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Image: A matrix

Markov chain Monte Carlo for computing probabilities of rare events in a heavy-tailed random walk

Thorbjörn Gudmundsson and Henrik Hult

Department of Mathematics KTH Stockholm

KTH, June 2012

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Consider a random variable X with known distribution F and the objective of computing

$$p = \mathbb{P}(X \in A),$$

where $\{X \in A\}$ is thought as rare in the sense that p is small.

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Background		



Consider a random variable X with known distribution F and the objective of computing

$$p = \mathbb{P}(X \in A),$$

where $\{X \in A\}$ is thought as rare in the sense that *p* is small.

Example. Random walk $S_m = Y_1 + \cdots + Y_m$ with non-negative steps *Y*'s with known heavy-tailed distribution F_Y and objective of computing

$$p=\mathbb{P}\Big(rac{S_m}{m}>a\Big),$$

where *a* is much larger than $\mathbb{E}[Y]$.

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Problem

Problem: compute
$$p = \mathbb{P}\left(\frac{S_m}{m} > a\right)$$
.

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Problem

Problem: compute
$$p = \mathbb{P}\Big(\frac{S_m}{m} > a\Big)$$
.

- Sometimes no analytical solution known,
- Monte Carlo simulation approach computationally inefficient for small p.

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Background

Problem

Problem: compute
$$p = \mathbb{P}\Big(\frac{S_m}{m} > a\Big)$$
.

- Sometimes no analytical solution known,
- Monte Carlo simulation approach computationally inefficient for small p.
- Goal: construct an efficient estimator \hat{p} in the sense that

$$\mathsf{RE}(\hat{\pmb{
ho}}) := rac{\mathbb{V}\textit{ar}(\hat{\pmb{
ho}})}{p^2}$$

is bounded or tends to zero as $p \rightarrow 0$.

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Importance sampling

Goal: construct an efficient estimator \hat{p} .

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Importance sampling

Goal: construct an efficient estimator \hat{p} . The importance sampling approach (Dupuis et al 2007)

- Generate *n* copies of *X* independently from a sampling distribution *G*.
- Compute empirical estimate

$$\hat{p} = \frac{1}{n} \sum_{k=1}^{n} \frac{dF}{dG}(X_k) \mathbb{I}\{X_k \in A\}.$$

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Background

Importance sampling continued

Reduces to finding a suitable sampling distribution G.

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Background

Importance sampling continued

- Reduces to finding a suitable sampling distribution G.
- The zero-variance distribution

$$F_A(x) = \mathbb{P}(X \le x | X \in A).$$

Seems difficult sampling directly from F_A since it requires knowledge of $\mathbb{P}(X \in A)$!

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Idea		

Want: sample from $F_A(x) = \mathbb{P}(X \le x | X \in A)$. Assuming the existence of a density, it takes the form

$$f_{\mathcal{A}}(x) = rac{f(x)\mathbb{I}\{x\in \mathcal{A}\}}{\mathbb{P}(X\in \mathcal{A})}.$$

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Idea		

Want: sample from $F_A(x) = \mathbb{P}(X \le x | X \in A)$. Assuming the existence of a density, it takes the form

$$f_{\mathcal{A}}(x) = rac{f(x)\mathbb{I}\{x\in \mathcal{A}\}}{\mathbb{P}(X\in \mathcal{A})}.$$

The main idea is to construct a Markov chain $(X_k)_{k\geq 1}$ for which f_A is the invariant density via MCMC. Then *extract* information about the normalising constant from the sample.

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■ Construct a Markov chain (X_k)_{k≥1} via MCMC sampler, with the zero-variance distribution F_A as its invariant distribution.

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MCMC approach		



- Construct a Markov chain (X_k)_{k≥1} via MCMC sampler, with the zero-variance distribution F_A as its invariant distribution.
- For any $v \ge 0$ such that $\int_A v(x) dx = 1$, consider

$$u\bigl((X_k)_{k\geq 1}\bigr)=\frac{1}{n}\sum_{k=1}^n\frac{v(X_k)\mathbb{I}\{X_k\in A\}}{f(X_k)}.$$

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 Random Walk with Heavy-tails

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Estimator continued

For $\int_A v(x) dx = 1$ it holds

$$\mathbb{E}_{F_A}\left[\frac{1}{n}\sum_{k=1}^n \frac{v(X_k)\mathbb{I}\{X_k \in A\}}{f(X_k)}\right] = \int_A \frac{v(x)}{f(x)} \frac{f(x)}{p} dx$$
$$= \frac{1}{p} \int_A v(x) dx$$
$$= \frac{1}{p}.$$

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 Random Walk with Heavy-tails

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Estimator continued

For $\int_A v(x) dx = 1$ it holds

$$\mathbb{E}_{F_A}\left[\frac{1}{n}\sum_{k=1}^n \frac{v(X_k)\mathbb{I}\{X_k \in A\}}{f(X_k)}\right] = \int_A \frac{v(x)}{f(x)}\frac{f(x)}{p}dx$$
$$= \frac{1}{p}\int_A v(x)dx$$
$$= \frac{1}{p}.$$

• Define
$$\hat{p} = \left(\frac{1}{n}\sum_{k=1}^{n} \frac{v(X_k)\mathbb{I}\{X_k \in A\}}{f(X_k)}\right)^{-1}$$
.

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MCMC approach

Design issues

Estimator
$$\hat{p} = \left(\frac{1}{n}\sum_{k=1}^{n}\frac{v(X_k)\mathbb{I}\{X_k \in A\}}{f(X_k)}\right)^{-1}$$
.

Choice of v: controls the variance, set to ensure rare-event efficiency of the algorithm

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Design issues

Estimator
$$\hat{p} = \left(\frac{1}{n}\sum_{k=1}^{n}\frac{v(X_k)\mathbb{I}\{X_k \in A\}}{f(X_k)}\right)^{-1}$$
.

Choice of v: controls the variance, set to ensure rare-event efficiency of the algorithm

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Choice of the MCMC sampler: crucial to control the dependence of the Markov chain

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Controlling the variance

Goal: ensure $\mathbb{V}ar(\hat{p})/p^2$ is bounded as $p \to 0$.

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Controlling the variance

Goal: ensure $\mathbb{V}ar(\hat{p})/p^2$ is bounded as $p \to 0$.

Taylor expansion of g(Z) around $\mathbb{E}[Z]$ leads to

$$\mathbb{V}ar(g(Z)) \approx \mathbb{V}ar(g(\mathbb{E}[Z]) + g'(\mathbb{E}[Z])(Z - \mathbb{E}[Z]))$$

= $(g'(\mathbb{E}[Z]))^2 \mathbb{V}ar(Z).$

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Controlling the variance

Goal: ensure $\mathbb{V}ar(\hat{p})/p^2$ is bounded as $p \to 0$. Taylor expansion of g(Z) around $\mathbb{E}[Z]$ leads to $\mathbb{V}ar(g(Z)) \approx \mathbb{V}ar(g(\mathbb{E}[Z]) + g'(\mathbb{E}[Z])(Z - \mathbb{E}[Z]))$ $= (g'(\mathbb{E}[Z]))^2 \mathbb{V}ar(Z).$

Applied to
$$g(Z) = 1/Z$$
 and $Z = \frac{1}{n} \sum_{k=1}^{n} u(X_k)$ where

$$u(x) = \frac{v(x)\mathbb{I}\{x \in A\}}{f(x)},$$

then leads to

$$\mathbb{V}ar_{F_A}(\hat{p}) \approx p^4 \mathbb{V}ar\Big(\frac{1}{n}\sum_{k=1}^n u(X_k)\Big) \leq C \cdot p^4 \mathbb{V}ar(u(X)).$$

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Controlling the variance continued

Proposition

If $p^2 \mathbb{V}ar_{F_A}(u(X)) \to 0$ as $p \to 0$ then \hat{p} has vanishing relative error (is sufficient).

How do we choose v to fulfill this proposition?

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Controlling the variance continued

Consider the term

$$p^{2} \mathbb{V}ar(u(X)) = p^{2} (\mathbb{E}[u(X)^{2}] - \mathbb{E}[u(X)]^{2})$$

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

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Controlling the variance continued

Consider the term

$$p^{2} \mathbb{V}ar(u(X)) = p^{2} (\mathbb{E}[u(X)^{2}] - \mathbb{E}[u(X)]^{2})$$

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

• choosing
$$v(x) = f_A(x) = f(x)\mathbb{I}\{x \in A\}/p$$
 implies
 $p^2 \mathbb{V}ar(u(X)) = p \int_A \frac{f^2(x)/p^2}{f(x)} dx - 1 = \frac{1}{p} \int_A f(x) dx - 1 = 0.$

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Controlling the variance continued

Consider the term

$$p^{2} \mathbb{V}ar(u(X)) = p^{2} \left(\mathbb{E}[u(X)^{2}] - \mathbb{E}[u(X)]^{2} \right)$$

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

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

• choosing $v(x) = f_A(x) = f(x)\mathbb{I}\{x \in A\}/p$ implies

$$p^2 \mathbb{V}ar(u(X)) = p \int_A \frac{f^2(x)/p^2}{f(x)} dx - 1 = \frac{1}{p} \int_A f(x) dx - 1 = 0.$$

Choose *v* as an approximation of the zero-variance density!

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Sample $(X_k)_{k\geq 1}$ under F_A via MCMC

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Sample (X_k)_{k≥1} under F_A via MCMC Show p² Var(u(X)) → 0 as p → 0

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- Sample $(X_k)_{k\geq 1}$ under F_A via MCMC
- Show $p^2 \mathbb{V}ar(u(X)) \to 0$ as $p \to 0$
- Show $(X_k)_{k\geq 1}$ is geometric ergodic

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Formulation		

Setup

Consider a random walk S_m = Y₁ + ··· + Y_m with non-negative steps Y's with known heavy-tailed distribution F_Y and objective of computing

$$p = \mathbb{P}\Big(rac{S_m}{m} > a\Big),$$

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where *a* is much larger than $\mathbb{E}[Y]$.

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Formulation		

Setup

Consider a random walk S_m = Y₁ + ··· + Y_m with non-negative steps Y's with known heavy-tailed distribution F_Y and objective of computing

$$p = \mathbb{P}\Big(rac{S_m}{m} > a\Big),$$

where *a* is much larger than $\mathbb{E}[Y]$.

Construct $(\mathbf{Y}_k)_{k>1}$ via MCMC with invariant density

$$f_{\mathcal{A}}(\mathbf{y}) = \frac{f_{\mathbf{Y}}(\mathbf{y})\mathbb{I}\{y_1 + \dots + y_m > am\}}{\mathbb{P}(S_m > am)}$$

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Formulation		

Setup

Consider a random walk S_m = Y₁ + ··· + Y_m with non-negative steps Y's with known heavy-tailed distribution F_Y and objective of computing

$$p = \mathbb{P}\Big(rac{S_m}{m} > a\Big),$$

where *a* is much larger than $\mathbb{E}[Y]$.

Construct $(\mathbf{Y}_k)_{k>1}$ via MCMC with invariant density

$$f_{A}(\mathbf{y}) = \frac{f_{\mathbf{Y}}(\mathbf{y})\mathbb{I}\{y_{1} + \dots + y_{m} > am\}}{\mathbb{P}(S_{m} > am)}$$

A typical such a random walk has a m – 1 number of "small" steps and one "large" step.

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Gibbs sampler

Initial state $\mathbf{Y}_0 = (Y_{0,1}, \dots, Y_{0,m})$ such that $Y_{0,1} > am$ and $Y_{0,i} = 0$ for other indices. Given $\mathbf{Y}_k = (Y_{k,1}, \dots, Y_{k,m})$, $k = 0, 1, \dots$ the next state \mathbf{Y}_{k+1} is sampled as follows

Take a copy of the current state, let $Y_{k+1,i} = Y_{k,i}$,

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Gibbs sampler

Initial state $\mathbf{Y}_0 = (Y_{0,1}, \dots, Y_{0,m})$ such that $Y_{0,1} > am$ and $Y_{0,i} = 0$ for other indices. Given $\mathbf{Y}_k = (Y_{k,1}, \dots, Y_{k,m})$, $k = 0, 1, \dots$ the next state \mathbf{Y}_{k+1} is sampled as follows

- **Take a copy of the current state, let** $Y_{k+1,i} = Y_{k,i}$,
- Draw a random index $j \in \{1, \ldots, m\}$,

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Gibbs sampler

Initial state $\mathbf{Y}_0 = (Y_{0,1}, \dots, Y_{0,m})$ such that $Y_{0,1} > am$ and $Y_{0,i} = 0$ for other indices. Given $\mathbf{Y}_k = (Y_{k,1}, \dots, Y_{k,m})$, $k = 0, 1, \dots$ the next state \mathbf{Y}_{k+1} is sampled as follows

- Take a copy of the current state, let $Y_{k+1,i} = Y_{k,i}$,
- Draw a random index $j \in \{1, \ldots, m\}$,
- Sample $Y_{k+1,j}$ from the conditional distribution of Y given that the sum exceeds the threshold,

$$\mathbb{P}(Y_{k+1,j} \in \cdot) = \mathbb{P}(Y \in \cdot \mid Y + \sum_{i \neq j} Y_{k,i} > am).$$

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Gibbs sampler

Initial state $\mathbf{Y}_0 = (Y_{0,1}, \dots, Y_{0,m})$ such that $Y_{0,1} > am$ and $Y_{0,i} = 0$ for other indices. Given $\mathbf{Y}_k = (Y_{k,1}, \dots, Y_{k,m})$, $k = 0, 1, \dots$ the next state \mathbf{Y}_{k+1} is sampled as follows

- Take a copy of the current state, let $Y_{k+1,i} = Y_{k,i}$,
- Draw a random index $j \in \{1, \ldots, m\}$,
- Sample $Y_{k+1,j}$ from the conditional distribution of Y given that the sum exceeds the threshold,

$$\mathbb{P}(Y_{k+1,j} \in \cdot) = \mathbb{P}(Y \in \cdot \mid Y + \sum_{i \neq j} Y_{k,i} > am).$$

Permutate the steps in \mathbf{Y}_{k+1}.

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Gibbs sampler continued

Proposition

The Markov chain $(\mathbf{Y}_k)_{k\geq 1}$ constructed using the proposed Gibbs sampler has the conditional distribution F_A as its invariant distribution.

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MCMC estimator

■ The MCMC estimator $\hat{p} = \left(\frac{1}{n}\sum_{k=1}^{n} \frac{v(\mathbf{y}_k)\mathbb{I}\{S_m > am\}}{f(\mathbf{y}_k)}\right)^{-1}$. The steps are heavy-tailed in the sense that

$$\frac{\mathbb{P}(\textit{M}_m > \textit{am})}{\mathbb{P}(\textit{S}_m > \textit{am})} \to 1,$$

where $M_m = \max_i \{y_{k,i}\}$.

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MCMC estimator

■ The MCMC estimator $\hat{p} = \left(\frac{1}{n}\sum_{k=1}^{n} \frac{v(\mathbf{y}_k)\mathbb{I}\{S_m > am\}}{f(\mathbf{y}_k)}\right)^{-1}$. The steps are heavy-tailed in the sense that

$$\frac{\mathbb{P}(\textit{M}_m > \textit{am})}{\mathbb{P}(\textit{S}_m > \textit{am})} \to 1,$$

where $M_m = \max_i \{y_{k,i}\}$.

Therefore seems smart to use

 $\mathbb{P}(\mathbf{Y} \in \cdot \mid \textit{M}_m > \textit{am}) \ \text{ as a proxy for } \ \mathbb{P}(\mathbf{Y} \in \cdot \mid \textit{S}_m > \textit{am}).$

Propose

$$v(\mathbf{y}_k) = \frac{f(\mathbf{y}_k)\mathbb{I}\{M_m > am\}}{\mathbb{P}(M_m > am)}$$

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MCMC estimator continued

Choosing
$$v(\mathbf{y}) = \frac{f(\mathbf{y})\mathbb{I}\{M_m > am\}}{\mathbb{P}(M_m > am)}$$
 yields
$$u(\mathbf{y}) = \frac{v(\mathbf{y})\mathbb{I}\{S_m > am\}}{f(\mathbf{y})} = \frac{\mathbb{I}\{M_m > am\}}{\mathbb{P}(M_m > am)}.$$

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MCMC estimator continued

Choosing
$$v(\mathbf{y}) = \frac{f(\mathbf{y})\mathbb{I}\{M_m > am\}}{\mathbb{P}(M_m > am)}$$
 yields

$$u(\mathbf{y}) = \frac{v(\mathbf{y})\mathbb{I}\{S_m > am\}}{f(\mathbf{y})} = \frac{\mathbb{I}\{M_m > am\}}{\mathbb{P}(M_m > am)}.$$

$$\hat{p} = \mathbb{P}(M_m > am) \left(\frac{1}{n} \sum_{k=1}^n \mathbb{I}\{M_m(k) > am\}\right)^{-1}$$

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$$p^{2}\mathbb{V}ar_{F_{A}}(u(\mathbf{Y})) = \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}}\mathbb{V}ar_{F_{A}}(\mathbb{I}\{M_{m} > am\})$$

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$$p^{2} \mathbb{V}ar_{F_{A}}(u(\mathbf{Y})) = \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \mathbb{V}ar_{F_{A}}(\mathbb{I}\{M_{m} > am\})$$
$$= \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \left(\mathbb{E}_{F_{A}}[\mathbb{I}\{M_{m} > am\}] - \mathbb{E}_{F_{A}}[\mathbb{I}\{M_{m} > am\}]^{2}\right)$$

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Efficiency

$$p^{2} \mathbb{V}ar_{F_{A}}(u(\mathbf{Y})) = \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \mathbb{V}ar_{F_{A}}(\mathbb{I}\{M_{m} > am\})$$

$$= \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \left(\mathbb{E}_{F_{A}}[\mathbb{I}\{M_{m} > am\}] - \mathbb{E}_{F_{A}}[\mathbb{I}\{M_{m} > am\}]^{2}\right)$$

$$= \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \left(\frac{\mathbb{P}(M_{m} > am)}{\mathbb{P}(S_{m} > am)} - \frac{\mathbb{P}(M_{m} > am)^{2}}{\mathbb{P}(S_{m} > am)^{2}}\right)$$

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Application

Efficiency

$$p^{2} \mathbb{V}ar_{F_{A}}(u(\mathbf{Y})) = \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \mathbb{V}ar_{F_{A}}(\mathbb{I}\{M_{m} > am\})$$

$$= \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \left(\mathbb{E}_{F_{A}}[\mathbb{I}\{M_{m} > am\}] - \mathbb{E}_{F_{A}}[\mathbb{I}\{M_{m} > am\}]^{2}\right)$$

$$= \frac{\mathbb{P}(S_{m} > am)^{2}}{\mathbb{P}(M_{m} > am)^{2}} \left(\frac{\mathbb{P}(M_{m} > am)}{\mathbb{P}(S_{m} > am)} - \frac{\mathbb{P}(M_{m} > am)^{2}}{\mathbb{P}(S_{m} > am)^{2}}\right)$$

$$= \frac{\mathbb{P}(S_{m} > am)}{\mathbb{P}(M_{m} > am)} - 1 \rightarrow 0 \quad \text{as } p \rightarrow 0.$$

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Markov chain Monte Carlo for computing probabilities of rare events in a heavy-tailed random walk

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Geometric ergodicity

■ The design of the Gibbs sampler ensures that the Markov chain (**Y**_{*k*})_{*k*≥1} is (uniformly) ergodic.

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Geometric ergodicity

- The design of the Gibbs sampler ensures that the Markov chain (Y_k)_{k≥1} is (uniformly) ergodic.
- This guarantees that the chain mixes sufficiently and hence that Var(p̂) → 0 as n → ∞ at same speed as 1/n.

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Geometric ergodicity

- The design of the Gibbs sampler ensures that the Markov chain (Y_k)_{k≥1} is (uniformly) ergodic.
- This guarantees that the chain mixes sufficiently and hence that Var(p̂) → 0 as n → ∞ at same speed as 1/n.
- The proof is technical ...

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Concluding remarks

- p̂ is an efficient estimator for heavy-tailed random walk for increasing (but fixed) number of steps.
- Extension to heavy-tailed random sum $\sum_{k=1}^{N} Y_k$ where *N* is stochastic.
- Other models such as recursion formulas, queues, ...

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Tables and figures

Assumptions

- The MCMC estimator p̂ tested against importance sampling and standard Monte Carlo.
- Steps are Pareto(2) distributed.
- Number of batches: 25, simulations per batch: 10,000.

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Tables and figures



т	а	MCMC	IS	MC	
5	10	3.40e-3	2.91e-3	2.83e-3	Avg. est.
		(0.81e-4)	(1.77e-4)	(4.74e-4)	(Std. dev.)
		[4.1]	[3.4]	[0.7]	[Avg. time (ms)]
10	20	3.34e-4	3.02e-4	2.68e-4	Avg. est.
		(5.83e-6)	(2.02e-6)	(162.58e-6)	(Std. dev.)

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Tables and figures

10,000 simulations for m = 10 and a = 20



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