Markov Chain Monte Carlo in Rare-Event Simulation

Asymptotics and Simulation of Heavy-Tailed Processes

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Importance Sampling in a Heavy-Tailed Setting

Markov Chain Monte Carlo in Rare-Event Simulation

Outline

1 Introduction to Rare-Event Simulation

- The Problem with Monte Carlo
- Importance Sampling
- 2 Importance Sampling in a Heavy-Tailed Setting
 - The Conditional Mixture Algorithm for Random Walks
 - Performance of the Conditional Mixture Algorithm
- Markov Chain Monte Carlo in Rare-Event Simulation
 Efficient Sampling for a Heavy-Tailed Random Walk
 Efficient Sampling of Heavy-Tailed Random Sums



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Markov Chain Monte Carlo in Rare-Event Simulation

Simulation of Heavy-Tailed Processes

- Goal: improve on the computational efficiency of standard Monte Carlo.
- Design: The large deviations analysis lead to a heuristic way to design efficient algorithms.
- Efficiency Analysis: The large deviations analysis can be applied to theoretically quantify the computational performance of algorithms.



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The Performance of Monte Carlo

- Let X^1, \ldots, X^N be independent copies of X.
- The Monte Carlo estimator is

$$\widehat{\rho} = \frac{1}{N} \sum_{k=1}^{N} I\{X^k > b\}.$$

Its standard deviation is

$$\mathsf{std} = \frac{1}{\sqrt{N}} \sqrt{\rho(1-\rho)}$$

To obtain a Relative Error (std/p) of 1% you need to take N such that

$$\frac{\frac{1}{\sqrt{N}}\sqrt{p(1-p)}}{p} \leq 0.01 \quad \Leftrightarrow N \geq 10^4 \frac{1-p}{p}$$



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Introduction to Importance Sampling¹

- The problem with Monte Carlo is that few samples hit the rare event.
- This problem can be fixed by sampling from a distribution which puts more mass on the rare event.
- Must compensate for not sampling from the original distribution.
- Key issue: How to select an appropriate sampling distribution?



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¹See e.g. [1] for an introduction.

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Monte Carlo and Importance Sampling

The Basics for Computing $F(A) = \mathbb{P}\{X \in A\}$

Monte Carlo

- Sample X¹,..., X^N from *F*.
- Empirical measure

$$\mathbf{F}_{N}(\cdot) = \frac{1}{N} \sum_{k=1}^{N} \delta_{X^{k}}(\cdot).$$

Plug-in estimator

$$\widehat{p} = \mathbf{F}_N(A).$$

Importance Sampling

- Sample $\widetilde{X}^1, \ldots, \widetilde{X}^N$ from \widetilde{F} .
- Weighted empirical measure

$$\widetilde{\mathbf{F}}_{N}^{\mathsf{W}}(\cdot) = \frac{1}{N} \sum_{k=1}^{N} \frac{dF}{d\widetilde{F}}(\widetilde{X}^{k}) \delta_{\widetilde{X}^{k}}(\cdot).$$

Plug-in estimator

 $\widehat{\rho} = \widetilde{\mathbf{F}}_{N}^{w}(A) = \frac{1}{N} \sum_{k=1}^{N} \frac{dF}{d\widetilde{F}}(\widetilde{X}^{k}) I\{\widetilde{X}^{k} \in A\}.$

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Monte Carlo and Importance Sampling

The Basics for Computing $F(A) = \mathbb{P}\{X \in A\}$

Monte Carlo

- Sample X^1, \ldots, X^N from F.
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$$\widetilde{\mathbf{F}}_{N}^{\mathsf{w}}(\cdot) = \frac{1}{N} \sum_{k=1}^{N} \frac{dF}{d\widetilde{F}}(\widetilde{X}^{k}) \delta_{\widetilde{X}^{k}}(\cdot).$$

Plug-in estimator

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Importance Sampling

The importance sampling estimator is unbiased:

$$\widetilde{E}\Big[rac{dF}{d\widetilde{F}}(\widetilde{X})I\{\widetilde{X}\in A\}\Big]=\int_{A}rac{dF}{d\widetilde{F}}d\widetilde{F}=\int_{A}dF=F(A).$$

Its variance is

$$\operatorname{Var}\left(\frac{dF}{d\widetilde{F}}(\widetilde{X})I\{\widetilde{X}\in A\}\right) = \widetilde{E}\left[\left(\frac{dF}{d\widetilde{F}}\right)^2 I\{\widetilde{X}\in A\}\right] - F(A)^2$$
$$= \int_A \left(\frac{dF}{d\widetilde{F}}\right)^2 d\widetilde{F} - F(A)^2$$
$$= \int_A \frac{dF}{d\widetilde{F}} dF - F(A)^2$$
$$= E\left[\frac{dF}{d\widetilde{F}}I\{X\in A\}\right] - F(A)^2.$$



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Importance Sampling

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Illustration

Sampling the tail

Monte Carlo

Importance Sampling



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Quantifying Efficiency

Variance Based Efficiency Criteria

- Basic idea: variance roughly the size of p^2 .
- Embed in a sequence of problems such that

$$p_n = \mathbb{P}\{X_n \in A\} \to 0.$$

■ Logarithmic Efficiency: for some $\epsilon > 0$

$$\limsup_{n\to\infty}\frac{\operatorname{Var}(\widehat{p}_n)}{p_n^{2-\epsilon}}<\infty.$$

Strong Efficiency/Bounded Relative Error:

$$\sup_n \frac{\operatorname{Var}(\widehat{p}_n)}{p_n^2} < \infty.$$

Vanishing relative error:

$$\limsup_n \frac{\operatorname{Var}(\widehat{\rho}_n)}{\rho_n^2} = 0.$$



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The Zero-Variance Change of Measure

There is a best choice of sampling distribution, the zero-variance change of measure, given by

$$F_A(\cdot) = \mathbb{P}\{X_n \in \cdot \mid X_n \in A\}.$$

For this choice

$$\frac{dF}{dF_A}(\mathbf{x}) = \mathbb{P}\{X_n \in A\} I\{X_n \in A\} = p_n I\{X_n \in A\},\$$

and hence

$$\operatorname{Var}(\widehat{p}_n) = E\Big[p_n I\{X_n \in A\}\Big] - F(A)^2 = 0.$$



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Example Problem

A Random Walk with Heavy Tails

- Let $\{Z_k\}$ be iid non-negative and regularly varying (index α) with density *f*.
- Put $S_m = Z_1 + \cdots + Z_m$.
- Compute $\mathbb{P}{S_m > n}$.

The zero-variance sampling distribution is

$$\mathbb{P}\{(Z_1,\ldots,Z_m)\in\cdot\mid S_m>n\}.$$

By regular variation we know that

$$\mathbb{P}\{(Z_1,\ldots,Z_m)\in\cdot\mid S_m>n\}\to\mu(\cdot),$$

where μ is concentrated on the coordinate axis. But μ and *F* are singular!



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The Conditional Mixture Algorithm for Random Walks

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The Conditional Mixture Algorithm for Random Walks

The Conditional Mixture Algorithm²

Suppose S_{i-1} = s. Sample Z_i as follows
1 If s ≥ n, sample Z_i from the original density f.
2 If s ≤ n, sample Z_i from the mixture p_if(z) + (1 − p_i) f̃_i(y | s), 1 ≤ i ≤ m − 1,

 $\tilde{f}_m(y \mid s), \quad i = m.$

Idea: take \tilde{f}_i to produce large values of Z_i .

²This algorithm is due to [4]

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The Conditional Mixture Algorithm for Random Walks

The Conditional Mixture Algorithm

• We can take \tilde{f}_i 's to be the conditional distributions of the form

$$egin{aligned} & ilde{f}_i(z\mid s) = rac{f(z)I\{z > a(n-s)\}}{\mathbb{P}\{Z > a(n-s)\}}, & i \leq m-1, \ & ilde{f}_m(z\mid s) = rac{f(z)I\{z > n-s\}}{\mathbb{P}\{Z > n-s\}}, \end{aligned}$$

where $a \in (0, 1)$. Note: \tilde{f}_i is the conditional distribution of *Z* given that *Z* is large.

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Performance of the Conditional Mixture Algorithm

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Performance of the Conditional Mixture Algorithm

The Performance of the Conditional Mixture Algorithm

The normalized second moment is

$$\begin{aligned} &\frac{E[\widehat{p}_n]}{p_n^2} = \frac{1}{p_n^2} \int \frac{dF}{d\widetilde{F}}(z_1, \dots, z_m) I\{s_m > n\} F(dz_1, \dots, dz_m) \\ &\sim \frac{1}{m^2 \mathbb{P}\{Z_1 > n\}^2} \int \frac{dF}{d\widetilde{F}}(z_1, \dots, z_m) I\{s_m > n\} F(dz_1, \dots, dz_m) \\ &\sim \frac{1}{m^2} \int \frac{1}{\mathbb{P}\{Z_1 > n\}} \frac{dF}{d\widetilde{F}}(nz_1, \dots, nz_m) I\{s_m > 1\} \frac{F(ndz_1, \dots, ndz_m)}{\mathbb{P}\{Z_1 > n\}}. \end{aligned}$$



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The Performance of the Conditional Mixture Algorithm

Weak convergence:

$$\frac{F(n \cdot)}{\mathbb{P}\{Z_1 > n\}} \rightarrow \sum_{k=1}^m \int I\{ze_k \in \cdot\}\mu_\alpha(dz)$$

The normalized likelihood ratio is bounded:

$$\sup_{n} \frac{1}{\mathbb{P}\{Z_1 > n\}} \frac{dF}{d\widetilde{F}}(nz_1, \dots, nz_m) I\{s_m > 1\} < \infty.$$



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The Performance of the Conditional Mixture Algorithm

The above enables us to show that the normalized second moment converges:

$$\lim_{n} \frac{E[\hat{p}_{n}]}{p_{n}^{2}} = \frac{1}{m^{2}} \Big(\sum_{i=1}^{m-1} \frac{a^{-\alpha}}{1-p_{i}} \prod_{j=1}^{i-1} \frac{1}{p_{j}} + \prod_{j=1}^{m-1} \frac{1}{p_{j}} \Big).$$

It is minimized at

$$p_i = \frac{(m-i-1)a^{-\alpha/2}+1}{(m-i)a^{-\alpha/2}+1},$$

with minimum

$$\frac{1}{m^2}\Big((m-1)a^{-\alpha/2}+1\Big)^2.$$



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The Performance of the Conditional Mixture Algorithm

- The conditional mixture algorithm has (almost) vanishing relative error.
- Heavy-tailed heuristics indicate how to design the algorithm.
- Heavy-tailed asymptotics needed to prove efficiency of the algorithm.



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MCMC for Rare Events³

- Let X be random variable with density f and compute $p = \mathbb{P}\{X \in A\}$, where A is a rare event.
- The zero-variance sampling distribution is

$$F_A(\cdot) = \mathbb{P}\{X \in \cdot \mid X \in A\}, \quad \frac{dF_A}{dx}(x) = \frac{f(x)I\{x \in A\}}{p}.$$

- It is possible to sample from F_A by constructing a Markov chain with stationary distribution F_A (e.g. Gibbs sampler or Metropolis-Hastings).
- Idea: sample from F_A and extract the normalizing constant p.



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MCMC for Rare Events

- Let X_0, \ldots, X_{T-1} be a sample of a Markov chain with stationary distribution F_A .
- Consider a non-negative function v(x) with $\int_A v(x) dx = 1$. The sample mean

$$\widehat{q}_T = rac{1}{T}\sum_{t=0}^{T-1}rac{v(X_t)I\{X_t\in A\}}{f(X_t)},$$

is an estimator of

$$E_{F_A}\Big[\frac{v(X)I\{X\in A\}}{f(X)}\Big] = \int_A \frac{v(x)}{f(x)}\frac{f(x)}{p}dx = \frac{1}{p}\int_A v(x)dx = \frac{1}{p}$$

Take \hat{q}_T as the estimator of 1/p.



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MCMC for Rare Events

- The rare-event properties of *q*_T are determined by the choice of *v*.
- The large sample properties of \hat{q}_T are determined by the ergodic properties of the Markov chain.



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The Normalized Variance

The rare-event efficiency (p small) is determined by the normalized variance:

$$p^{2} \operatorname{Var}_{F_{A}}\left(\frac{v(X)}{f(X)}I\{X \in A\}\right)$$

$$= p^{2}\left(E_{F_{A}}\left[\left(\frac{v(X)}{f(X)}I\{X \in A\}\right)^{2}\right] - \frac{1}{p^{2}}\right)$$

$$= p^{2}\left(\int \frac{v^{2}(x)}{f^{2}(x)}\frac{f(x)}{p}dx - \frac{1}{p^{2}}\right)$$

$$= p\int_{A}\frac{v^{2}(x)}{f(x)}dx - 1.$$

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The Optimal Choice of *v*

It is optimal to take v as f(x)/p. Indeed, then

$$p^2 \operatorname{Var}_{F_A}\left(rac{v(X)}{f(X)} I\{X \in A\}
ight) = p \int_A rac{v^2(x)}{f(x)} dx - 1 = 0.$$

Insight: take v as an approximation of the conditional density given the event.



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Efficient Sampling for a Heavy-Tailed Random Walk

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Efficient Sampling for a Heavy-Tailed Random Walk

- Let $\{Z_k\}$ be iid with density *f*.
- Put $S_n = Z_1 + \cdots + Z_n$.
- Compute $\mathbb{P}{S_n > a_n}$.
- Heavy-tailed assumption:

$$\lim_{n\to\infty}\frac{\mathbb{P}\{S_n>a_n\}}{\mathbb{P}\{M_n>a_n\}}=1.$$

(includes subexponential distributions, see [3]).



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Gibbs Sampling of a Heavy-Tailed Random Walk

- 1 Start from a state with $Z_1 > a_n$.
- 2 Update the steps in a random order according to j_1, \ldots, j_n (uniformly without replacement).
- **3** Update Z_{j_k} by sampling from

$$\mathbb{P}\{Z \in \cdot \mid Z + \sum_{i \neq j_k} Z_i > n\}.$$

The vector $(Z_{t,1}, \ldots, Z_{t,n})'$ forms a uniformly ergodic Markov chain with stationary distribution

$$\mathcal{F}_{\mathcal{A}}(\cdot) = \mathbb{P}\{(Z_1,\ldots,Z_n)' \in \cdot \mid Z_1 + \ldots Z_n > a_n\}.$$



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Rare-Event Efficiency

The Choice of v

Take *v* to be the density of P{(Z₁,...,Z_n)' ∈ · | M_n > a_n}.
 Then

$$\frac{v(z_1,\ldots,z_n)}{f(z_1,\ldots,z_n)}=\frac{1}{\mathbb{P}\{M_n>a_n\}}I\{\vee_{i=1}^n z_i>a_n\}.$$

Rare event efficiency:

$$p_n^2 \operatorname{Var}_{F_A} \left(\frac{v(Z_1, \dots, Z_n)}{f(Z_1, \dots, Z_n)} I\{Z_1 + \dots + Z_n > a_n\} \right) \\ = \frac{\mathbb{P}\{S_n > a_n\}^2}{\mathbb{P}\{M_n > a_n\}^2} \mathbb{P}\{M_n > a_n \mid S_n > a_n\} \mathbb{P}\{M_n \le a_n \mid S_n > a_n\} \\ = \frac{\mathbb{P}\{S_n > a_n\}}{\mathbb{P}\{M_n > a_n\}} \left(1 - \frac{\mathbb{P}\{M_n > a_n\}}{\mathbb{P}\{S_n > a_n\}} \right) \to 0.$$



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 Then

$$\frac{v(z_1,\ldots,z_n)}{f(z_1,\ldots,z_n)}=\frac{1}{\mathbb{P}\{M_n>a_n\}}I\{\vee_{i=1}^n z_i>a_n\}.$$

Rare event efficiency:

$$p_{n}^{2} \operatorname{Var}_{F_{A}} \left(\frac{v(Z_{1}, \dots, Z_{n})}{f(Z_{1}, \dots, Z_{n})} I\{Z_{1} + \dots + Z_{n} > a_{n}\} \right)$$

$$= \frac{\mathbb{P}\{S_{n} > a_{n}\}^{2}}{\mathbb{P}\{M_{n} > a_{n}\}^{2}} \mathbb{P}\{M_{n} > a_{n} \mid S_{n} > a_{n}\} \mathbb{P}\{M_{n} \le a_{n} \mid S_{n} > a_{n}\}$$

$$= \frac{\mathbb{P}\{S_{n} > a_{n}\}}{\mathbb{P}\{M_{n} > a_{n}\}} \left(1 - \frac{\mathbb{P}\{M_{n} > a_{n}\}}{\mathbb{P}\{S_{n} > a_{n}\}}\right) \to 0.$$



Image: Image:

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Numerical illustration

 $n = 5, \alpha = 2, a_n = an.$

$b = 25, T = 10^5, \alpha = 2, n = 5, a = 5, p_{max} = 0.737e-2$			
	MCMC	IS	MC
Avg. est.	1.050e-2	1.048e-2	1.053e-2
Std. dev.	3e-5	9e-5	27e-5
Avg. time per batch(s)	12.8	12.7	1.4
$b = 25, T = 10^5, \alpha = 2, n = 5, a = 20, p_{max} = 4.901e-4$			
	MCMC	IS	MC
Avg. est.	5.340e-4	5.343e-4	5.380e-4
Std. dev.	6e-7	13e-7	770e-7
Avg. time per batch(s)	14.4	13.9	1.5
$b = 20, T = 10^5, \alpha = 2, n = 5, a = 10^3, p_{max} = 1.9992e-7$			
	MCMC	IS	
Avg. est.	2.0024e-7	2.0027e-7	
Std. dev.	3e-11	20e-11	
Avg. time per batch(s)	15.9	15.9	
$b = 20, T = 10^5, \alpha = 2, n = 5, a = 10^4, p_{max} = 1.99992e-9$			
	MCMC	IS	
Avg. est.	2.00025e-9	2.00091e-9	
Std. dev.	7e-14	215e-14	
Avg. time per batch(s)	15.9	15.9	



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Efficient Sampling for a Heavy-Tailed Random Walk

Numerical Illustration

 $n = 20, \alpha = 2, a_n = an.$

$b = 25, T = 10^5, \alpha = 2, n = 20, a = 20, p_{max} = 1.2437e-4$			
	MCMC	IS	MC
Avg. est.	1.375e-4	1.374e-4	1.444e-4
Std. dev.	2e-7	3e-7	492e-7
Avg. time per batch(s)	52.8	50.0	2.0
$b = 25, T = 10^5, \alpha = 2, n = 20, a = 200, p_{max} = 1.2494e-6$			
	MCMC	IS	MC
Avg. est.	1.2614e-6	1.2615e-6	1.2000e-6
Std. dev.	4e-10	12e-10	33,166e-10
Avg. time per batch(s)	49.4	48.4	1.9
$b = 20, T = 10^5, \alpha$	= 2, <i>n</i> = 20, <i>a</i>	$= 10^3, p_{max} =$	4.9995e-8
	MCMC	IS	
Avg. est.	5.0091e-8	5.0079e-8	
Std. dev.	7e-12	66e-12	
Avg. time per batch(s)	53.0	50.6	
$b = 20, T = 10^5, \alpha = 2, n = 20, a = 10^4, p_{max} = 5.0000e-10$			
	MCMC	IS	
Avg. est.	5.0010e-10	5.0006e-10	
Std. dev.	2e-14	71e-14	
Avg. time per batch(s)	48.0	47.1	



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Markov Chain Monte Carlo in Rare-Event Simulation

Efficient Sampling of Heavy-Tailed Random Sums

Outline

- Introduction to Rare-Event Simulation
 The Problem with Monte Carlo
 - Importance Sampling
- Importance Sampling in a Heavy-Tailed Setting
 The Conditional Mixture Algorithm for Random Walks
 Performance of the Conditional Mixture Algorithm
- Markov Chain Monte Carlo in Rare-Event Simulation
 Efficient Sampling for a Heavy-Tailed Random Walk
 Efficient Sampling of Heavy-Tailed Random Sums



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Importance Sampling in a Heavy-Tailed Setting

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Efficient Sampling for a Heavy-Tailed Random Sum

- Let $\{Z_k\}$ be iid with density *f*.
- Put $S_n = Z_1 + \cdots + Z_n$ and let $\{N_n\}$ be independent of $\{Z_k\}$
- Compute $\mathbb{P}{S_{N_n} > a_n}$.
- Heavy-tailed assumption:⁴

$$\lim_{n\to\infty}\frac{\mathbb{P}\{S_{N_n}>a_n\}}{\mathbb{P}\{M_{N_n}>a_n\}}=1.$$

⁴See e.g. [6] for examples.

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Constructing the Gibbs Sampler

- Suppose we are in state $(N_t, Z_{t,1}, ..., Z_{t,N_t}) = (k_t, z_{t,1}, ..., z_{t,k_t})$.
- Let $k_t^* = \min\{j : z_{t,1} + \cdots + z_{t,j} > a_n\}.$
- Update the number of steps N_{t+1} from the distribution

$$p(k_{t+1} \mid k_t^*) = \mathbb{P}\{N = k_{t+1} \mid N \ge k^{*t}\}$$

- If $k_{t+1} > k_t$, sample $Z_{t+1,k_t+1}, \ldots, Z_{t+1,k_{t+1}}$ independently from F_Z .
- Proceed by updating all steps as before.
- Permute the steps.

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Properties of the algorithm

The Markov chain $\{(N_t, Z_{t,1}, ..., Z_{t,N_t})\}$ is uniformly ergodic with stationary distribution

$$F_{\mathcal{A}}(\cdot) = \mathbb{P}\{(Z_1,\ldots,Z_n)' \in \cdot \mid Z_1 + \ldots Z_n > a_n\}$$

• With v as the density of $\mathbb{P}\{(N, Z_1, \dots, Z_N) \in \cdot \mid M_N > a_n\}$ we have

$$\frac{v(k, z_1, \dots, z_k)}{f(k, z_1, \dots, z_k)} = \frac{1}{\mathbb{P}\{M_N > a_n\}} I\{\max z_1, \dots, z_k > a_n\}$$
$$= \frac{1}{1 - g_N(F_Z(a_n))} I\{\max z_1, \dots, z_k > a_n\}.$$

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The algorithm has vanishing normalized variance.



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Asymptotics and Simulation of Heavy-Tailed Processes

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Numerical illustration

Geometric(ρ) number of steps: $\rho = 0.05$, $\alpha = 1$, $a_n = a/\rho$.

$b=25,T=10^5,lpha=1, ho=0.2,a=10^2, ho_{ m max}=0.990$ e-2					
	MCMC	IS	MC		
Avg. est.	1.149e-2	1.087e-2	1.089e-2		
Std. dev.	4e-5	6e-5	35e-5		
Avg. time per batch(s)	25.0	11.0	1.2		
$b = 25, T = 10^5, \alpha = 1, \rho = 0.2, a = 10^3, p_{max} = 0.999e-3$					
	MCMC	IS	MC		
Avg. est.	1.019e-3	1.012e-3	1.037e-3		
Std. dev.	1e-6	3e-6	76e-6		
Avg. time per batch(s)	25.8	11.1	1.2		
$b = 20, T = 10^{6}, \alpha = 1, \rho = 0.2, a = 5 \cdot 10^{7}, p_{max} = 2.000000e-8$					
	MCMC	IS			
Avg. est.	2.000003e-8	1.999325e-8			
Std. dev.	6e-14	1114e-14			
Avg. time per batch(s)	385.3	139.9			
$b = 20, T = 10^{6}, \alpha = 1, \rho = 0.2, a = 5 \cdot 10^{9}, p_{max} = 2.0000e-10$					
	MCMC	IS			
Avg. est.	2.0000e-10	1.9998e-10			
Std. dev.	0	13e-14			
Avg. time per batch(s)	358.7	130.9			



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Numerical Illustration

Geometric(ρ) number of steps: $\rho = 0.05$, $\alpha = 1$, $a_n = a/\rho$.

$b = 25, T = 10^5, \alpha = 1, \rho = 0.05, a = 10^3, p_{max} = 0.999e-3$					
	MCMC	IS	MC		
Avg. est.	1.027e-3	1.017e-3	1.045e-3		
Std. dev.	1e-6	4e-6	105e-6		
Avg. time per batch(s)	61.5	44.8	1.3		
$b = 25, T = 10^{\circ}, \alpha = 1, \rho = 0.05, a = 5 \cdot 10^{\circ}, p_{max} = 1.9999e-6$					
	MCMC	IS	MC		
Avg. est.	2.0002e-6	2.0005e-6	3.2000e-6		
Std. dev.	1e-10	53e-10	55,678e-10		
Avg. time per batch(s)	60.7	45.0	1.3		



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For Further Reading I



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