1}{N}[\ \mathrm{var}(Z) + (1-P_1)\mathbb{E}(Z)^2] \tag{18}$$

$$= \frac{(P_1 P_2..P_{k+2})^2}{N}\Big[\sum_{i=0}^{k+1} \frac{1}{r_i}(\frac{1}{P_{i+1|0}} - \frac{1}{P_{i|0}})\Big] \tag{19}$$

Thus for M thresholds

$$\mathrm{var}(\hat{P}) = \frac{P^2}{N}\Big[\sum_{i=0}^{M} \frac{1}{r_i}(\frac{1}{P_{i+1|0}} - \frac{1}{P_{i|0}})\Big] \tag{20}$$

Remark 3.1 *The induction principle has a concrete interpretation : if in a simulation with M steps, the retrials generated in the first level are not taken into account except one that we call* main trial*, we have a simulation with $M-1$ steps.*

3.2 Optimization of the parameters

As said in the introduction our aim is to minimize the variance for a fixed budget, giving optimal values for N,R_1,..,R_M, $P_1,..,P_{M+1}$ and M. Therefore, we have to describe the cost of a given simulation : each time a particle is launched, it generates an average cost function h. We assume that

- the cost h for a particle to reach B_i starting from B_{i-1} depends only on P_i (and not on the starting level),
- h is decreasing in x (which means that the smaller the transition probability is, the harder the transition is and the higher is the cost),
- h is non-negative,
- h converges to a constant (in general small) when x converges to 1.

The (average) cost is then

$$C = \mathbb{E}(Nh(P_1) + R_1 N_1 h(P_2) + R_2 N_2 h(P_3) + .. + R_M N_M h(P_{M+1})) \tag{21}$$

where N_i is the number of trials that have reached threshold i. Finally,

$$C = N\sum_{i=0}^{M} r_i h(P_{i+1}) P_{i|0} \tag{22}$$

Example 3.1 *We want to study the model of the simple random walk on* $\mathbb{Z}$ *starting from* 0 *that we kill as soon as it reaches the level* -1 *or* k *(success if we reach* k*, failure otherwise).*
So let X_n *such that* $X_0 = 0$ *and* $X_n = \sum_{i=1}^{n} Y_n$ *where* $\{Y_n\}$ *is a sequence of random variables valued in* $\{-1, 1\}$ *with* $\mathbb{P}(Y_n = 1) = \mathbb{P}(Y_n = -1) = \frac{1}{2}$ *and define* $T_k = \inf\{n \geq 0 \ : \ X_n = -1 \text{ or } k\}$.
One can easily check that X_n *and* $X_n^2 - n$ *are martingales. By the Doob's stopping theorem,* $\mathbb{E}(X_{T_k}) = 0$ *and* $\mathbb{E}(X_{T_k}^2) = \mathbb{E}(T_k)$ *which yields to*

$$p := \mathbb{P}(X_{T_k} = k) = \frac{1}{k+1} \quad \text{and} \quad \mathbb{E}(T_k) = k = \frac{1}{p} - 1 \tag{23}$$

i.e. the cost needed to reach the next level is $\frac{1}{p} - 1$ *if* p *is the success probability.*

To minimize the variance of $\hat{P}$, the optimal values are derived in three steps :

1. The optimal values of $N, R_1, .., R_M$ are derived when we consider that $P_1, .., P_{M+1}$ are constant (i.e. the thresholds B_i are fixed).
2. Replacing these optimal values in the variance, we derive the optimal transition probabilities : $P_1, .., P_{M+1}$.
3. Replacing these optimal values in the variance, we derive M the optimal number of thresholds.

Optimal values for $N, R_1, .., R_M$**.** Using the method of Lagrange multipliers, we get

$$R_i = \frac{r_i}{r_{i-1}} = \sqrt{\frac{h(P_i)}{h(P_{i+1})}}\sqrt{\frac{1}{P_i P_{i+1}}}\sqrt{\frac{1-P_{i+1}}{1-P_i}} \quad i = 1, .., M \tag{24}$$

$$N = \frac{1}{\sqrt{h(P_1)}} \frac{C\sqrt{1/P_1 - 1}}{\sum_{i=1}^{M+1} \sqrt{h(P_i)}\sqrt{\frac{1}{P_i} - 1}} \tag{25}$$

Optimal values for $P_1, .., P_{M+1}$**.** Thus the variance becomes

$$\text{var}(\hat{P}) = \frac{P^2}{C}\Big[\sum_{i=1}^{M+1} \sqrt{h(P_i)}\sqrt{\frac{1}{P_i} - 1}\Big]^2 \tag{26}$$

Proceeding as previously under the constraint $P = P_1..P_{M+1}$, we obtain that all the P_i's satisfy $2\sqrt{C}\lambda\sqrt{h(x)(\frac{1}{x} - 1)} = h'(x)(1-x) - \frac{h(x)}{x}$. If we assume that there exists a unique solution to this equation, we have $P_i = g(\lambda)$, hence $P = g(\lambda)^{M+1}$ and $g(\lambda) = P^{\frac{1}{M+1}}$.

Finally $$P_i = P^{\frac{1}{M+1}} \quad i = 1, .., M+1 \tag{27}$$

Optimal value for M. The optimal values for $P_1, .., P_{M+1}$ imply that the optimal R_i become $1/P_i$, $i = 1, .., M$ and thus

$$\mathrm{var}(\hat{P}) = \frac{P^2}{C}(M+1)^2 h(P^{1/M+1})(P^{-1/M+1} - 1) \tag{28}$$

that we want to minimize in M. Remark that $R_i P_i = 1$. Let

$$f(M) = \frac{P^2}{C}(M+1)^2 h(P^{1/M+1})(P^{-1/M+1} - 1), \tag{29}$$

whose derivative cancels in

$$F(y) := (2(1-e^y)+y)h(e^y) - y(1-e^y)e^y h'(e^y) = 0, \text{ with } y = \frac{\ln P}{M+1} \tag{30}$$

In general, this does not give an integer. We have $y_0 = \frac{\ln P}{M+1}$ i.e. $M+1 = [\frac{\ln P}{y_0}]$ or $[\frac{\ln P}{y_0}] + 1$. Let $\frac{\ln P}{y_0} = n + x$ with $0 < x < 1$. Then

- if we take $M + 1 = n$, $y = \frac{\ln P}{n}$,
- if we take $M + 1 = n + 1$, $y = \frac{\ln P}{n+1}$.

and the value of the ratio $\rho := \frac{f(n-1)}{f(n)}$ gives the best choice for M :

- if $\rho < 1$, $M = n - 1$,
- if $\rho > 1$, $M = n$.

Thus the optimal number of thresholds is given by $M = [\frac{\ln P}{y_0}] - 1$ or $M = [\frac{\ln P}{y_0}]$ where y_0 solves $F(y) = 0$. Then M minimizes

$$\mathrm{var}(\hat{P}) = \frac{P^2}{C}(\ln P)^2 y^{-2} h(e^y)(e^{-y} - 1) \tag{31}$$

Example 3.2 *For $h = 1$, we have to solve $y = 2(e^y - 1)$. We get $y_1 = 0$ and $y_2 \approx -1.5936$. y_2 is a minimum and the optimal value of M is*

$$M = [-0.6275 \ln P] - 1 \quad or \quad [-0.6275 \ln P] \tag{32}$$

With $P = 10^{-k}$,

k	n	*ratio*(ρ) >1,<1	M	k	n	*ratio*(ρ) >1,<1	M
1	*1*	>	*1*	*6*	*8*	>	*8*
2	*2*	>	*2*	*9*	*13*	<	*12*
3	*4*	<	*3*	*12*	*17*	<	*16*
4	*5*	>	*5*	*15*	*21*	>	*21*
5	*7*	<	*6*	*18*	*26*	<	*25*

Note that M increases while P decreases and with this value of M, each R_i and P_i become

$$R_i \approx 5 \quad \text{and} \quad P_i \approx \frac{1}{5}. \tag{33}$$

Thus the optimal sampling number and the optimal transition probabilities are independent of the rare event probability.
Moreover, asymptotically, $M = n = [\frac{\ln P}{y_0}] - 1$, thus

$$P_i = P^{\frac{1}{M+1}} = e^{\frac{\ln P}{M+1}} = e^{y_0} \quad \text{and} \quad P = e^{-(n+1)|y_0|} \tag{34}$$

Application 3.1 *In approximate counting, remind that the goal is to estimate the number of Knapsack solutions i.e. the cardinal of* Ω *defined by*

$$\Omega := \{x \in \{0,1\}^n \ : \ \mathbf{a}.\mathbf{x} := \sum_{i=1}^{n} a_i x_i \leq b\}$$

for given positive real vector $\mathbf{a} = (a_i)_{i=1}^n$ *and real number* b*. We might try to apply the Markov Chain Monte-Carlo method (MCMC) [9] : construct a Markov chain* $\mathcal{M}_{Knap}$ *with state space* $\Omega = \{x \in \{0,1\}^n : \mathbf{a}.\mathbf{x} \leq b\}$ *and transitions from each state* $x = (x_1, .., x_n) \in \Omega$ *defined by*

- *with probability* $\frac{1}{2}$ *let* $y = x$ *; otherwise*
- *select* i *uniformly at random in* $\{1, .., n\}$ *and let* $y' = (x_1, .., x_{i-1}, 1 - x_i, x_{i+1}, .., x_n)$
- *if* $a.y' \leq b$ *then let* $y = y'$ *else let* $y = x$

the new state is y*. This random walk on the hypercube truncated by the hyperplane* $\mathbf{a}.\mathbf{x} = b$ *converges to the uniform distribution over* Ω*. This suggests a procedure for selecting Knapsack solutions almost uniformly at random. Starting in state* $(0, .., 0)$*, simulate* $\mathcal{M}_{Knap}$ *for sufficiently many steps that the distribution over states is "close"*[1] *to uniform, then return the current state. Of course sampling over* Ω *is not the same as estimating the size of* Ω*. But the first task leads to the second.*

Keep on taking the vector $\mathbf{a}$ *fixed but allow* b *to vary. Note* $\Omega(b)$ *and* $\mathcal{M}_{Knap}(b)$ *instead of* Ω *and* $\mathcal{M}_{Knap}$ *to emphasize on the dependence on* b*. Assume without loss of generality that* $a_1 \leq .. \leq a_n$ *and define* $b_1 = 0$ *and* $b_i = \min\{b, \sum_{i=1}^{i-1} a_j\}$*. One can check that*

$$|\Omega(b_{i-1})| \leq |\Omega(b_i)| \leq (n+1)|\Omega(b_{i-1})| \tag{35}$$

Now write

$$|\Omega(b)| = |\Omega(b_{n+1})| = \frac{|\Omega(b_{n+1})|}{|\Omega(b_n)|} \frac{|\Omega(b_n)|}{|\Omega(b_{n-1})|} .. \frac{|\Omega(b_2)|}{|\Omega(b_1)|} |\Omega(b_1)| := \rho_n^{-1} .. \rho_1^{-1} \tag{36}$$

[1] The problem is to bound the number of steps necessary to make the Markov chain $\mathcal{M}_{Knap}(b)$ "close" to stationarity. More precisely, we need a bound of the *mixing time* :

$$\tau_{mix}(\nu) := \min\{t : \Delta_x(t') \leq \nu \text{ for all } t' \geq t\}$$

where $\Delta_x(t) = \max_{S \subset \Omega} |P^t(x, S) - \Pi(S)|$ and Π the stationary distribution. In [7], it is shown that $\mathcal{O}(n^{9/2+\nu})$ steps suffice.

The ratio $\rho_i = \frac{|\Omega(b_i)|}{|\Omega(b_{i+1})|}$ *may be estimated by sampling almost uniformly from* $\Omega(b_{i+1})$ *using the Markov chain* $\mathcal{M}_{Knap}(b_{i+1})$ *and computing the fraction of the samples that lie within* $\Omega(b_i)$.

Now take $a = [1, 2, 3, 4]$, $b = 3$, $h = 1$, $R = 5$ *and* $C = 2600$. *We chose the levels as proposed : first define* $b_1 = 0$, $b_2 = 1$, $b_3 = 3$, $b_4 = 3$ *and* $b_5 = b$, *secondly* $B_0 = \Omega$, $B_1 = \Omega(b_4)$, $B_2 = \Omega(b_3)$, $B_3 = \Omega(b_2)$ *and* $B_4 = \Omega(b_1)$. *Thus here* $M = n - 1$, $N = C/n$ *and* $n_{step} = 1020$. *Obviously Card*$(\Omega) = 5$. *We run 3 different simulations : the first suggested in [7] consisting in estimating the n ratios independently, the crude and splitting ones. We obtain different estimations for Card*(Ω) *:*

- *estimation by crude simulation* $= 4.088$,
- *estimation by the n ratios independently* $= 5.44$,
- *and estimation by splitting* $= 5.019$.

Even though the levels are not optimal, splitting carries out an improvement.

Let us describe briefly the possible solutions of (30). Remind we want to solve (30) i.e. if $z = e^y$ and $z \neq 0, 1$

$$H(z) := \frac{h'(z)}{h(z)} = \frac{1}{z}\left(\frac{2}{\ln z} + \frac{1}{1-z}\right) =: \frac{l'(z)}{l(z)} =: L(z) \tag{37}$$

First of all, let z_0 be the solution of $2(z-1) = \ln z$. Since $h' \leq 0$, H is negative and a quick survey shows that L is positive on $]0, z_0[$ and negative on $]z_0, 1[$. As a consequence, the solutions of (37) lie in $]z_0, 1[$, if there exist. Thus solving (30) is equivalent to study the intersections between H and L. A quick survey of these functions shows that we have 2 cases (see Figure 3) :

- case 1 : an odd number of intersections between L and H

$$\Leftrightarrow \quad H(z) > L(z) \quad \text{near} \quad 1 \tag{38}$$

$$\Leftrightarrow \quad h''(1) < 0 \tag{39}$$

- case 2 : an even number of intersections or 0 between L and H

Note that $y = 0$ is a solution of (30). In case 1, it corresponds to a maximum and in case 2, to a minimum. And the second case is excluded since we made the assumption $h(1) > 0$.

Remark 3.2 *The solution* $y = 0$ *corresponds to the following optimal values*

$$M = \infty, \quad P_i = 1, \quad R_i = 1, \quad N \sim_{M\to\infty} \frac{C}{(M+1)h(1) + \ln(P)h'(1)} \tag{40}$$

But $P_i = 1$ *implies that* $P = 1$ *and* $R_i = 1$ *means that we just perform a crude simulation.*

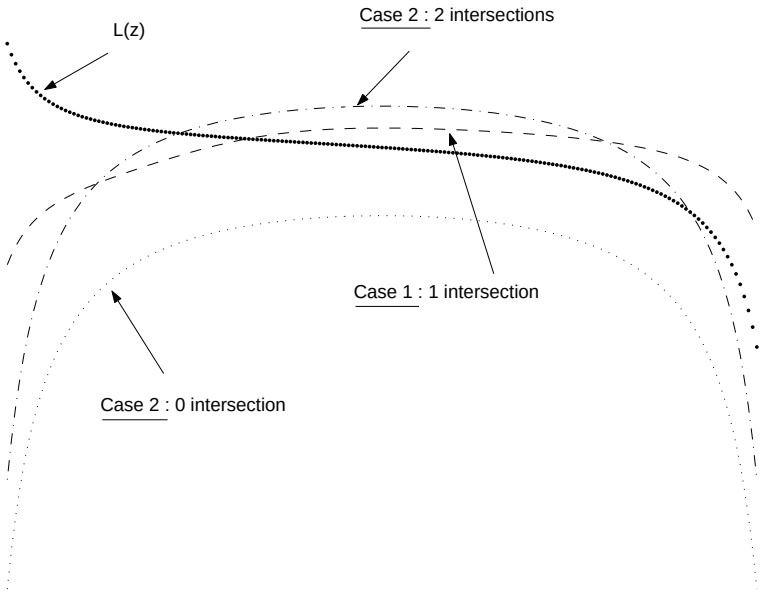


FIG. 3 – Behavior of H and L

Example 3.3 *Here* $P = 10^{-12}$ *and* $C = 10^4$.
1) In Example 3.1, $h(1) = 0$ *and we are in the 2nd case : the unique solution* $y = 0$ *is the minimum.*
2) Let $h(x) = \frac{1}{x} - 8x^2 + 12x - 5$. $h(1) = 0$ *and we are in the first case :* $y = 0$ *and* $y \approx -0.9919$ *are the solutions.* $y = 0$ *is the maximum and the other solution the minimum. Taking* $y \approx -0.9919$*, we obtain*

$$M = 26, \quad P_0 \approx 0.3594, \quad R \approx 2.7826 \quad \textit{and} \quad N \approx 22.9 \tag{41}$$

and we can take $R = 3$ *and* $N = 23$.
3) Let $h(x) = (\frac{1}{x} - 1)^2 e^{6x}$. $h(1) = 0$ *and we are in the 2nd case :* $y = 0$*,* $y_1 \approx -0.4612$ *and* $y_2 \approx -0.5645$ *are the solutions.* $y = 0$ *is the minimum and the second solution the maximum.*
4) Let $h(x) = \frac{1}{x}$*. Here* $h(1) = 1$*. We aim at solving (30) whose solutions are* $y = 0$ *and* $y \approx -0.6438$*. Taking* $y \approx -0.6438$*, we obtain*

$$M = 41, \quad P_0 \approx 0.5179, \quad R \approx 1.9307 \quad \textit{and} \quad N \approx 34.5 \tag{42}$$

and we can take $R = 2$ *and* $N = 34$.

Thus the control of the variance of $\hat{P}$ gives a crude confidence interval for P. Indeed, we get

$$\begin{aligned}
\mathbb{P}(\frac{|\hat{P}-P|}{P} \geq \alpha) &\leq \frac{1}{P^2\alpha^2}\mathbb{E}((\hat{P}-\mathbb{E}(\hat{P}))^2) && (43)\\
&\leq \frac{1}{\alpha^2 C}[(M+1)^2(P^{-1/M+1}-1)h(P^{\frac{1}{M+1}})] && (44)\\
&\approx \frac{4(M+1)}{\alpha^2 N}h(P^{\frac{1}{M+1}}) && (45)
\end{aligned}$$

This estimation is in general useless. For example, for $h=1$, $M=12$ and $\alpha=10^{-2}$, the upper bound becomes $\approx \frac{5.10^5}{N}$. To obtain a bound lower than 1, we need $N \geq 5.10^5$. To improve it, we shall use Chernoff's bounding method instead of Markov inequality : for all $\lambda > 0$,

$$\begin{aligned}
\mathbb{P}(\hat{P} \geq P(1+\alpha)) &= \mathbb{P}(\frac{1}{N}\sum_{i=1}^{N}\hat{P}_i \geq P(1+\alpha)) && (46)\\
&= \mathbb{P}(e^{\lambda\sum_{i=1}^{N}\hat{P}_i} \geq e^{\lambda NP(1+\alpha)}) && (47)\\
&\leq e^{-\lambda NP(1+\alpha)}\mathbb{E}(e^{\lambda\hat{P}_1})^N && (48)\\
&\leq e^{-N[\lambda P(1+\alpha)-\psi(\lambda)]} && (49)
\end{aligned}$$

where $\psi(\lambda) = \mathbb{E}(e^{\lambda\hat{P}_1})$ is the log-Laplace of $\hat{P}_1$. Optimization on $\lambda > 0$ provides

$$\mathbb{P}(\hat{P} \geq P(1+\alpha)) \leq e^{-N\sup_{\lambda>0}[\lambda P(1+\alpha)-\psi(\lambda)]} \quad (50)$$

Similarly, $\mathbb{P}(\hat{P} \leq P(1+\alpha)) \leq e^{-N\sup_{\lambda<0}[\lambda P(1-\alpha)-\psi(\lambda)]}$
Let ψ^* be the Crämer transform of ψ : $\psi^*(\tau) = \sup_\lambda[\lambda\tau - \psi(\lambda)]$. Thus

$$\begin{aligned}
\mathbb{P}(\frac{|\hat{P}-P|}{P} \geq \alpha) &\leq e^{-N\psi^*(P(1-\alpha))} + e^{-N\psi^*(P(1+\alpha))} && (51)\\
&\leq 2e^{-N\min(\psi^*(P(1-\alpha)),\psi^*(P(1-\alpha)))} && (52)
\end{aligned}$$

So we aim at obtaining an accurate lower bound of ψ^*.

Remark 3.3 *Although we would therefore like to take R_i so that $R_iP_i = 1$, we are constrained to choose R_i to be a positive integer. Hereafter we suppose that we are in the good case where $R_i = 1/P_i$ is an integer.*

4 Laplace transform of $\hat{P}_1$

To study the Laplace transform of $\hat{P}_1$, we turn to the theory of branching processes (see Harris [6], Lyons [8] and Athreya and Ney [2]). More precisely we consider our splitting model as a Galton-Watson process, the thresholds representing the different generations.

4.1 Description of the model and first results

We consider a Galton-Watson model (Z_n) where the size of the n-th generation Z_n is the number of particles that have reached the level B_n, with one particle run at the beginning. Then $Z_0 = 1$ and Z_n satisfies the following recurrence relation

$$Z_{n+1} = \sum_{i=1}^{Z_n} X_i^n \tag{53}$$

where X_i^n is the number of particles among R_i that have reached the $n+1$-th level. The $(X_i^n)_{n\geq 1}$ are i.i.d. with common law Binomial with parameters (R_n, P_{n+1}) and $X_i^0 \sim Ber(P_1)$. Take the optimal values of 3.2 :

$$R_i = R \;\; i = 1, .., M, \qquad P_i = P_0 \;\; i = 1, .., M+1. \tag{54}$$

Let $f(s) = \mathbb{E}(s^{Z_1})$ the g.f. of Z_1. Then the g.f. of Z_n is the n-th iterate of f. Since $\hat{P}_1 = \frac{1}{R^M} Z_{M+1}$, we get

$$\mathbb{E}(e^{\lambda \hat{P}_1}) = \mathbb{E}(e^{\frac{\lambda}{R^M} Z_{M+1}}) = g(f_M(e^{\lambda/R^M})) = g(f^{oM}(e^{\lambda/R^M})) \tag{55}$$

where g is the g.f. of a $Ber(P_0)$ and f the one of a $Bin(R, P_0)$. Thus we are interested in the expression of f_M the M-th functional iterate of f.

Here $m = \mathbb{E}(Z_1) = RP_0 = 1$, so we are in the critical case of the branching process that ensures us the algorithm of the simulation stops with probability one when $M \to \infty$, see [6], since if $f^{(3)}(1) < \infty$,

$$\lim_{n\to\infty} \mathbb{P}(\frac{2Z_n}{nf"(1)} > u | Z_n \neq 0) = e^{-u}, u \geq 0. \tag{56}$$

This emphasizes on the rarity character when the number M of thresholds increases and the probabilities between the levels decrease.
In our case

$$f(s) \;\; = [P_0 s + (1 - P_0)]^R = [P_0(s-1) + 1]^R \tag{57}$$

The iterated function f_M has no explicit tractable form and we shall derive bounds for $f_M(s)$ around $s = 1$. To do this, we state a general result on the Laplace transform in critical Galton-Watson models, which we could not find in the literature.

4.2 Bounds of $f_n(s)$ for $0 \leq s < 1$ and $m = 1$

Remark 4.1 *Remind that f_n and its derivatives are convex. Furthermore for all $0 \leq s \leq 1$, $s \leq f(s) \leq f(1) = 1$, and by induction $f(s) \leq f_2(s) \leq .. \leq 1$. Finally we obtain $f_n(s) \to 1$ since $f_n(s) \geq f_n(0)$.*

Proposition 4.1 *Let* $\alpha_1 = \frac{f''(1)}{2}$, $C = \frac{\max_{s\in[0,1]} f'''(s)}{6\alpha_1}$ *and* $\gamma_n = n\alpha_1[1 - \frac{C}{n}(\log n + 1)] - \alpha_1$. *Then, for* s *close to 1 and large* n

$$1 - \frac{1-s}{1+\gamma_n(1-s)} \le f_n(s) \le 1 - \frac{(1-s)[1-\alpha_1(1-s)]}{1+\alpha_1(1-s)(n-1-\frac{\alpha_1^2(1-s)^2}{2})} \tag{58}$$

Proof. Upper bound : Using Taylor's expansion, with $f_n(s) \le \theta_n \le f_n(1) = 1$,

$$f_{n+1}(s) = f(f_n(s)) = f(1) + (f_n(s)-1)f'(1) + \frac{(f_n(s)-1)^2}{2} f''(\theta_n) \tag{59}$$

$$= f_n(s) + \frac{(f_n(s)-1)^2}{2} f''(\theta_n), \tag{60}$$

since $f'(1) = 1$. Let $r_n = 1 - f_n(s)$, r_n satisfies

$$r_{n+1} = r_n - r_n^2 \frac{f''(\theta_n)}{2}. \tag{61}$$

Now let $\alpha_0 = \frac{f''(0)}{2}$. Define the decreasing sequences (a_n) and (b_n) satisfying

$$a_{n+1} = a_n - a_n^2\alpha_1, \qquad b_{n+1} = b_n - b_n^2\alpha_0, \qquad a_0 = b_0 = 1-s \tag{62}$$

Then
$$a_n \le r_n \le b_n. \tag{63}$$

1) b_n's upper bound : since $0 \le b_j \le 1$ we have

$$\frac{1}{b_n} = \frac{1}{b_{n-1}} + \alpha_0 \frac{1}{1-\alpha_0 b_{n-1}} = \frac{1}{b_0} + \alpha_0 \sum_{j=0}^{n-1} \frac{1}{1-\alpha_0 b_j} \ge \frac{1}{b_0} + n\alpha_0 \tag{64}$$

Thus
$$b_n \le \frac{1-s}{1+\alpha_0 n(1-s)}. \tag{65}$$

2) a_n's lower bound : apply this upper bound to a_n (α_0 becoming α_1).

$$a_n \le \frac{1-s}{1+n\alpha_1(1-s)}. \tag{66}$$

By injecting (66) in $\frac{1}{a_n} = \frac{1}{a_0} + \alpha_1 \sum_{j=0}^{n-1} \frac{1}{1-\alpha_1 a_j}$, we get

$$a_n \ge \frac{(1-s)[1-\alpha_1(1-s)]}{1+\alpha_1(1-s)(n-1-\frac{\alpha_1^2(1-s)^2}{2})}. \tag{67}$$

Finally (63) and (67) lead to the upper bound of f_n in (58).

Lower bound : In fact, we prove by induction

$$h_{\hat\gamma_n}(s) := 1 - \frac{1-s}{1+\hat\gamma_n(1-s)} \le f_n(s) \quad \text{with} \quad \begin{cases} \hat\gamma_{n+1} = c_n + \hat\gamma_n \\ \hat\gamma_1 = 0 \\ c_n = \alpha_1(1-\frac{C}{n}) \end{cases} \tag{68}$$

For $n = 1$, the left hand side of (68) is given by the Remark 4.1. Then note that $h_{\hat{\gamma}_n}(s) \to_{n\to\infty} 1$ thus for n large enough $1 - h_{\hat{\gamma}_n}(s) \leq \frac{1}{n}$. For all $1 - \frac{1}{n} \leq s \leq 1$,

$$\begin{aligned} h_{c_n}(s) &= 1 + (s-1) + c_n(s-1)^2 + \frac{(s-1)^3}{6} h'''_{c_n}(\theta_n^1) && (69)\\ &\leq 1 + (s-1) + c_n(s-1)^2 && (70)\\ &= f(s) - (s-1)^2[\frac{s-1}{6} f'''(\theta_n^2) + \frac{C\alpha_1}{n}] && (71)\\ &\leq f(s) \qquad \text{by definition of} \quad C && (72) \end{aligned}$$

But by induction, we have $h_{\hat{\gamma}_n}(s) \leq f_n(s)$, and so, since f is increasing, taking $s = h_{\hat{\gamma}_n}(t)$,

$$h_{c_n}(h_{\hat{\gamma}_n}(t)) = h_{c_n+\hat{\gamma}_n}(t) \leq f(h_{\hat{\gamma}_n}(t)) \leq f(f_n(t)) = f_{n+1}(t) \qquad (73)$$

i.e. $h_{\hat{\gamma}_{n+1}}(t) \leq f_{n+1}(t)$ where $\hat{\gamma}_{n+1} = c_n + \hat{\gamma}_n$.
Note that $\gamma_n \sim \hat{\gamma}_n$, more precisely we have $\gamma_n \leq \hat{\gamma}_n$ and we finally obtain the left hand side of (58) since $\gamma \to h_\gamma$ is increasing.■

In the particular case of $f(s) = (P_0 s + 1 - P_0)^R$, we can derive a more precise lower bound :

Proposition 4.2 *For s close to 1,*

$$1 - \frac{1-s}{1 + n\alpha_1(1-s)} \leq f_n(s) \qquad (74)$$

Observe that this is precise at $s = 1$.

Proof. Let $h(s) = 1 - \frac{1-s}{1+\alpha_1(1-s)}$. Since $f(1) = h(1) = 1$, $f'(1) = h'(1) = 1$ and $f''(1) = h''(1) = 2\alpha_1$, the sign of $f - h$ trivially depends on the sign of the third derivative of $f - h$ which is here obviously negative. Then $h \leq f$. Since f is increasing, we deduce (74) by induction.■

We plot in Figure 4.1 the upper bound and the two lower bounds for $P = 10^{-12}$ and s near 1.

4.3 Bounds of $f_n(s)$ for $1 \leq s$ and $m = 1$

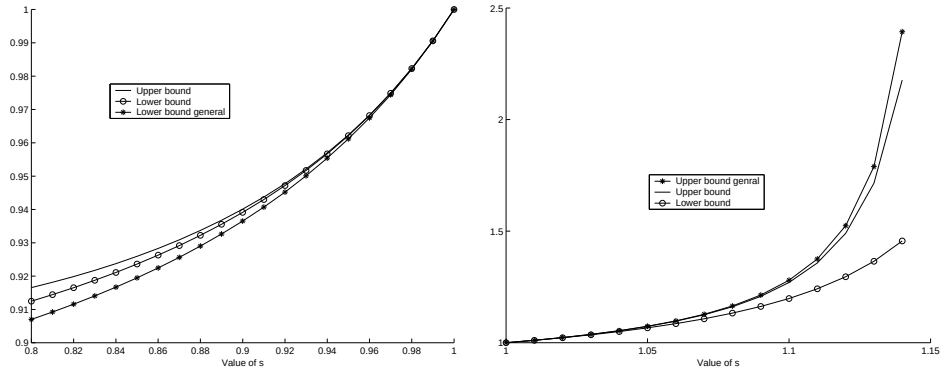
Remark 4.2 *First, let us note that by convexity, for all $s \geq 1$*

$$(s-1)f'(1) \leq f(s) - f(1) = f(s) - 1, \qquad (75)$$

hence $f(s) \geq s$ and by induction on n

$$f_{n+1}(s) \geq f_n(s) \geq .. \geq f(s) \geq s \geq 1. \qquad (76)$$

We remark that for $s > 1$, the iterated function increases rapidly to infinity.



1. for $0 \leq s \leq 1$ 2. for $1 \leq s$

FIG. 4 – Bounds of $f_M(s)$

Proposition 4.3 *Let* $\gamma'_n = n\alpha_1[1 + \frac{C}{n}(\log n + 1)] - \alpha_1$. *Then, for* s *close to 1 and large* n,

$$1 + \frac{(s-1)}{1 - n\alpha_1 s_n^{P_0-2}(s-1)} \leq f_n(s) \leq 1 + \frac{s-1}{1 - n\gamma'_n(s-1)} \tag{77}$$

Proof. Proceeding as done in Proposition 4.1 leads to the upper bound. Here $f_n \rightarrow_{n\rightarrow+\infty} \infty$ which prevents us to make a Taylor expansion around 1. To overcome this difficulty, consider k_n the inverse function of f_n, it is the n-th functional iterate of the g.f. k (inverse function of f) which takes the value 1 in 1, whose derivative is 1 in 1, second derivative is negative and $k_n \rightarrow_{n\rightarrow+\infty} 1$. Thus making a Taylor development and using the same tools as previously, we get

$$1 + \frac{(s-1)(1-\alpha_1(s-1))}{1 + (n-1)\alpha_1(s-1)} \leq k_n(s) \leq 1 + \frac{s-1}{1 + n\alpha_1 s_n^{P_0-2}(s-1)} \tag{78}$$

where $\beta_2 = \frac{k"(s)}{2}$ and $s_n := 1 + \frac{1}{n\alpha_1}$. Using the link between k_n and f_n and the upper bound of k_n,

$$1 + \frac{(s-1)}{1 - n\alpha_1 s_n^{P_0-2}(s-1)} \leq f_n(s). \tag{79}$$

The lower bound of k_n leads to an upper bound of f_n. But it provides us no improvement.■

As done before, we can derive a more precise upper bound in the particular case of $f(s) = (P_0 s + 1 - P_0)^R$:

Proposition 4.4 *For s close to* 1,

$$f_n(s) \leq 1 + \frac{s-1}{1 - n\alpha_1(s-1)} \tag{80}$$

We plot in Figure 4.2 these three bounds for $P = 10^{-12}$ and s near 1.

About the geometric distribution If the law of X is such that the probabilities p_k are in a geometric proportion : $p_k = \mathbb{P}(X = k) = bc^{k-1}$ for $k = 1, 2...$ and $p_0 = 1 - p_1 - p_2...$ with $b, c > 0$ and $b \leq 1 - c$, then the associated g.f. is a rational function :

$$h(s) = 1 - \frac{b}{1-c} + \frac{bs}{1-cs}. \tag{81}$$

Taking $b = (1-c)^2$ and $c = \frac{\alpha_1}{1+\alpha_1}$ leads to

$$h(s) = 1 + \frac{s-1}{1 - \alpha_1(s-1)} \tag{82}$$

So we have compared the n-th functional iterate of a Binomial g.f. to the one of a geometric g.f.. It suggests us to compare the importance splitting models with Binomial and with geometric laws. The second one is set in the following way : we run particles one after the other. As long as the next level is not reached we keep on generating particles, then we start again from it (the geometric distribution is the law of the first success).

This link is also underlined by Cosnard and Demangeot in [4] : for $m = 1$ and $\sigma^2 = f''(1) = 2\alpha_1$, the asymptotic behavior of f^{2^n} is the same as the one of a geometric with the same variance i.e. h.

4.4 Optimization of the Crämer transform

Remind that

$$\psi^*(P(1+\alpha)) = \sup_{\lambda > 0} \{\lambda P(1+\alpha) - \ln(P_0 f_M(e^{\lambda/R^M}) + 1 - P_0)\} \tag{83}$$

$$\psi^*(P(1-\alpha)) = \sup_{\lambda < 0} \{\lambda P(1-\alpha) - \ln(P_0 f_M(e^{\lambda/R^M}) + 1 - P_0)\} \tag{84}$$

Considering the gradient of the functions, we prove that the supremum for $\lambda \geq 0$ is reached near 0. So we can use the upper bounds for f_M obtained in the previous section which leads to lower bounds for ψ^* :

$$\psi^*(P(1+\alpha)) \geq F(P(1+\alpha)) \text{ and } \psi^*(P(1-\alpha)) \geq G(P(1-\alpha)), \tag{85}$$

where $F(x) = \sup_{\lambda>0}[\lambda x - \ln(1 + P_0 \frac{(e^{\lambda/R^M}-1)}{1-M\alpha_1(e^{\lambda/R^M}-1)})]$ and
$G(x) = \sup_{\lambda<0}[\lambda x - \ln(1 - P_0 \frac{(1-e^{\lambda/R^M})[1-\alpha_1(1-e^{\lambda/R^M})]}{u_0})]$. Finally

$$\mathbb{P}(\frac{|\hat{P}-P|}{P} \geq \alpha) \leq 2e^{-N \min(F(P(1+\alpha)),G(P(1-\alpha))}. \tag{86}$$

And one can easily obtain explicit but complex expressions for $F(x)$ and $G(x)$. We plot in Figure 5 the upper bounds obtained by the variance and by the Laplace transform, for different values of α, the prescribed error of the confidence interval. We take $P = 10^{-9}$ and the optimal values obtained above for the parameters. Note that the upper bound given by the

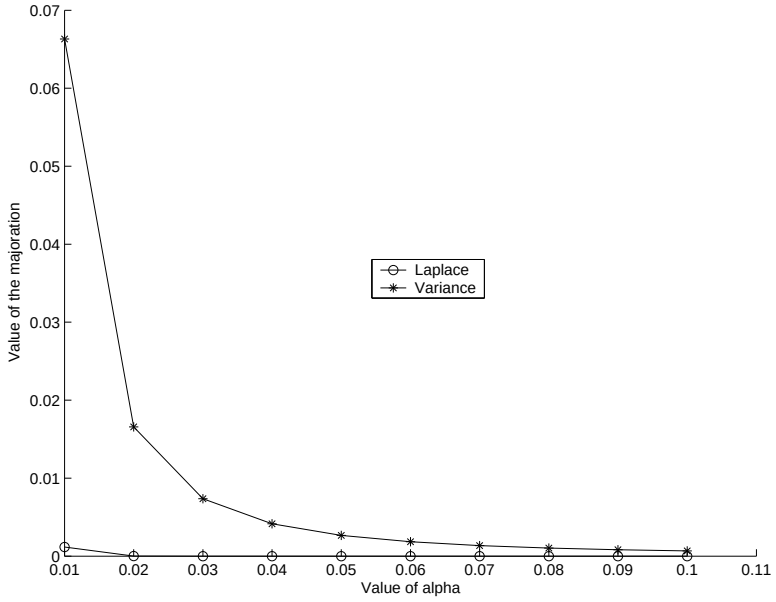


FIG. 5 – Upper bounds obtained by the variance and the Laplace transform

Laplace transform is better than the other one (with the variance). We obtain $\mathbb{P}(\frac{|\hat{P}-P}{P}| \geq \alpha) \leq L$. In the preceding example where $P = 10^{-9}$, if we fix $\alpha = 0.05$ and L close to 0.01, then the corresponding costs needed are $3 * 10^7$ for the variance and $3 * 10^6$ for the Laplace transform.

5 Conclusion

The simplified model described here has 2 main defaults. First, we cannot choose in general the optimal level P_i. In practice, we just have empirical estimation on them, and we can bound to adjust the levels according to them. A more precise analysis is then needed to get confidence intervals

of the estimation. Moreover, the optimal sampling number at each level is not an integer in general. Therefore, in practice, the number of particles generated at each step should be chosen at random, either such that $\mathbb{E}(R) = \frac{1}{P_0}$ or $\mathbb{E}(\frac{1}{R}) = P_0$. Thus, we finally need to work in random environment. This requires a precise asymptotic of random iterates of Laplace transform where analysis is more delicate than the one presented here and shall be the purpose of a forthcoming paper.

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