# Some recent improvements to importance splitting*

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**Abstract**

The estimation of rare event probability is a crucial issue in areas such as reliability, telecommunications, aircraft management. In complex systems, analytical study is out of question and one has to use Monte Carlo methods. When rare is really rare, which means a probability less than $10^{-9}$, naive Monte Carlo becomes unreasonable. A widespread technique consists in multilevel splitting, but this method requires enough knowledge about the system to decide where to put the levels at hand and select the branching rates. In this paper, we propose to improve the importance splitting algorithm by using adaptive branching rates.This variant of the algorithm may be described by the formalism of Feynman-Kac Formula, providing a very elegant way of studying its properties. We also propose a second variant

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using adaptive splitting levels, for which only partial convergence results have been obtained. We will give some numerical examples, including the computation of large self avoiding random walks on the 2D lattice.

**Keywords :** rare events, multilevel splitting, Feynman-Kac formula, genetic models, quantiles

# 1 Introduction

Throughout this paper, we will consider the following type of problems: given a strong Markov process $X$, we want to estimate the probability that it enters some measurable set $R$ before visiting some recurrent set $A_0$. Moreover, we would like not only to estimate this probability, but as well end up with realizations of the Markov process that reach the rare set. The probability of the event of interest is unknown, but assumed too small to be estimated by naive Monte-Carlo. In the rare event community this problem is usually addressed by using an *importance splitting* algorithm. The basic idea is to use a family of nested sets

$$R = B_{m+1} \subset B_m \subset \cdots \subset B_1 \subset B_0 \ , \tag{1}$$

and replicate $R_j$ times each trajectory reaching $B_j$ for the first time. It is quite intuitive, and it is well known (see [12, 9]) that this approach is only efficient when $1/R_j$ is close to $P_j$, where $P_j$ is the probability of reaching $B_j$ given the trajectory has already reached $B_{j-1}$. Moreover (see [12]), the variance is minimal when all the $P_j$'s are equal. Even if this approach has already proved to be very attractive for rare event simulation, it is not always obvious how to choose the sets $B_j$ and the corresponding branching rates $R_j$. In the sequel, we will develop new variants of the basic splitting algorithm, the first one solving the problem of choosing the branching rates, and the second one partially solving the problem of the choice of the sets $B_j$.

# 2 Adaptive branching rates

## 2.1 Mathematical setting

We assume that $X$ is a strong Markov process taking its values in a Polish space $S$, with almost surely right continuous, left limited trajectories (RCLL, or càdlàg), and that $R$ is closed. We assume to be given a family of nested, closed, subsets of $S$ satisfying (1), where $R$ denote the event of interest. We also denote by $A_0$ a closed recurrent set for the process $X$, and assume that $A_0 \cap B_0 = \emptyset$. We now define for any Borel set $B$ in $S$ the following stopping time:

$$T_B = \inf\{t \geq 0, X_t \in B\}.$$

With this notation, the rare event is simply $E_R = \{T_R \leq T_{A_0}\}$. It is also quite obvious that we can express its probability as

$$\mathbb{P}(T_R \leq T_{A_0}) = \mathbb{E}[\mathbb{1}_{T_R \leq T_{A_0}}] = \mathbb{E}[\mathbb{1}_{X_{T_R \wedge T_{A_0}} \in R}].$$

For any $1 \leq k \leq m+1$, we denote

$$T_k = T_{B_k} \wedge T_{A_0}.$$

Then for any functional $\phi$ of the trajectory up to $T_{m+1} = T_R \wedge T_{A_0}$, we can express the conditional expectation given the rare event by

$$\mathbb{E}[\phi(X_t, t \leq T_{m+1}) | T_R \leq T_{A_0}] = \frac{\mathbb{E}[\phi(X_t, t \leq T_{m+1}) \prod_{k=0}^{m+1} \mathbb{1}_{X_{T_k} \in B_k}]}{\mathbb{E}[\prod_{k=0}^{m+1} \mathbb{1}_{X_{T_k} \in B_k}]}, \tag{2}$$

and

$$\mathbb{P}(T_R \leq T_{A_0}) = \mathbb{E}[\prod_{k=0}^{m+1} \mathbb{1}_{X_{T_k} \in B_k}]. \tag{3}$$

Now what have we gained by putting it in such a cumbersome form ?

## 2.2 Feynman-Kac model interpretation

The interest of equation (2) is that it rewrites a conditional expectation given a rare event in the form of a (discrete time) Feynman-Kac formula, for which a great deal of developments have been carried out by P. Del Moral in recent years (see [5]). This theory gives a general algorithm to construct a numerical approximation and numerous convergence results as soon as we are interested in expressions of the form

$$\hat{\eta}_n(\phi) = \frac{\mathbb{E}[\phi(Z_1, \dots, Z_n) \prod_{k=0}^{n} G_k(Z_k)]}{\mathbb{E}[\prod_{k=0}^{n} G_k(Z_k)]} \tag{4}$$

where $G_k$ are measurable non-negative functions called potentials. Many practical problems can take this form (arising in non linear Bayesian filtering, statistical physics, directed polymers simulation...).
To see that equation (2) fits exactly in equation (4), we can consider the discrete time Markov chain of the excursions of $X$ between two consecutive stopping times $T_k$ and $T_{k+1}$, that is $\mathcal{X}_k = \{X_t, T_k \leq t \leq T_{k+1}\}$ (see [3] for a more careful check).

## 2.3 Algorithm

This formalism gives a nice way to construct a discrete approximation to the measure $\hat{\eta}_n$ using a particle approximation. Basically, we start with a set of *particles*, which is an i.i.d. $N$-sample $\xi_0^k, k = 1, \dots, N$ of the law of $X_0$. Then we associate to each sample $k$ a weight proportional to $G_0(\xi_0^k)$, and normalize them such that their sum is equal to 1. We denote the corresponding weights by $w_0^k$. Then we re-sample according to the weights. This step will give offspring to particles with high weights, and will remove the ones with very little weights. To go to the next time step we draw independently for each $k$ a new position using the transitions of the Markov chain $\mathbb{P}(X_1 \in dx | X_0 = \xi_0^k)$, recompute the weights using $G_1$, re-sample, and iterate the process until the final time. Note that in general there are many different ways to practically implement the re-sampling step, but we will not discuss this topic here. In fact, our un-normalized weights being either 0 or 1, this discussion would not be much relevant here (see [7] for a review on practical aspects of these methods).
This family of algorithms is often referred to as *genetic* as they can be decomposed into a *mutation* step, the drawing of new states using the transitions of the chain, and a *selection* step, which is the re-sampling, favoring the best fitted according to the potential. It is also referred to as *genealogical* because we can keep track of all the previous states occupied by a given particle, constructing a kind of genealogical tree for the particle system.
Note that in the case of rare event simulation, unlike many other applications, we are also interested in computing the denominator of equation (4), as it is precisely the probability of the rare event (see equation (3)). Obviously we can write, as usual with splitting methods:

$$\mathbb{P}(T_R \leq T_{A_0}) = \prod_{k=1}^{m+1} \mathbb{P}(X_{T_k} \in B_k | X_{T_{k-1}} \in B_{k-1}) = \prod_{k=1}^{m+1} \mathbb{E}[\mathbb{1}_{B_k}(X_{T_k}) | X_{T_{k-1}} \in B_{k-1}].$$

Now each term in the product is the normalizing constant at each step of the algorithm, and we can reconstruct the global normalizing constant by multiplying the local ones. Practically, as in any splitting method, we then will estimate the global probability of success as the product of all the probabilities of reaching the next level set $B_k$ given that we succeeded to hit $B_{k-1}$.
Applying these ideas to equation (2) we end up with algorithm 1.

### Algorithm 1

**Parameters**

$N$ the number of particles.

**Initialization**

Draw an i.i.d. $N$-sample $\xi_k, k = 1, \dots, N$ of the law of $X_0$.

for $k = 1$ to $N$, $T_0^k \leftarrow 0$.

**Iterations**

for $h = 0$ to $m$ /* level number */

let $I_1$ be the set of indices for which $\xi_k(T_k^h) \in B_h$, and $I_0$ its complement in $1, \dots, N$.

$P_h \leftarrow |I_1|/N$.

for $k \in I_0$, let $\xi_k$ be a copy of $\xi_\ell$ where $\ell$ is chosen randomly in $I_1$ with uniform probabilities.

for $k \in 1, \dots, N$, extend each trajectory $\xi_k$ using the transition probabilities of $X$, until time $T_k^{h+1}$ when it first hits $B_{h+1} \cup A_0$.

endfor

let $P_{m+1}$ be the proportion of trajectories that actually hit $R$.

**Output**

estimate the probability of the rare event by $\hat{P}_1 = \prod_{h=0}^{m+1} P_h$.

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We have therefore constructed an algorithm that does not need to specify any branching rate. Note that just as in the plain splitting algorithm, there is a (hopefully small but) non zero probability of extinction (i.e. $I_1 = \emptyset$ at some stage). In this case, if we do not accept to estimate the probability by 0, we need to restart the whole process. We should also mention a variant in which we do not stop the computation until a fixed number of successes has been reached, which was proposed in [13]. As mentioned in [3], for algorithm 1, the probability of extinction is exponentially small as $N \to +\infty$, and restricted on realizations such that the particle system does not die, the probability estimator $\hat{P}_1$ is unbiased.

## 2.4 Convergence results

We briefly present here some convergence results, following general results on Feynman-Kac models (see [3, 6, 2] for details). As in algorithm 1, we denote by $\hat{P}_1$ our estimate of the probability of the rare event, and $\mathbb{1}_{\hat{P}_1>0}$ the indicator function of the non extinction set of realizations. Then we have a strong law of large numbers:

$$\sqrt{N}\mathbb{E}[|\hat{P}_1.\mathbb{1}_{\hat{P}_1>0} - \mathbb{P}(T_R \leq T_{A_0})|^p]^{\frac{1}{p}} \leq C_p,$$

for any positive $p$, and for some finite constant $C_p$ depending on $p$, and on the model. We also have the same kind of estimates for any functional of the trajectory, given that the rare event is hit.
We also have a CLT type result: the sequence of random variables

$$\sqrt{N}(\hat{P}_1.\mathbb{1}_{\hat{P}_1>0} - \mathbb{P}(T_R \leq T_{A_0}))$$

converges in distribution to a Gaussian $N(0, \sigma^2)$ with

$$\sigma^2 = c.\mathbb{P}(T_R \leq T_{A_0})^2.$$

The square of the probability here characterizes an efficient simulation method, like standard splitting methods. But unfortunately the expression for the constant $c$ is not very simple in general. In dimension 1 however, the asymptotic variance reduces to

$$\sigma^2 = \sum_{h=0}^{m+1} \left( \frac{1}{\mathbb{P}(T_h \leq T_{A_0} | T_{h-1} \leq T_{A_0})} - 1 \right), \tag{5}$$

which is the same variance as given in [12], with optimal branching rates. This suggests that our variant is strictly better than standard splitting because it is asymptotically as efficient as the standard one with optimal branching rates, and with the same algorithmic complexity.
Note that a variant of this algorithm, better fitted for hybrid models, has been developed and applied to practical problems in [11].

# 3 Adaptive levels

Having solved the problem of choosing the branching rates, it still remains that of choosing the family of nested sets $B_k, k = 0, \ldots, m+1$, and even the number $m$.
We will assume here that $R$ is the super level set of some scalar function $\Phi$:

$$R = \{x \in S : \Phi(x) \geq \lambda_R\},$$

for some $\lambda_R \in \mathbb{R}$. We assume that $\Phi$ is upper semi continuous to ensure that its level sets are closed. In the rare event literature such a function $\Phi$ is often referred to as an importance function.

## 3.1 Algorithm

The main idea is to construct recursively $\Phi$ level sets such that the probability to reach the next one will approximately be some value given as a parameter. Following [4] we give the details below in algorithm 2 of the proposed approach.

### Algorithm 2

**Parameters**

$N$ the number of particles.

$K$ the number of succeeding particles at each step.

**Initialization**

Draw an i.i.d. $N$-sample $\xi_k, k = 1, \ldots, N$ of the trajectory of $X$ until new stopping time $T_k^0$ when it hits $A_0$, re-compute $S_k = \sup_{0 \leq t \leq T_k^0} \Phi(\xi_k(t))$, and $T_k^S = \inf\{0 \leq t \leq T_k^0, \Phi(\xi_k(t)) \geq S_k\}$.

Sort the $S_k$, $k = 1, \ldots, N$ in decreasing order, and reorder the $\xi_k$, $T_k^0$, and $T_k^S$ accordingly.

$m \leftarrow 0$.

**Iterations**

while $S_K < \lambda_R$ do

$m \leftarrow m + 1$.

for $k = K+1, \ldots, N$

Choose at random an index $\ell$ in $1, \ldots, K$ with uniform probability.

Let $\xi_k = \xi_\ell$ until time $T_k^S$, and extend the trajectory by simulation until $T_k^0$ when it hits $A_0$, compute $S_k = \sup_{0 \leq t \leq T_k^0} \Phi(\xi_k(t))$, and $T_k^S = \inf\{0 \leq t \leq T_k^0, \Phi(\xi_k(t)) \geq S_k\}$.

endfor

Sort the $S_k$, $k = 1, \ldots, N$ in decreasing order, and reorder the $\xi_k$, $T_k^0$, and $T_k^S$ accordingly.

endwhile

let $\tilde{P}$ be the proportion of trajectories that actually hit $R$.

**Output**

estimate the probability of the rare event by $\hat{P}_2 = \tilde{P}.(\frac{K}{N})^m$.

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The fact that the number of iterations is not fixed should not be a problem, as it is very unlikely, for $N$ reasonably large, to be different from the ratio of logarithms $\lfloor \frac{\log \mathbb{P}(T_M \leq T_0)}{\log K - \log N} \rfloor + 1$.
For simplicity we run all the trajectories up to the time they hit $A_0$. In fact, if we do not need the trajectories after hitting $R$, we just stop them at their first hitting time $T_{A_0} \wedge T_R$. In that case, the simulation time is exactly the same as it would be using algorithm 1.
Note that the complexity is only increased by the need to sort the suprema, that is by an $N \log N$ (in the mean) term if we use a Quicksort algorithm.
We should also mention that the idea of using quantiles to construct the level sets was already presented in [8]. But unlike in algorithm 2, the trajectories used to find the level sets were thrown away, and a classical splitting algorithm was then used.

## 3.2 Convergence results

The use of quantiles in the algorithm adds complex dependencies between trajectories and makes it unsuitable for Feynman-Kac representation. So there is no easy approach to show convergence results and so far only partial results have been obtained.
We consider here the framework of [4], where some partial convergence results are proved.
The most restrictive assumption is that the state space is $\mathbb{R}$. We consider a strong Markov process starting at some fixed $x_0 > 0$. We assume that $X$ has a.s. continuous trajectories. We assume that 0 is an attractive point and $M \gg 0$ is a barrier the process is very unlikely to reach. We would like to estimate the probability that the process reaches $M$ before 0. We define

$$T_0 = \inf\{t \geq 0, X_t = 0\},$$

and

$$T_M = \inf\{t \geq 0, X_t = M\}.$$

We further assume that the distribution function $F$ of the random variable $S = \sup_{0 \leq t \leq T_0} X_t^{x_0}$ is continuous. Under this set of assumptions, we have the almost sure convergence:

$$\hat{P}_2(N, K) \xrightarrow{a.s.} \mathbb{P}(T_M \leq T_0) \text{ as } N \to +\infty,$$

and with $K = \lfloor pN \rfloor$ for some fixed $p > 0$.
Furthermore, we have the following CLT type result. Let us define $r$ as $r = \mathbb{P}(T_M \leq T_0).p^{-q}$ with $q = \lfloor \frac{\log \mathbb{P}(T_M \leq T_0)}{\log p} \rfloor$. We have

$$\sqrt{N}(\hat{P}_2(N, K) - \mathbb{P}(T_M \leq T_0)) \xrightarrow{\mathcal{D}} N(0, \sigma^2), \text{ as } N \to +\infty,$$

where the asymptotic variance is

$$\sigma^2 = \mathbb{P}(T_M \leq T_0)^2.(q\frac{1-p}{p} + \frac{1-r}{r}).$$

Assume that $\mathbb{P}(T_M \leq T_0) = p^q$ for some $q \in \mathbb{N}$, that is $r = 1$. It is remarkable then that this expression for the variance is exactly the same as equation (5), with the optimal choice for the levels, i.e. $\mathbb{P}(T_h \leq T_{A_0} | T_{h-1} \leq T_{A_0}) = p$ for all $k$ (see [12] for a discussion of this optimality).
We did not succeed to prove that the estimate $\hat{P}_2(N, K)$ is unbiased, because from numerical evidence it is not. But as discussed in the next section, the bias is small compared with the standard deviation.

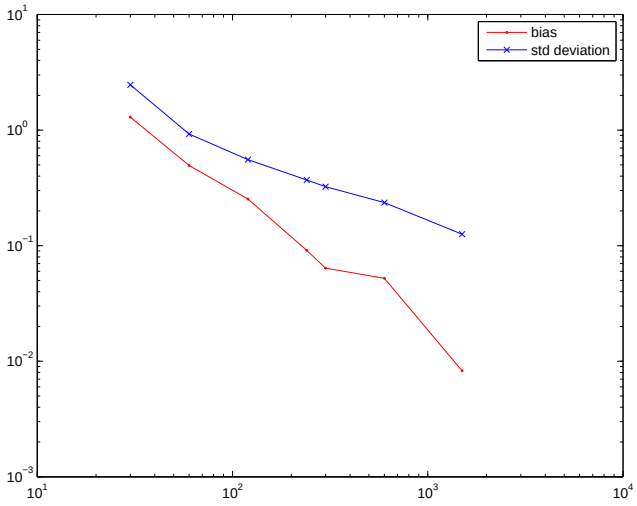


Figure 1: Bias and standard deviation

## 3.3 Numerical results

### 3.3.1 Brownian motion with drift

Let $B$ denote the standard Brownian motion. Let $X_t^{(\mu)} = B_t + \mu t$ be the Brownian motion with drift $\mu$. We note $H_{a,b} = H = \min\{s > 0, X_s^{(\mu)} \notin [a,b]\}$. The expression of the probability of reaching $b$ before $a$ starting from $x \in [a,b]$ is given in [1]:

$$\mathbb{P}_x(\, X_H^{(\mu)} = b\,) = e^{\mu(b-x)} \frac{\sinh\,(\,(x-a)|\mu|\,)}{\sinh\,(\,(b-a)|\mu|\,)}.$$

This explicit and simple expression makes the Brownian motion with drift a good non trivial candidate to compute the bias of our estimator given by algorithm 2.
Figure 1 shows the computed bias and standard deviation of $\hat{P}_2(K,K)$ as functions of $N$, with $K = N/2$, in logarithmic scales. The other parameters are $\mu = -1$, $a = 0$, $b = 10$, $x = 1$, making a true rare event probability of $1.317 \times 10^{-8}$. The computation was carried out for $N$ varying from 30 to $3,000$. For each value, the bias and variance were estimated from 300 runs. The figure clearly shows that the bias is small compared with the standard deviation for reasonably large $N$. From this we can conjecture that the bias is of order $N^{-1}$ when the standard deviation is of order $N^{-\frac{1}{2}}$.
Concerning the choice of $K$, from this and several other numerical computations it seems that good choices are in the range $N/2 \leq K \leq 3N/4$.

### 3.3.2 Self avoiding walks

We have implemented this with self-Avoiding Walks in $\mathbb{Z}^2$, which is a simplified model for molecular chains (for more informations see [15, 10]). A SAW is simply a random walk on $\mathbb{Z}^2$, conditioned on the fact that it never visited twice the same site. The proportion of such trajectories upon all possible chains decreases very fast with its length $n$, making it a very rare event. See [14] for a monograph on SAW. We can then calculate the probability of having long chains and draw some of them using algorithm 2 (see examples in figure 2).

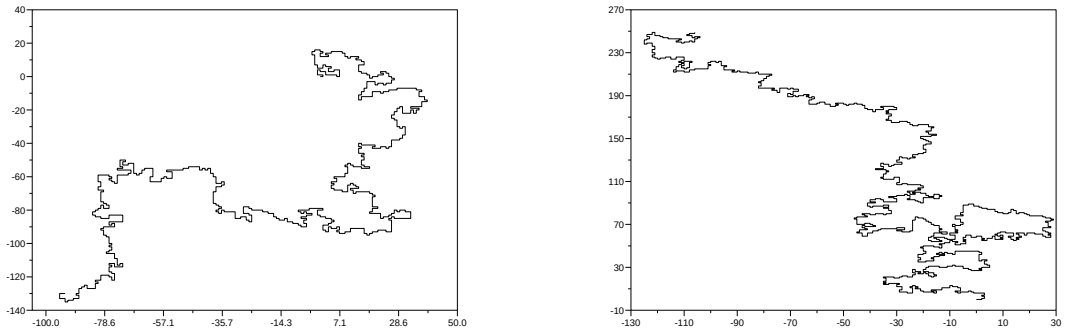


Figure 2: SAW in $\mathbb{Z}^2$ of length 1000 and 1500,
the estimated probabilities are respectively of order $10^{-204}$ and $10^{-305}$.

The function $\Phi$ here is simply the length of the chain before it hits itself[1]. As in the historical paper [15] we focused on the extension of the chain. The extension of a SAW $X$ of length $n$ is defined as

$$s(n) = \mathbb{E}[X(n)^2].$$

It is proved that the limit

$$\lim_{n \to +\infty} \frac{s(n)}{n^\gamma}$$

exists and is finite for some $\gamma > 0$. But in $\mathbb{Z}^2$ the exact value of $\gamma$ is still unknown, and it is conjectured [14] that $\gamma = 3/2$. In figure 3, we present estimates of $s(n)$ as a function of $n$. These were computed for $n \leq 150$ with $N = 150,000$, and $K = 50,000$. To estimate $\gamma$ we decided to remove the beginning because we are not yet in the asymptotic regime. Keeping the values for $50 \leq n \leq 150$, and fitting the logarithms with a simple linear regression, we found $\gamma \simeq 1.511$, which is compatible with the conjecture.

# 4 Conclusion

The first algorithm presented is strictly better than ordinary importance splitting because it is unbiased, its convergence is well understood, it has asymptotically the same variance, and virtually needs the same amount of computation, but without the need to tune the branching rates.
The second algorithm is less understood, but still promising from both partial convergence results and numerical computations. It is better than the first one if there is an obvious choice for $\Phi$.
The question of the choice of $\Phi$ is still open.

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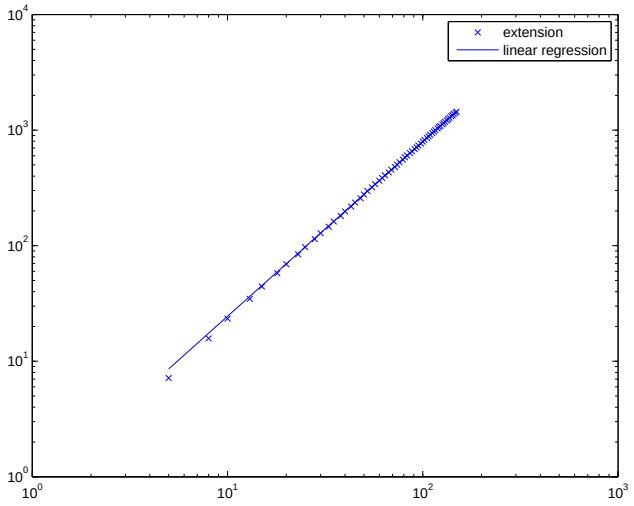


Figure 3: SAW extension

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