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A VANILLA RAO–BLACKWELLISATION OF METROPOLIS–HASTINGS ALGORITHMS

BY RANDAL DOUC AND CHRISTIAN P. ROBERT

Telecom SudParis, Evry, France

CEREMADE, Université Paris Dauphine, and CREST, INSEE, Paris

Casella and Robert (1996) presented a general Rao–Blackwellisation principle for accept–reject and Metropolis–Hastings schemes that leads to significant decreases in the variance of the resulting estimators, but at a high cost in computing and storage. Adopting a completely different perspective, we introduce instead a universal scheme that guarantees variance reductions in all Metropolis–Hastings based estimators while keeping the computing cost under control. We establish a central limit theorem for the improved estimators and illustrate their performances on toy examples.

1. Introduction. As its accept–reject predecessor, the Metropolis–Hastings simulation algorithm relies in part on the generation of uniform variables to achieve given acceptance probabilities. More precisely, given a target density f wrt to a dominating measure on the space \mathcal{X} , if the Metropolis–Hastings proposal is associated with the density $q(x|y)$ (wrt the same dominating measure), the acceptance probability of the corresponding Metropolis–Hastings iteration at time t is

$$\alpha(x^{(t)}, y_t) = \min \left\{ 1, \frac{\pi(y_t)}{\pi(x^{(t)})} \frac{q(x^{(t)}|y_t)}{\pi(x^{(t)})q(y_t|x^{(t)})} \right\}$$

when $y_t \sim q(y_t|x^{(t)})$ is the proposed value for $x^{(t+1)}$. In practice, this means that a uniform $u_t \sim \mathcal{U}(0, 1)$ is first generated and that $x^{(t+1)} = y_t$ if, and only if, $u_t \leq \alpha(x^{(t)}, y_t)$.

Since the uniformity of the u_t 's is an extraneous (albeit necessary) noise, in that it does not directly bring information upon the target f (but only through its acceptance rate), Casella and Robert (1996) took advantage of this flow of auxiliary variables u_t to reduce the variance of the resulting estimators while preserving their unbiasedness by integrating out the u_t 's conditional on all simulated y_t 's. Unfortunately, this strategy has a non-negligible cost of $O(N^2)$ for a given sample of size N . While extensions have

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be proposed in the literature (Casella and Robert, 1998, Perron, 1999), this solution is not often considered in practice, in part due to this very cost. The current paper reproduces the Rao–Blackwellisation argument of Casella and Robert (1996) by a different representation that allows to reduce the variance at a fixed computing cost. Section 2 exposes the Rao–Blackwellisation technique and validates the resulting variance reduction, including a derivation of the asymptotic variance of the improved estimators, while Section 3 presents some illustrations of the improvement on toy examples.

2. The Rao–Blackwellisation solution. When considering the outcome of a Metropolis–Hastings experiment, $(x^{(t)})_t$, and the way it is used in Monte Carlo approximations,

$$(1) \quad \delta = \frac{1}{N} \sum_{t=1}^N h(x^{(t)}),$$

alternative representations of this estimator are

$$\delta = \frac{1}{N} \sum_{t=1}^N \sum_{j=1}^t h(y_j) \mathbb{I}_{x^{(t)}=y_j} \quad \text{and} \quad \delta = \frac{1}{N} \sum_{i=1}^M \mathbf{n}_i h(\mathfrak{z}_i),$$

where the y_j 's are the proposed Metropolis–Hastings moves, the \mathfrak{z}_i 's are the accepted y_j 's, M is the number of accepted y_j 's till time N , and \mathbf{n}_i is the number of times \mathfrak{z}_i appears in the sequence $(x^{(t)})_t$. The first representation is the one used by Casella and Robert (1996), who integrate out the random elements of the outer sum given the sequence of y_t 's. The second representation is also found in Gåsemyr (2002), Sahu and Zhigljavsky (1998, 2003) and is the basis for our construction.

Let us first recall the basic properties of the pairs $(\mathfrak{z}_i, \mathbf{n}_i)$:

LEMMA 1. *The sequence $(\mathfrak{z}_i, \mathbf{n}_i)$ satisfies*

1. $(\mathfrak{z}_i, \mathbf{n}_i)_i$ is a Markov chain;
2. \mathfrak{z}_{i+1} and \mathbf{n}_i are independent given \mathfrak{z}_i ;
3. \mathbf{n}_i is distributed as a geometric random variable with probability parameter

$$(2) \quad p(\mathfrak{z}_i) := \int \alpha(\mathfrak{z}_i, y) q(y|\mathfrak{z}_i) dy;$$

4. $(\mathfrak{z}_i)_i$ is a Markov chain with transition kernel $\tilde{Q}(\mathfrak{z}, dy) = \tilde{q}(y|\mathfrak{z})dy$ and stationary distribution $\tilde{\pi}$ such that

$$\tilde{q}(\cdot|\mathfrak{z}) \propto \alpha(\mathfrak{z}, \cdot) q(\cdot|\mathfrak{z}) \quad \text{and} \quad \tilde{\pi}(\cdot) \propto \pi(\cdot)p(\cdot).$$

PROOF. We only prove the last point of the lemma. The transition kernel density \tilde{q} of the Markov chain $(\mathfrak{z}_i)_i$ is obtained by integrating out the geometric waiting time, namely $\tilde{q}(\cdot|\mathfrak{z}_i) = \alpha(\mathfrak{z}_i, \cdot) q(\cdot|\mathfrak{z}_i) / p(\mathfrak{z}_i)$. Thus,

$$\tilde{\pi}(x)\tilde{q}(y|x) = \frac{\pi(x)p(x)}{\int \pi(u)p(u)du} \frac{\alpha(x, y)q(y|x)}{p(x)} = \tilde{\pi}(x)\tilde{q}(x|y),$$

where we have used the detailed balance property of the original Metropolis–Hastings algorithm, namely that $\pi(x)q(y|x)\alpha(x, y) = \pi(y)q(x|y)\alpha(y, x)$. This shows that the Markov chain $(\mathfrak{z}_i)_i$ also satisfies a detailed balance property with respect to $\tilde{\pi}$, thus that it is $\tilde{\pi}$ -reversible, which concludes the proof. \square

Since the Metropolis–Hastings estimator δ only involves the \mathfrak{z}_i 's, i.e. the accepted y_t 's, an optimal weight for those random variables would be the importance weight $1/p(\mathfrak{z}_i)$, leading to the corresponding importance sampling estimator

$$\delta^* = \frac{1}{N} \sum_{i=1}^M \frac{h(\mathfrak{z}_i)}{p(\mathfrak{z}_i)},$$

but this quantity is usually unavailable in closed form and needs to be estimated by an unbiased estimator. The geometric \mathbf{n}_i is the obvious solution that is used in the original Metropolis–Hastings estimate, but solutions with smaller variance also are available, as shown by the following results:

LEMMA 2. *If $(y_j)_j$ is an iid sequence with distribution $q(y|\mathfrak{z}_i)$, the quantity*

$$\hat{\xi}_i = 1 + \sum_{j=1}^{\infty} \prod_{\ell \leq j} \{1 - \alpha(\mathfrak{z}_i, y_\ell)\}$$

is an unbiased estimator of $1/p(\mathfrak{z}_i)$ which variance, conditional on \mathfrak{z}_i , is lower than the conditional variance of \mathbf{n}_i , $\{1 - p(\mathfrak{z}_i)\}/p^2(\mathfrak{z}_i)$.

PROOF. Since \mathbf{n}_i can be written as

$$\mathbf{n}_i = 1 + \sum_{j=1}^{\infty} \prod_{\ell \leq j} \mathbb{I}\{u_\ell \geq \alpha(\mathfrak{z}_i, y_\ell)\},$$

where the u_j 's are iid $\mathcal{U}(0, 1)$, given that the sum actually stops with the first pair (u_j, y_j) such that $u_j \leq \alpha(\mathfrak{z}_i, y_j)$, a Rao–Blackwellised version of \mathbf{n}_i

consists in its expectation conditional on the sequence $(y_j)_j$:

$$\begin{aligned}\hat{\xi}_i &= 1 + \sum_{j=1}^{\infty} \mathbb{E} \left[\prod_{\ell \leq j} \mathbb{I}\{u_\ell \geq \alpha(\mathfrak{z}_i, y_\ell)\} \middle| (y_t)_{t \geq 1} \right] \\ &= 1 + \sum_{j=1}^{\infty} \prod_{\ell \leq j} \mathbb{P}(u_\ell \geq \alpha(\mathfrak{z}_i, y_\ell) | (y_t)_{t \geq 1}) \\ &= 1 + \sum_{j=1}^{\infty} \prod_{\ell \leq j} \{1 - \alpha(\mathfrak{z}_i, y_\ell)\}.\end{aligned}$$

Therefore, since $\hat{\xi}_i$ is a conditional expectation of \mathbf{n}_i , its variance is necessarily smaller. \square

Given that $\alpha(\mathfrak{z}_i, y_j)$ involves a ratio of probability densities, $\alpha(\mathfrak{z}_i, y_j)$ takes the value 1 with positive probability and the sum $\hat{\xi}_i$ is therefore almost surely finite. This may however requires far too many iterations to be realistically computed or it may involve too much variability in the number of iterations thus required. An intermediate estimator with a fixed computational cost is fortunately available:

PROPOSITION 1. *If $(y_j)_j$ is an iid sequence with distribution $q(y|\mathfrak{z}_i)$ and $(u_j)_j$ is an iid uniform sequence, for any $k \geq 0$, the quantity*

$$(3) \quad \hat{\xi}_i^k = 1 + \sum_{j=1}^{\infty} \prod_{1 \leq \ell \leq k \wedge j} \{1 - \alpha(\mathfrak{z}_i, y_j)\} \prod_{k+1 \leq \ell \leq j} \mathbb{I}\{u_\ell \geq \alpha(\mathfrak{z}_i, y_\ell)\}$$

is an unbiased estimator of $1/p(\mathfrak{z}_i)$ involving an almost sure finite number of terms. Moreover, for $k \geq 1$,

$$\mathbb{V} \left[\hat{\xi}_i^k | \mathfrak{z}_i \right] = \frac{1 - p(\mathfrak{z}_i)}{p^2(\mathfrak{z}_i)} - \frac{1 - (1 - 2p(\mathfrak{z}_i) + r(\mathfrak{z}_i))^k}{2p(\mathfrak{z}_i) - r(\mathfrak{z}_i)} \left(\frac{2 - p(\mathfrak{z}_i)}{p^2(\mathfrak{z}_i)} \right) (p(\mathfrak{z}_i) - r(\mathfrak{z}_i)),$$

where p is defined in (2) and $r(\mathfrak{z}_i) := \int \alpha^2(\mathfrak{z}_i, y) q(y|\mathfrak{z}_i) dy$. Therefore, we have

$$\mathbb{V} \left[\hat{\xi}_i | \mathfrak{z}_i \right] \leq \mathbb{V} \left[\hat{\xi}_i^k | \mathfrak{z}_i \right] \leq \mathbb{V} \left[\hat{\xi}_i^0 | \mathfrak{z}_i \right] = \mathbb{V} \left[\mathbf{n}_i | \mathfrak{z}_i \right].$$

The truncation at the k -th proposal thus allows for a calibration of the computational effort since computing $\hat{\xi}_i^k$ costs on average k additional simulations of y_j and computations of $\alpha(\mathfrak{z}_i, y_j)$, when compared with the regular Metropolis–Hastings weight \mathbf{n}_i .

PROOF. Define $y = (y_j)_{j \geq 1}$ and $u_{k:\infty} = (u_\ell)_{\ell \geq k}$. Note that $\hat{\xi}_i^0 = \mathbf{n}_i$ and therefore, the conditional variance of $\hat{\xi}_i^0$ is the variance of a geometric variable. Now, obviously $\hat{\xi}_i^{k+1} = \mathbb{E} \left[\hat{\xi}_i^k \mid \mathfrak{z}_i, y, u_{k+2:\infty} \right]$; thus, we have

$$\mathbb{V} \left[\hat{\xi}_i^k \mid \mathfrak{z}_i \right] = \mathbb{V} \left[\hat{\xi}_i^{k+1} \mid \mathfrak{z}_i \right] + \mathbb{E} \left[\mathbb{V} \left[\hat{\xi}_i^k \mid \mathfrak{z}_i, y, u_{k+2:\infty} \right] \mid \mathfrak{z}_i \right].$$

To get a closed-form expression of the second term of the rhs, we first introduce a geometric random variable T_k defined by

$$T_k = 1 + \sum_{j=1}^{\infty} \prod_{\ell \leq j} \mathbb{I} \{ u_{k+\ell} \geq \alpha(\mathfrak{z}_i, y_{k+\ell}) \}.$$

Then, by straightforward algebra, $\hat{\xi}_i^k$ may be rewritten as

$$\hat{\xi}_i^k = C + \left(\prod_{\ell=1}^k \{1 - \alpha(\mathfrak{z}_i, y_\ell)\} \right) T_{k+2} \mathbb{I} \{ u_{k+1} > \alpha(\mathfrak{z}_i, y_{k+1}) \}$$

where C does not depend on u_1, \dots, u_{k+1} . Thus,

$$\mathbb{V} \left[\hat{\xi}_i^k \mid \mathfrak{z}_i, y, u_{k+2:\infty} \right] = \left(\prod_{\ell=1}^k \{1 - \alpha(\mathfrak{z}_i, y_\ell)\} \right)^2 T_{k+2}^2 \alpha(\mathfrak{z}_i, y_{k+1}) \{1 - \alpha(\mathfrak{z}_i, y_{k+1})\},$$

Taking the expectation of the above expression, we obtain

$$\mathbb{E} \left(\mathbb{V} \left[\hat{\xi}_i^k \mid \mathfrak{z}_i, y, u_{k+2:\infty} \right] \right) = (1 - 2p(\mathfrak{z}_i) + r(\mathfrak{z}_i))^k \left(\frac{2 - p(\mathfrak{z}_i)}{p^2(\mathfrak{z}_i)} \right) (p(\mathfrak{z}_i) - r(\mathfrak{z}_i)),$$

which concludes the proof. \square

Using those Rao-Blackwellised versions of δ brings an asymptotic improvement for the estimation of $\mathbb{E}_\pi[h(X)]$, as shown by the following result which, for any $M > 0$, compares the estimators ($k \geq 0$)

$$\delta_M^k = \frac{\sum_{i=1}^M \hat{\xi}_i^k h(\mathfrak{z}_i)}{\sum_{i=1}^M \hat{\xi}_i^k}.$$

For any positive function φ , we denote $\mathcal{C}_\varphi = \{h; |h/\varphi|_\infty < \infty\}$ the set of functions bounded by φ up to a constant and we assume throughout that the reference (if unavailable) importance sampling estimator is sufficiently well-behaved, in that there exist positive functions $\varphi \geq 1$ and ψ such that

$$(4) \quad \forall h \in \mathcal{C}_\varphi, \quad \frac{\sum_{i=1}^M h(\mathfrak{z}_i)/p(\mathfrak{z}_i)}{\sum_{i=1}^M 1/p(\mathfrak{z}_i)} \xrightarrow{\mathbb{P}} \pi(h)$$

$$(5) \quad \forall h \in \mathcal{C}_\psi, \quad \sqrt{M} \left(\frac{\sum_{i=1}^M h(\mathfrak{z}_i)/p(\mathfrak{z}_i)}{\sum_{i=1}^M 1/p(\mathfrak{z}_i)} - \pi(h) \right) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Gamma(h))$$

THEOREM 1. *Under the assumption that $\pi(p) > 0$, the following convergence properties hold:*

i) If h is in \mathcal{C}_φ , then

$$\delta_M^k \xrightarrow[M \rightarrow \infty]{\mathbb{P}} \pi(h)$$

ii) If, in addition, $h^2/p \in \mathcal{C}_\varphi$ and $h \in \mathcal{C}_\psi$, then

$$(6) \quad \sqrt{M}(\delta_M^k - \pi(h)) \xrightarrow[M \rightarrow \infty]{\mathcal{L}} \mathcal{N}(0, V_k[h - \pi(h)]),$$

where $V_k(h) := \pi(p) \int \pi(d\mathfrak{z}) \mathbb{V} \left[\hat{\xi}_i^k \mid \mathfrak{z} \right] h^2(\mathfrak{z}) p(\mathfrak{z}) + \Gamma(h)$.

PROOF. We will prove that, for all $g \in \mathcal{C}_\varphi$,

$$(7) \quad M^{-1} \sum_{i=1}^M \hat{\xi}_i^k g(\mathfrak{z}_i) \xrightarrow{\mathbb{P}} \pi(g)/\pi(p).$$

Then, *i)* directly follows from (7) applied to both $g = h$ and $g = 1$. Now, denote by \mathcal{F}_i the σ -field $\mathcal{F}_i := \sigma(\mathfrak{z}_1, \dots, \mathfrak{z}_{i+1}, \hat{\xi}_1^k, \dots, \hat{\xi}_i^k)$. Since $\mathbb{E} \left[\hat{\xi}_i^k g(\mathfrak{z}_i) \mid \mathcal{F}_{i-1} \right] = g(\mathfrak{z}_i)/p(\mathfrak{z}_i)$, we have

$$M^{-1} \sum_{i=1}^M \hat{\xi}_i^k g(\mathfrak{z}_i) = \left(\sum_{i=1}^M U_{M,i} - \mathbb{E} [U_{M,i} \mid \mathcal{F}_{i-1}] \right) + M^{-1} \sum_{i=1}^M g(\mathfrak{z}_i)/p(\mathfrak{z}_i),$$

with $U_{M,i} := M^{-1} \hat{\xi}_i^k g(\mathfrak{z}_i)$. First consider the second term of the rhs. Since $\varphi \geq 1$, the function p is in \mathcal{C}_φ ; then, Eq. (4) implies that $M/\{\sum_{i=1}^M 1/p(\mathfrak{z}_i)\} \xrightarrow{\mathbb{P}} \pi(p) > 0$ and therefore that

$$(8) \quad \forall g \in \mathcal{C}_\varphi, \quad M^{-1} \sum_{i=1}^M g(\mathfrak{z}_i)/p(\mathfrak{z}_i) \xrightarrow{\mathbb{P}} \pi(g)/\pi(p).$$

It remains to check that $\sum_{i=1}^M U_{M,i} - \mathbb{E} [U_{M,i} \mid \mathcal{F}_{i-1}] \xrightarrow{\mathbb{P}} 0$. We use asymptotic results for conditional triangular arrays of random variables established in Douc and Moulines (2008, Theorem 11). Obviously, since $|g| \in \mathcal{C}_\varphi$,

$$\sum_{i=1}^M \mathbb{E} [|U_{M,i}| \mid \mathcal{F}_{i-1}] = M^{-1} \sum_{i=1}^M |g(\mathfrak{z}_i)|/p(\mathfrak{z}_i) \xrightarrow{\mathbb{P}} \pi(|g|)/\pi(p),$$

and we only need to show that $\sum_{i=1}^M \mathbb{E} [|U_{M,i}| \mathbb{I}\{|U_{M,i}| > \epsilon\} \mid \mathcal{F}_{i-1}] \xrightarrow{\mathbb{P}} 0$. Let $C > 0$ and note that $\{|U_{M,i}| > \epsilon\} \subset \{|g(\mathfrak{z}_i)| > (\epsilon M)/C\} \cup \{\hat{\xi}_i^k > C\}$. Using

again $\mathbb{E} \left[\hat{\xi}_i^k g(\mathfrak{z}_i) \middle| \mathcal{F}_{i-1} \right] = g(\mathfrak{z}_i)/p(\mathfrak{z}_i)$, we have

$$(9) \quad \sum_{i=1}^M \mathbb{E} \left[|U_{M,i}| \mathbb{I}\{|U_{M,i}| > \epsilon\} \middle| \mathcal{F}_{i-1} \right] \leq \frac{1}{M} \sum_{i=1}^M \frac{|g(\mathfrak{z}_i)| \mathbb{I}\{|g(\mathfrak{z}_i)| > (\epsilon M)/C\}}{p(\mathfrak{z}_i)} + \frac{1}{M} \sum_{i=1}^M \frac{F_C(\mathfrak{z}_i)}{p(\mathfrak{z}_i)},$$

with $F_C(\mathfrak{z}_i) := |g(\mathfrak{z}_i)| \mathbb{E} \left[\hat{\xi}_i^k \mathbb{I}\{\xi_i^k > C\} \middle| \mathfrak{z}_i \right] p(\mathfrak{z}_i)$. Since $F_C \leq |g|$, we have $F_C \in \mathcal{C}_\varphi$. Then, using again (8),

$$\begin{aligned} \frac{1}{M} \sum_{i=1}^M \frac{|g(\mathfrak{z}_i)| \mathbb{I}\{|g(\mathfrak{z}_i)| > (\epsilon M)/C\}}{p(\mathfrak{z}_i)} &\xrightarrow{\mathbb{P}} 0, \\ \frac{1}{M} \sum_{i=1}^M \frac{F_C(\mathfrak{z}_i)}{p(\mathfrak{z}_i)} &\xrightarrow{\mathbb{P}} \pi(F_C)/\pi(p), \end{aligned}$$

which can be arbitrarily small when taking C sufficiently large. Indeed, using Lebesgue's theorem in the definition of F_C , for any fixed \mathfrak{z} , $\lim_{C \rightarrow \infty} F_C(\mathfrak{z}) = 0$ and then, using again Lebesgue's theorem, $\lim_{C \rightarrow \infty} \pi(F_C) = 0$. Finally, (7) is proved. The proof of *i*) follows.

We now consider *ii*). Without loss of generality, we assume that $\pi(h) = 0$. Write

$$\sqrt{M} \delta_M^k = \frac{M^{-1/2} \sum_{i=1}^M \hat{\xi}_i^k h(\mathfrak{z}_i)}{M^{-1} \sum_{i=1}^M \hat{\xi}_i^k}.$$

By (7), the denominator of the rhs converges in probability to $1/\pi(p)$. Thus, by Slutsky's Lemma, we only need to prove a CLT for the numerator of the rhs. Set $U_{M,i} := M^{-1/2} \hat{\xi}_i^k h(\mathfrak{z}_i)$ and write:

$$M^{-1/2} \sum_{i=1}^M \hat{\xi}_i^k h(\mathfrak{z}_i) = \left(\sum_{i=1}^M U_{M,i} - \mathbb{E} [U_{M,i} \middle| \mathcal{F}_{i-1}] \right) + M^{-1/2} \sum_{i=1}^M h(\mathfrak{z}_i)/p(\mathfrak{z}_i).$$

Since $h \in \mathcal{C}_\psi$ and $M^{-1} \sum_{i=1}^M 1/p(\mathfrak{z}_i) \xrightarrow{\mathbb{P}} 1/\pi(p)$, the second term, thanks again to Slutsky's lemma and Eq. (5), converges in distribution to $\mathcal{N}(0, \Gamma(h)/\pi^2(p))$. Now, consider the first term of the rhs. We will once again use asymptotic results on triangular arrays of random variables (as in Douc and

Moulines, 2008, Theorem 13). We have

$$\begin{aligned} & \sum_{i=1}^M \mathbb{E} \left[U_{M,i}^2 \middle| \mathcal{F}_{i-1} \right] - (\mathbb{E} [U_{M,i} \middle| \mathcal{F}_{i-1}])^2 \\ &= M^{-1} \sum_{i=1}^M \left(h^2(\mathfrak{z}_i) \mathbb{V} \left[\hat{\xi}_i^k \middle| \mathfrak{z}_i \right] p(\mathfrak{z}_i) \right) / p(\mathfrak{z}_i) \xrightarrow{\mathbb{P}} \pi \left[\mathbb{V} \left[\hat{\xi}_i^k \middle| \cdot \right] h^2(\cdot) p(\cdot) \right] / \pi(p), \end{aligned}$$

by (8) applied to the non negative function $\mathfrak{z}_i \mapsto h^2(\mathfrak{z}_i) \mathbb{V} \left[\hat{\xi}_i^k \middle| \mathfrak{z}_i \right] p(\mathfrak{z}_i)$ which is in \mathcal{C}_φ since it is bounded from above by $h^2/p \in \mathcal{C}_\varphi$. It remains for us to show that, for any $\epsilon > 0$,

$$(10) \quad \sum_{i=1}^M \mathbb{E} \left[|U_{M,i}|^2 \mathbb{I}_{|U_{M,i}| > \epsilon} \middle| \mathcal{F}_{i-1} \right] \xrightarrow{\mathbb{P}} 0.$$

Following the same lines as in the proof of *i*), note that for any $C > 0$, we have $\{|U_{M,i}| > \epsilon\} \subset \{|h(\mathfrak{z}_i)| > (\epsilon\sqrt{M})/C\} \cup \{\hat{\xi}_i^k > C\}$. Using that

$$\mathbb{E} \left[\left(\hat{\xi}_i^k \right)^2 \middle| \mathcal{F}_{i-1} \right] = \mathbb{V} \left[\hat{\xi}_i^k \middle| \mathfrak{z}_i \right] + \left(\mathbb{E} \left[\hat{\xi}_i^k \middle| \mathfrak{z}_i \right] \right)^2 \leq 2/p^2(\mathfrak{z}_i),$$

we have

$$\begin{aligned} & \sum_{i=1}^M \mathbb{E} \left[|U_{M,i}| \mathbb{I}_{\{|U_{M,i}| > \epsilon\}} \middle| \mathcal{F}_{i-1} \right] \\ & \leq \frac{2}{M} \sum_{i=1}^M \frac{h^2(\mathfrak{z}_i) \mathbb{I}_{\{|h(\mathfrak{z}_i)| > (\epsilon\sqrt{M})/C\}}}{p^2(\mathfrak{z}_i)} + \frac{1}{M} \sum_{i=1}^M \frac{F_C(\mathfrak{z}_i)}{p(\mathfrak{z}_i)} \end{aligned}$$

with $F_C(\mathfrak{z}_i) := h^2(\mathfrak{z}_i) \mathbb{E} \left[\left(\hat{\xi}_i^k \right)^2 \mathbb{I}_{\{\hat{\xi}_i^k > C\}} \middle| \mathfrak{z}_i \right] p(\mathfrak{z}_i)$. Since $F_C \leq (2h^2)/p$ and $h^2/p \in \mathcal{C}_\varphi$, we have $F_C \in \mathcal{C}_\varphi$. Then, using again Eq. (8),

$$\begin{aligned} & \frac{1}{M} \sum_{i=1}^M \frac{(h^2(\mathfrak{z}_i)/p(\mathfrak{z}_i)) \mathbb{I}_{\{|h(\mathfrak{z}_i)| > (\epsilon\sqrt{M})/C\}}}{p(\mathfrak{z}_i)} \xrightarrow{\mathbb{P}} 0, \\ & \frac{1}{M} \sum_{i=1}^M \frac{F_C(\mathfrak{z}_i)}{p(\mathfrak{z}_i)} \xrightarrow{\mathbb{P}} \pi(F_C)/\pi(p), \end{aligned}$$

which can be arbitrarily small by taking C sufficiently large. Indeed, as in the proof of *i*), one can use Lebesgue's theorem in the definition of F_C so that for any fixed \mathfrak{z} , $\lim_{C \rightarrow \infty} F_C(\mathfrak{z}) = 0$. Then, using again by Lebesgue's theorem, $\lim_{C \rightarrow \infty} \pi(F_C) = 0$. Finally, (10) is proved. The proof of *ii*) follows. \square

The main consequence of this CLT is thus that, asymptotically, the correlation between the ξ_i 's vanishes, hence that the variance ordering on the ξ_i 's extends to the same ordering on the δ_M 's.

It remains for us to link the CLT of the usual MCMC estimator (1) with the CLT expressed in (6) with $k = 0$ associated with the accepted values. We will need some additional assumptions, starting with a maximal inequality for the Markov chain $(\mathfrak{z}_i)_i$: there exists a measurable function ζ such that for any starting point x ,

$$(11) \quad \forall h \in \mathcal{C}_\zeta, \quad \mathbb{P}_x \left(\left| \sup_{0 \leq i \leq N} \sum_{j=0}^i [h(\mathfrak{z}_j) - \tilde{\pi}(h)] \right| > \epsilon \right) \leq \frac{C_h(x)}{(\epsilon N)^2}$$

where \mathbb{P}_x is the probability measure induced by the Markov chain $(\mathfrak{z}_i)_{i \geq 0}$ starting from $\mathfrak{z}_0 = x$.

Moreover, we assume that there exists a measurable function $\phi \geq 1$ such that for any starting point x ,

$$(12) \quad \forall h \in \mathcal{C}_\phi, \quad \tilde{Q}^n(x, h) \xrightarrow{\mathbb{P}} \tilde{\pi}(h) = \pi(ph)/\pi(p),$$

where \tilde{Q} is the transition kernel of $(\mathfrak{z}_i)_i$ expressed in Lemma 1.

THEOREM 2. *In addition to the assumptions of Theorem 1, assume that h is a measurable function such that $h/p \in \mathcal{C}_\zeta$ and $\{C_{h/p}, h^2/p^2\} \subset \mathcal{C}_\phi$. Assume moreover that*

$$\sqrt{M} \left(\delta_M^0 - \pi(h) \right) \xrightarrow{\mathcal{L}} \mathcal{N}(0, V_0[h - \pi(h)]).$$

Then, for any starting point x ,

$$\sqrt{M_N} \left(\frac{\sum_{t=1}^N h(x^{(t)})}{N} - \pi(h) \right) \xrightarrow{\mathcal{L}}_{N \rightarrow \infty} \mathcal{N}(0, V_0[h - \pi(h)]),$$

where M_N is defined by

$$(13) \quad \sum_{i=1}^{M_N} \hat{\xi}_i^0 \leq N < \sum_{i=1}^{M_N+1} \hat{\xi}_i^0.$$

PROOF. Without loss of generality, we assume that $\pi(h) = 0$. In this proof, we will denote by \mathbb{P}_x (resp. \mathbb{E}_x) the probability (resp. expectation) associated to the Markov chain $(x^{(t)})_{t \geq 0}$ starting from a fixed point x . Using (7) with $g = 1$, one may divide (13) by M_N and let N go to infinity. This

yields that $M_N/N \xrightarrow{\mathbb{P}} \pi(p) > 0$. Then, by Slutski's lemma, Theorem 2 will be proved if we are able to show that

$$\sqrt{N} \left(\frac{\sum_{t=1}^N h(x^{(t)})}{N} - \pi(h) \right) \xrightarrow{\mathcal{L}}_{N \rightarrow \infty} \mathcal{N}(0, V_0[h - \pi(h)]/\pi(p)).$$

To that purpose, consider the following decomposition:

$$N^{-1/2} \sum_{t=1}^N h(x^{(t)}) := \Delta_{N,1} + \Delta_{N,2} + \Delta_{N,3},$$

where $M_N^* := \lfloor N\pi(p) \rfloor$,

$$\begin{aligned} \Delta_{N,1} &:= N^{-1/2} \left(N - \sum_{i=1}^{M_N} \hat{\xi}_i^0 \right) h(\mathfrak{z}_{M_N+1}), \\ \Delta_{N,2} &:= N^{-1/2} \left(\sum_{i=1}^{M_N} \hat{\xi}_i^0 h(\mathfrak{z}_i) - \sum_{i=1}^{M_N^*} \hat{\xi}_i^0 h(\mathfrak{z}_i) \right), \\ \Delta_{N,3} &:= N^{-1/2} \sum_{i=1}^{M_N^*} \hat{\xi}_i^0 h(\mathfrak{z}_i). \end{aligned}$$

Using that $0 \leq N - \sum_{i=1}^{M_N} \hat{\xi}_i^0 \leq \hat{\xi}_{M_N+1}^0$ and Markov's inequality,

$$\mathbb{P}_x(|\Delta_{N,1}| > \epsilon) \leq \frac{\mathbb{E}_x(\hat{\xi}_{M_N+1}^0 |h(\mathfrak{z}_{M_N+1})|)}{\epsilon \sqrt{N}} = \frac{\tilde{Q}^{M_N+1}(x, |h|/p)}{\epsilon \sqrt{N}}$$

which converges in probability to 0 using that $|h|/p \leq h^2/p^2 + 1$ and $\{h^2/p^2, 1\} \subset \mathcal{C}_\phi$. Thus, $\Delta_{N,1} \xrightarrow{\mathbb{P}} 0$. We now consider $\Delta_{N,2}$. Note that

$$(14) \quad \mathbb{P}_x(|\Delta_{N,2}| > \epsilon) \leq \mathbb{P}_x(|A_N| > \epsilon \sqrt{N}/2) + \mathbb{P}_x(|B_N| > \epsilon \sqrt{N}/2)$$

with

$$A_N = \sum_{i=M_N \wedge M_N^*}^{M_N \vee M_N^*} h(\mathfrak{z}_i)/p(\mathfrak{z}_i) \quad \text{and} \quad B_N = \sum_{i=M_N \wedge M_N^*}^{M_N \vee M_N^*} (\hat{\xi}_i^0 - 1/p(\mathfrak{z}_i))h(\mathfrak{z}_i).$$

Now, pick an arbitrary $\alpha \in (0, 1)$ and set $\underline{M}_N := M_N^*(1 - \alpha)$ and $\overline{M}_N := M_N^*(1 + \alpha)$. Since $M_N/N \xrightarrow{\mathbb{P}} \pi(p)$, for all $\eta > 0$, there exists N_0 such that

for all $N \geq N_0$, $\mathbb{P}_x(\underline{M}_N \leq M_N \leq \overline{M}_N) \geq 1 - \eta$. Then, obviously for $N \geq N_0$, the first term of the rhs of (14) is bounded by

$$(15) \quad \mathbb{P}_x(|A_N| > \epsilon\sqrt{N}/2) \leq \eta + \mathbb{P}_x \left(\sup_{M_N^* \leq i \leq \overline{M}_N} \left| \sum_{j=M_N^*}^i h(\mathfrak{z}_j)/p(\mathfrak{z}_j) \right| > \epsilon\sqrt{N}/2 \right) \\ + \mathbb{P}_x \left(\sup_{\underline{M}_N \leq i \leq M_N^*} \left| \sum_{j=i}^{M_N^*} h(\mathfrak{z}_j)/p(\mathfrak{z}_j) \right| > \epsilon\sqrt{N}/2 \right).$$

Using (11), the second term of the rhs is bounded by $4(\overline{M}_N - M_N^*)\mathbb{E}_x[C_{h/p}(\mathfrak{z}_{M_N^*})]/\epsilon^2 N$, which converges to $4\alpha\pi(p)\tilde{\pi}(C_{h/p})/\epsilon^2$ as N goes to infinity using that $C_{h/p} \in \mathcal{C}_\phi$. The obtained bound can thus be arbitrarily small as α goes to 0. Similarly, one can bound the third term of the rhs of (15) and let N go to infinity. Letting again α go to 0, we obtain that $A_N/\sqrt{N} \xrightarrow{\mathbb{P}} 0$. Similarly, the second term of the rhs of (14) is bounded by

$$(16) \quad \mathbb{P}_x(|B_N| > \epsilon\sqrt{N}/2) \leq \eta + \\ \mathbb{P}_x \left(\sup_{M_N^* \leq i \leq \overline{M}_N} \left| \sum_{j=M_N^*}^i \left(\hat{\xi}_j^0 - \frac{1}{p(\mathfrak{z}_j)} \right) h(\mathfrak{z}_j) \right| > \epsilon\sqrt{N}/2 \right) \\ + \mathbb{P}_x \left(\sup_{\underline{M}_N \leq i \leq M_N^*} \left| \sum_{j=i}^{M_N^*} \left(\hat{\xi}_j^0 - \frac{1}{p(\mathfrak{z}_j)} \right) h(\mathfrak{z}_j) \right| > \epsilon\sqrt{N}/2 \right)$$

Denote $R_N = \sum_{\ell=1}^N \left(\hat{\xi}_\ell^0 - \frac{1}{p(\mathfrak{z}_\ell)} \right) h(\mathfrak{z}_\ell)$. Clearly, (R_N) is a \mathcal{F} -martingale where $\mathcal{F} = (\mathcal{F}_i)_{i \geq 1}$ and \mathcal{F}_i is the σ -field $\mathcal{F}_i := \sigma(\mathfrak{z}_1, \dots, \mathfrak{z}_{i+1}, \hat{\xi}_1^0, \dots, \hat{\xi}_i^0)$. Then, by Kolmogorov's inequality, one can bound the second term of (16) in the following way:

$$\mathbb{P}_x \left(\sup_{M_N^* \leq i \leq \overline{M}_N} |R_i - R_{M_N^*}| > \epsilon\sqrt{N}/2 \right) \leq 4 \frac{\mathbb{E}_x \left[(R_{M_N^*} - R_{M_N^*})^2 \right]}{\epsilon^2 N} \\ = \frac{4}{\epsilon^2 N} \mathbb{E}_x \left[\sum_{i=M_N^*}^{\overline{M}_N} \frac{1 - p(\mathfrak{z}_i)}{p^2(\mathfrak{z}_i)} h^2(\mathfrak{z}_i) \right] = \frac{4(\overline{M}_N - M_N^* + 1) \sum_{i=M_N^*}^{\overline{M}_N} \tilde{Q}^i(x, \frac{1-p}{p^2} h^2)}{\epsilon^2 N (\overline{M}_N - M_N^* + 1)} \\ \xrightarrow{\mathbb{P}} \frac{4\alpha\pi \left(\frac{1-p}{p} h^2 \right)}{\epsilon^2},$$

which can be arbitrarily small as α goes to 0. Similarly, one can bound the third term of (16) and let N go to infinity. Finally, letting α go to 0, we

obtain that $B_N/\sqrt{N} \xrightarrow{\mathbb{P}} 0$. Thus, $\Delta_{N,2} \xrightarrow{\mathbb{P}} 0$. Finally, by Slutsky's lemma,

$$\Delta_{N,3} := (N/M_N^*)^{-1/2} \frac{\sum_{i=1}^{M_N^*} \hat{\xi}_i^0 h(\mathfrak{z}_i)}{\sqrt{M_N^*}} \xrightarrow{\mathcal{L}} \mathcal{N}(0, V_0[h - \pi(h)]/\pi(p)).$$

The proof now stands completed. \square

3. Illustrations. We first consider a random walk Metropolis–Hastings algorithm with target the $\mathcal{N}(0, 1)$ distribution and with proposal $q(y|x) = \varphi(x - y; \tau)$, i.e. a normal random walk with scale $\tau = 10$. The acceptance probability is then the ratio of the targets and Figure 1 illustrates the gain provided by the Rao–Blackwellisation scheme by repeating the simulation 250 times and by representing the 90% range as well as the whole range of both estimators. The gain provided by the Rao–Blackwellisation is not huge wrt to the overlap of both estimates, but one must consider that the variability of the estimator δ is due to two sources of randomness, one due to the \mathbf{n}_i 's and the other one to the \mathfrak{z}_i 's, and that the Rao–Blackwellisation only impact the first one.

Our second example is an independent Metropolis–Hastings algorithm with target the $\mathcal{N}(0, 1)$ distribution and with proposal a Cauchy $\mathcal{C}(0, .25)$ distribution. The outcome is quite similar to the first example, although producing a slightly superior improvement, as shown on Figure 2.

Our third example is an independent Metropolis–Hastings algorithm with target the $\mathcal{Exp}(\lambda)$ distribution and with proposal the $\mathcal{Exp}(\mu)$ distribution. In this case, the probability functions $p(x)$ in (2) and $r(x)$ in Proposition 1 can be derived in closed form as

$$p(x) = 1 - \frac{\lambda - \mu}{\lambda} e^{-\mu x} \quad \text{and} \quad r(x) = 1 - \frac{2(\lambda - \mu)}{2\lambda - \mu} e^{-\mu x}.$$

This special feature means that we can compare the variability of the original Metropolis–Hastings estimator with its Rao–Blackwellised version δ_M^∞ , but also with the optimal importance sampling version shown in (4). As illustrated by Figure 3, the gain brought by the Rao–Blackwellisation is significant when compared with the reduction in variance of the optimal importance sampling version.

Our fourth and final example is a geometric $\mathcal{Geo}(\beta)$ target associated with a one-step random walk proposal:

$$\pi(x) = \beta(1 - \beta)^x \quad \text{and} \quad 2q(y|x) = \begin{cases} \mathbb{I}_{|x-y|=1} & \text{if } x > 0, \\ \mathbb{I}_{|y|\leq 1} & \text{if } x = 0. \end{cases}$$

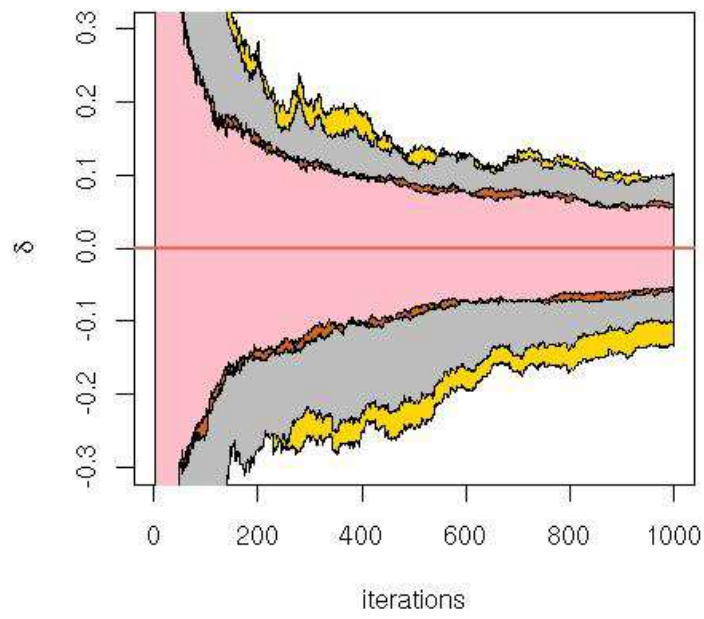


FIG 1. *Overlay of the variations of 250 iid realisations of the estimates δ (gold) and δ^∞ (grey) of $\mathbb{E}[X] = 0$ for 1000 iterations, along with the 90% interquantile range for the estimates δ (brown) and δ^∞ (pink), in the setting of a random walk Gaussian proposal with scale $\tau = 10$.*

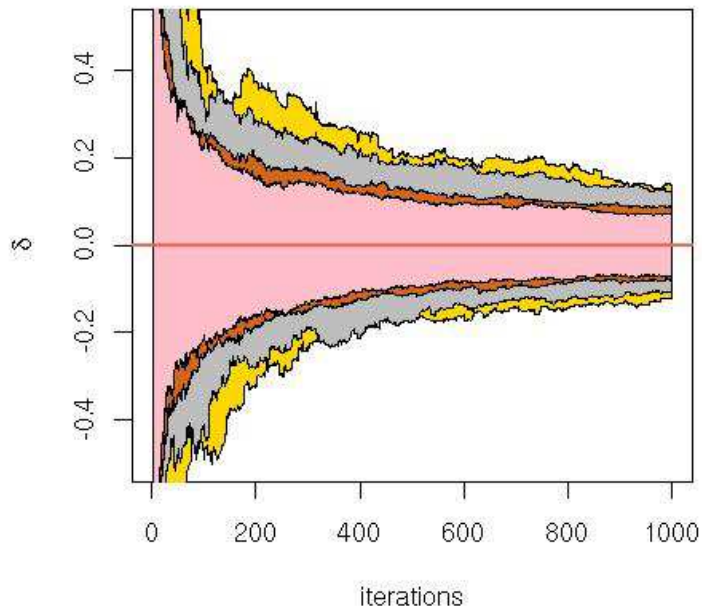


FIG 2. *Overlay of the variations of 250 iid realisations of the estimates δ (gold) and δ^∞ (grey) of $\mathbb{E}[X] = 0$ for 1000 iterations, along with the 90% interquantile range for the estimates δ (brown) and δ^∞ (pink), in the setting of an independent Cauchy proposal with scale 0.25.*

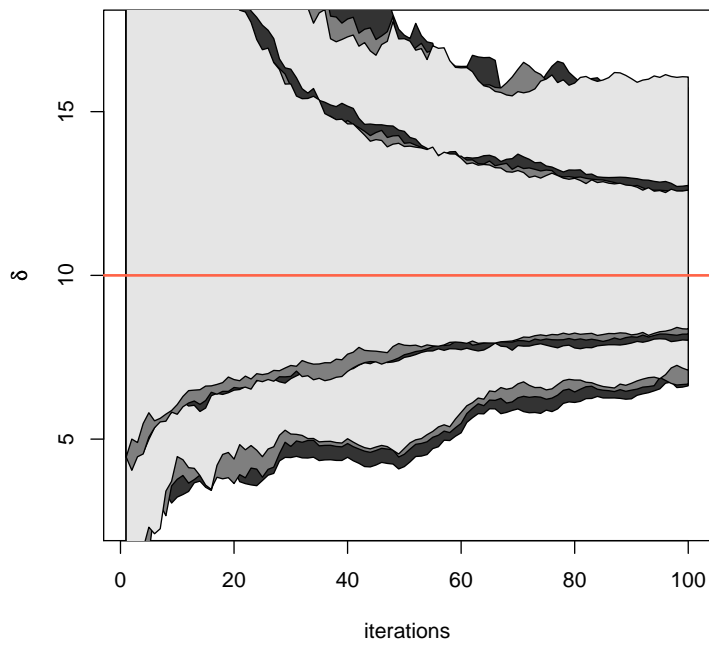


FIG 3. *Overlay of the variations of 500 iid realisations of the estimates δ (deep grey), δ^∞ (medium grey) and of the importance sampling version (light grey) of $\mathbb{E}[X] = 10$ when $X \sim \text{Exp}(.1)$ for 100 iterations, along with the 90% interquantile ranges (same colour code), in the setting of an independent exponential proposal with scale $\mu = 0.02$.*

For this problem,

$$p(x) = 1 - \beta/2 \text{ and } r(x) = 1 - \beta + \beta^2/2.$$

We can therefore compute the gain in variance

$$\frac{p(x) - r(x)}{2p(x) - r(x)} \frac{2 - p(x)}{p^2(x)} = 2 \frac{\beta(1 - \beta)(2 + \beta)}{(2 - \beta^2)(2 - \beta)^2}$$

which is optimal for $\beta = 0.174$, leading to a gain of 0.578 while the relative gain in variance is

$$\frac{p(x) - r(x)}{2p(x) - r(x)} \frac{2 - p(x)}{1 - p(x)} = \frac{(1 - \beta)(2 + \beta)}{(2 - \beta^2)}$$

which is decreasing in β .

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TELECOM SUDPARIS
91011 EVRY CEDEX, FRANCE
E-MAIL: Randal.Douc@it-sudparis.eu

CEREMADE
UNIVERSITÉ PARIS DAUPHINE
75775 PARIS CEDEX 16, FRANCE,
CREST-ENSAE, INSEE
92245 MALAKOFF CEDEX, FRANCE
E-MAIL: xian@ceremade.dauphine.fr