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DOES WASTE-RECYCLING REALLY IMPROVE METROPOLIS-HASTINGS MONTE CARLO ALGORITHM?

JEAN-FRANÇOIS DELMAS AND BENJAMIN JOURDAIN

ABSTRACT. The Metropolis Hastings algorithm and its multi-proposal extensions are aimed at the computation of the expectation $\langle \pi, f \rangle$ of a function f under a probability measure π difficult to simulate. They consist in constructing by an appropriate acceptance/rejection procedure a Markov chain $(X_k, k \geq 0)$ with transition matrix P such that π is reversible with respect to P and in estimating $\langle \pi, f \rangle$ by the empirical mean $I_n(f) = \frac{1}{n} \sum_{k=1}^n f(X_k)$. The waste-recycling Monte Carlo (WR) algorithm introduced by physicists is a modification of the Metropolis-Hastings algorithm, which makes use of all the proposals in the empirical mean, whereas the standard Metropolis-Hastings algorithm only uses the accepted proposals. In this paper, we extend the WR algorithm into a general control variate technique and exhibit the optimal choice of the control variate in terms of asymptotic variance. We also give an example which shows that in contradiction to the intuition of physicists, the WR algorithm can have an asymptotic variance larger than the one of the Metropolis-Hastings algorithm. However, in the particular case of the Metropolis-Hastings algorithm called Boltzmann algorithm, we prove that the WR algorithm is asymptotically better than the Metropolis-Hastings algorithm.

1. INTRODUCTION

The Metropolis-Hastings algorithm is used to compute the expectation $\langle \pi, f \rangle$ of a function f under a probability measure π difficult to simulate. It relies on the construction by an appropriate acceptance/rejection procedure of a Markov chain $(X_k, k \geq 0)$ with transition matrix P such that π is reversible with respect to P and the quantity of interest $\langle \pi, f \rangle$ is estimated by the empirical mean $I_n(f) = \frac{1}{n} \sum_{k=1}^n f(X_k)$. We shall recall the well-known properties of this estimation (consistency, asymptotic normality) in what follows. In particular the quality or precision of the algorithm is measured through the asymptotic variance of the estimator of $\langle \pi, f \rangle$.

The waste-recycling Monte Carlo (WR) algorithm, introduced by physicists, is a modification of the Metropolis-Hastings algorithm, which makes use of all the proposals in the empirical mean, whereas the standard Metropolis-Hastings algorithm only uses the accepted proposals. To our knowledge, the WR algorithm was first introduced in 1977 by Ceperley, Chester and Kalos in equation (35) p.3085 [3]. Without any proof, they claim that “The advantage of using this form is that some information about unlikely moves appears in the final answer, and the variance is lowered”. It is commonly assumed among the physicists and supported by most of the simulations that the WR algorithm is more efficient than the Metropolis-Hastings algorithm, that is the estimation given by the WR algorithm is consistent and has a smaller asymptotic variance. An other way to speed up the Metropolis-Hastings algorithm, that is to reduce the asymptotic variance, could be to use multiple proposals at

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each step instead of only one. According to Frenkel [5], the waste recycling can be particularly useful for these algorithms where many states are rejected.

Our aim is to clarify the presentation of the WR algorithms with one proposal and with multiple proposals and to present a first rigorous study of those algorithms. We will give in Section 2 an introduction to our results using a didactic point of view so that both the physicist and probabilistic communities could easily see the construction of the WR algorithm and the main results. In particular, we will stick to the finite state space case in the introduction and shall first state standard results on the consistency and asymptotic normality of the Metropolis-Hastings algorithm (and in particular we will recall the expression of the asymptotic variance using the solution of the Poisson equation). Our main new results are Theorem 3.3 and Corollary 3.7, which are a first step towards the comparison of the asymptotic variances. We shall detail their consequences in the didactic Section 2 for:

- the one proposal WR algorithm through Propositions 2.1 (consistency of the estimation), 2.2 (asymptotic normality) and 2.3 (a first partial answer to the initial question: Does waste-recycling really improve the Metropolis-Hastings Monte Carlo algorithm?),
- the multi-proposal WR algorithm through Propositions 2.6 (consistency of the estimation and asymptotic normality) and 2.7 (a second partial answer to the initial question: Does waste-recycling really improve the Metropolis-Hastings Monte Carlo algorithm?).

The study of the WR estimator in the form $I_n(f) + J_n(f)$, for a given functional J , leads us to rewrite the WR algorithm as a particular case of a general control variate problem by considering the estimators $I_n(f) + J_n(\psi)$ where the function ψ is possibly different from f . In the multi-proposal framework, the consistency (or convergence) of this general algorithm and its asymptotic normality are stated in Theorem 3.3 in Section 3. We also give its asymptotic variance. In Corollary 3.7, we prove the optimal choice of ψ in terms of asymptotic variance is the solution, F , of the Poisson equation (6). This choice achieves variance reduction, but the function F is difficult to compute and should be replaced by any approximation at hand. In some sense, f is such an approximation and for this particular choice we recover the Waste Recycling estimator introduced by physicists. In Section 3.4.2 we give a simple counterexample which shows that the WR algorithm does not in general improve the Metropolis-Hastings algorithm : the WR algorithm can have an asymptotic variance larger than the one of the Metropolis-Hastings algorithm. Since, Manuel Athènes [2] has also observed variance augmentation in some numerical computations of free energy. However, in the particular case of the Metropolis-Hastings algorithm called Boltzmann algorithm, we prove in Section 3.5 that the WR algorithm is asymptotically better than the Metropolis-Hastings algorithm (see Remark 2.4 on Boltzmann algorithm). Section 4 is devoted to the extension of the results to more general state spaces.

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2. DIDACTIC VERSION OF THE RESULTS

For simplicity, we assume that E is a finite set. Let $\langle \nu, h \rangle = \sum_{x \in E} \nu(x)h(x)$ denote the “integration” of a real function defined on E , $h = (h(x), x \in E)$, w.r.t. to a measure on E , $\nu = (\nu(x), x \in E)$.

Let π be a probability measure on E such that $\pi(x) > 0$ for all $x \in E$ and f a real function defined on E . The Metropolis-Hastings algorithm gives an estimation of $\langle \pi, f \rangle$ as the a.s. limit of the empirical mean of f , $\frac{1}{n} \sum_{k=1}^n f(X_k)$, as n goes to infinity, where $X = (X_n, n \geq 0)$ is a Markov chain which is reversible with respect to the probability measure π .

2.1. The Metropolis-Hastings algorithm. The Markov chain $X = (X_n, n \in \mathbb{N})$ of the Metropolis-Hastings algorithm is built in the following way. Let Q be an irreducible transition matrix over E : this means that $Q \in \mathbb{R}_+^{E \times E}$ is such that for all $x \in E$, $Q(x, \cdot)$ is a probability (i.e. $\sum_{y \in E} Q(x, y) = 1$) and for all $y \in E$, there exists $m \geq 1$ which may depend on (x, y) s.t. $Q^m(x, y) > 0$. We also assume that for all $x, y \in E$, if $Q(x, y) = 0$ then $Q(y, x) = 0$. The transition matrix Q is called the selection matrix.

For $x, y \in E$ such that $Q(x, y) > 0$, let $(\rho(x, y), \rho(y, x)) \in (0, 1]^2$ be such that

$$(1) \quad \rho(x, y)\pi(x)Q(x, y) = \rho(y, x)\pi(y)Q(y, x).$$

For example, one gets such a function ρ by setting

$$(2) \quad \rho(x, y) = \gamma \left(\frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)} \right), \quad \text{for all } x, y \in E \quad \text{s.t. } Q(x, y) > 0,$$

where γ is a function with values in $(0, 1]$ such that $\gamma(u) = u\gamma(1/u)$. Usually, one takes $\gamma(u) = \min(1, u)$ for the Metropolis algorithm. The case $\gamma(u) = u/(1+u)$ is known as the Boltzmann algorithm or Barker algorithm.

For convenience, we set $\rho(x, y) = 1$ if $Q(x, y) = 0$. Notice that $\rho(x, y) > 0$ for all $x, y \in E$. The function ρ is viewed as an acceptance probability.

Let X_0 be a random variable taking values in E with probability distribution ν_0 . At step n , X_0, \dots, X_n are given. The proposal at step $n+1$, \tilde{X}_{n+1} , is distributed according to $Q(X_n, \cdot)$. This proposal is accepted with probability $\rho(X_n, \tilde{X}_{n+1})$ and then $X_{n+1} = \tilde{X}_{n+1}$. If it is rejected, then we set $X_{n+1} = X_n$.

It is easy to check that $X = (X_n, n \geq 0)$ is a Markov chain with transition matrix P defined by

$$(3) \quad P(x, y) = \begin{cases} Q(x, y)\rho(x, y) & \text{if } x \neq y, \\ 1 - \sum_{z \neq x} P(x, z) & \text{if } x = y. \end{cases}$$

Furthermore X is reversible w.r.t. to the probability measure π : $\pi(x)P(x, y) = \pi(y)P(y, x)$ for all $x, y \in E$. This property is also called detailed balance. By summation over $y \in E$, one deduces that π is an invariant probability for P (i.e. $\pi P = \pi$). The irreducibility of Q implies that P is irreducible. Since the probability measure π is invariant for P , we deduce that X is positive recurrent with (unique) invariant probability measure π . In particular, for any real valued function f defined on E , the ergodic theorem (see e.g. [7]) implies the consistency of the estimation:

$$\lim_{n \rightarrow \infty} I_n(f) = \langle \pi, f \rangle \quad \text{a.s.},$$

where

$$(4) \quad I_n(f) = \frac{1}{n} \sum_{k=1}^n f(X_k).$$

The asymptotic normality of the estimator $I_n(f)$ is given by the following central limit theorem (see [4] or [7])

$$\sqrt{n}(I_n(f) - \langle \pi, f \rangle) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma(f)^2),$$

where $\mathcal{N}(0, \sigma^2)$ denotes the Gaussian distribution with mean 0 and variance σ^2 , $\sigma(f)^2$ is given by (5) below and the convergence holds in the distribution sense. Improving the Metropolis-Hastings algorithm means exhibiting other estimators of $\langle \pi, f \rangle$ that are still consistent (i.e. estimators which converge a.s. to $\langle \pi, f \rangle$) but with an asymptotic variance smaller than $\sigma(f)^2$.

Let us formally derive the expression of the asymptotic variance of the Metropolis-Hastings

algorithm. The variance of $\sqrt{n}I_n(f) = \frac{1}{\sqrt{n}} \sum_{k=1}^n f(X_k)$ is equal to

$$\frac{1}{n} \sum_{k,l=1}^n \text{Cov}(f(X_k), f(X_l)) = \frac{1}{n} \sum_{k=1}^n \left[\text{Var}(f(X_k)) + 2 \sum_{j=1}^{n-k} \text{Cov}(f(X_k), f(X_{k+j})) \right].$$

Intuitively it converges to $\sigma(f)^2 = \text{Var}_\pi(f(X_0)) + 2 \sum_{j \geq 1} \text{Cov}_\pi(f(X_0), f(X_j))$ where the subscript π means that X_0 is distributed according to π . One has

$$\sigma(f)^2 = \mathbb{E}_\pi[(f(X_0) - \langle \pi, f \rangle)^2] + 2\mathbb{E}_\pi \left[(f(X_0) - \langle \pi, f \rangle) P \sum_{k \geq 0} P^k (f - \langle \pi, f \rangle)(X_0) \right]$$

where for $R \in \mathbb{R}_+^{E \times E}$, $h : E \rightarrow \mathbb{R}$ and $x \in E$, we denote $Rh(x) = \sum_{y \in E} R(x, y)h(y)$. The function $F = \sum_{k \geq 0} P^k (f - \langle \pi, f \rangle)$ is a formal solution of the Poisson equation $F - PF = f - \langle \pi, f \rangle$. Plugging F in the formula for $\sigma(f)^2$ leads to

$$(5) \quad \sigma(f)^2 = \langle \pi, (F - PF)^2 \rangle + 2\langle \pi, (F - PF)PF \rangle = \langle \pi, F^2 \rangle - \langle \pi, (PF)^2 \rangle.$$

This intuitive derivation can be made rigorous. Since E is finite, the Poisson equation

$$(6) \quad F(x) - PF(x) = f(x) - \langle \pi, f \rangle, \quad x \in E,$$

admits a unique solution up to an additive constant and the asymptotic variance of $I_n(f)$ is indeed given by (5), see [4] or [7].

2.2. WR algorithm. The classical estimation of $\langle \pi, f \rangle$ by the empirical mean $I_n(f)$ makes no use of the proposals \tilde{X}_k which have been rejected. For a long time, physicists have claimed that the efficiency of the estimation can be improved by including these rejected states in the sampling procedure. They suggest to use the so-called Waste-Recycling Monte Carlo (WR) algorithm, which consists in replacing $f(X_k)$ in $I_n(f)$ by a weighted average of $f(X_{k-1})$ and $f(\tilde{X}_k)$. For the natural choice of weights corresponding to the conditional expectation of $f(X_k)$ w.r.t. (X_{k-1}, \tilde{X}_k) , one gets the following estimator of $\langle \pi, f \rangle$.

$$I_n^{WR}(f) = \frac{1}{n} \sum_{k=0}^{n-1} \rho(X_k, \tilde{X}_{k+1}) f(\tilde{X}_{k+1}) + (1 - \rho(X_k, \tilde{X}_{k+1})) f(X_k).$$

To our knowledge, the WR algorithm was first introduced in 1977 by Ceperley, Chester and Kalos in equation (35) p.3085 [3]. Without any proof, they claim that ‘‘The advantage of using this form is that some information about unlikely moves appears in the final answer, and the variance is lowered’’. Notice that the WR algorithm requires the evaluation of f for all the proposals whereas the Metropolis-Hastings algorithm evaluates f only for the accepted proposals. Other algorithms using all the proposals, such as the Rao-Blackwell Metropolis-Hasting algorithm, have been studied, see for example section 6.4.2 in [10] and references therein. In the Rao-Blackwell Metropolis-Hasting algorithm, the weight of $f(\tilde{X}_{k+1})$ depends on all the proposals $\tilde{X}_1, \dots, \tilde{X}_n$ and is difficult to compute.

One easily checks that $I_n^{WR}(f) - I_n(f) = J_n(f)$ where for any real function ψ defined on E ,

$$J_n(\psi) = \frac{1}{n} \sum_{k=0}^{n-1} \left[\left(\rho(X_k, \tilde{X}_{k+1}) - \mathbf{1}_{\{X_{k+1}=\tilde{X}_{k+1}\}} \right) \psi(\tilde{X}_{k+1}) + \left(1 - \rho(X_k, \tilde{X}_{k+1}) - \mathbf{1}_{\{X_{k+1}=X_k\}} \right) \psi(X_k) \right].$$

Notice that $J_n(\psi) = 0$ when ψ is constant. We can consider a more general estimator of $\langle \pi, f \rangle$ given by

$$I_n(f, \psi) = I_n(f) + J_n(\psi).$$

Notice that $I_n^{WR}(f) = I_n(f, f)$ and $I_n(f) = I_n(f, 0)$. Theorem 3.3 implies the following result on the estimator $I_n(f, \psi)$.

Proposition 2.1. *For any real functions ψ and f defined on E , we have:*

- *The bias of the estimator $I_n(f, \psi)$ does not depend on ψ : $\mathbb{E}[I_n(f, \psi)] = \mathbb{E}[I_n(f)]$.*
- *The estimator $I_n(f, \psi)$ of $\langle \pi, f \rangle$ is consistent: a.s. $\lim_{n \rightarrow \infty} I_n(f, \psi) = \langle \pi, f \rangle$.*

From this result, $J_n(\psi)$ can be seen as a control variate and it is natural to look for ψ which minimizes the variance or the asymptotic variance of $I_n(f, \psi)$. Another class of control variates has been studied in [1] in the particular case of the Independent Metropolis-Hastings algorithm where $Q(x, \cdot)$ does not depend on x .

The last part of Theorem 3.3 implies the following result.

Proposition 2.2. *For any real functions ψ and f defined on E , the estimator $I_n(f, \psi)$ of $\langle \pi, f \rangle$ is asymptotically normal with asymptotic variance $\sigma(f, \psi)^2$:*

$$\sqrt{n} (I_n(f, \psi) - \langle \pi, f \rangle) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma(f, \psi)^2).$$

Moreover, for fixed f , the asymptotic variance $\sigma(f, \psi)^2$ is minimal for $\psi = F$ where F solves the Poisson equation (6). In particular, this choice achieves variance reduction : $\sigma(f, F)^2 \leq \sigma(f)^2$.

Although optimal in terms of the asymptotic variance, the estimator $I_n(f, F)$ is not for use in practice, since computing a solution of the Poisson equation is more complicated than computing $\langle \pi, f \rangle$. Nevertheless, the Proposition suggests that using $I_n(f, \psi)$ where ψ is an approximation of F should lead to a smaller asymptotic variance than in the standard Metropolis-Hastings algorithm. In particular if a solution of a perturbed Poisson equation is available, it would be a natural candidate. Otherwise, some hint at the computation of an approximation of F by a Monte Carlo approach is for instance given in [8] p.418-419. Because of the series expansion $F = \sum_{k \geq 0} P^k(f - \langle \pi, f \rangle)$, f can be seen as an approximation of F of order 0. Hence the asymptotic variance of $I_n^{WR}(f) = I_n(f, f)$ should be smaller than the one of $I_n(f)$ in some situations. It is common belief in the physicist community, see [3] or [6], that the inequality is always true. Notice that, as remarked by Frenkel in a particular case [6], the variance of each term of the sum of $I_n^{WR}(f)$ is equal or smaller than the variance of each term of the sum of $I_n(f)$. Indeed, we have for any real valued function h

$$\mathbb{E}[\rho(X_{k-1}, \tilde{X}_k)h(X_{k-1}) + (1 - \rho(X_{k-1}, \tilde{X}_k))h(\tilde{X}_k)] = \mathbb{E}[h(X_k)]$$

and $\mathbb{E} \left[[\rho(X_{k-1}, \tilde{X}_k)h(X_{k-1}) + (1 - \rho(X_{k-1}, \tilde{X}_k))h(\tilde{X}_k)]^2 \right] \leq \mathbb{E}[h^2(X_k)],$

by Jensen inequality. But one has also to compare the covariance terms, which is not so obvious. We investigate whether the asymptotic variance of the WR algorithm is smaller than the one of the standard Metropolis algorithm and reach the following conclusion which contradicts the intuition.

Proposition 2.3.

- In the Metropolis case, that is when (2) holds with $\gamma(u) = \min(1, u)$, then it may happen that $\sigma^2(f, f) > \sigma^2(f)$.
- In the Boltzmann (or Barker) algorithm, that is when (2) holds with $\gamma(u) = \frac{u}{1+u}$, then we have $\sigma^2(f, f) \leq \sigma^2(f)$.

To prove the first assertion, we give an explicit counter-example such that $\sigma^2(f, f) > \sigma^2(f)$ in the Metropolis case (see Section 3.4.2 and equation (27)). The second assertion is proved in Section 3.5. In fact we prove a result slightly stronger in Proposition 3.10. We also give some natural conditions for this result to hold, see the comments following Proposition 3.10.

Remark 2.4. According to [9], since for all $u > 0$, $\frac{u}{1+u} < \min(1, u)$, in the absence of waste recycling, the asymptotic variance $\sigma^2(f)$ is smaller in the Metropolis case than in the Boltzmann case for given π , Q and f . So waste recycling always achieves variance reduction only for the worst choice of γ . This result is in a sense disappointing.

Remark 2.5. When the computation of Pg is feasible for any function $g : E \rightarrow \mathbb{R}$ (typically when, for every $x \in E$, the cardinal of $\{y \in E : Q(x, y) > 0\}$ is small), then it is possible to use $I_n(\psi - P\psi)$ as a control variate and approximate $\langle \pi, f \rangle$ by $I_n(f - (\psi - P\psi))$. Since π is invariant with respect to P , $\langle \pi, \psi - P\psi \rangle = 0$ and a.s. $I_n(f - (\psi - P\psi))$ converges to $\langle \pi, f \rangle$ as n tends to infinity. Moreover, the asymptotic variance of the estimator is $\sigma(f - \psi + P\psi)^2$. Last, remarking that

$$(7) \quad I_n(\psi - P\psi) = \frac{1}{n} \sum_{k=1}^n (\psi(X_k) - P\psi(X_{k-1})) + \frac{1}{n} (P\psi(X_0) - P\psi(X_n))$$

one obtains that the bias difference $\mathbb{E}[I_n(f - \psi + P\psi)] - \mathbb{E}[I_n(f)] = \frac{1}{n} \mathbb{E}[P\psi(X_0) - P\psi(X_n)]$ is smaller than $2 \max_{x \in E} |\psi(x)|/n$.

For the choice $\psi = F$, this control variate is perfect, since according to (6), for each $n \in \mathbb{N}^*$, $I_n(f - (F - PF))$ is constant and equal to $\langle \pi, f \rangle$.

For the choice $\psi = f$, the asymptotic variance of the estimator $I_n(Pf)$ is also smaller than the one of $I_n(f)$. Indeed setting $f_0 = f - \langle \pi, f \rangle$, we have

$$\begin{aligned} \sigma(f)^2 - \sigma(Pf)^2 &= \langle \pi, (f_0 + PF)^2 - 2(PF)^2 + (Pf_0 - PF)^2 \rangle \\ &= \langle \pi, f_0^2 + 2f_0P(F - PF) + (Pf_0)^2 \rangle = \langle \pi, (f_0 + Pf_0)^2 \rangle \end{aligned}$$

where we used (6) for the first and last equalities and the reversibility of π w.r.t. P for the second one.

Notice the control variate $J_n(\psi)$ is similar to $I_n(\psi - P\psi)$ except that the conditional expectation $P\psi(X_{k-1})$ of $\psi(X_k)$ given X_{k-1} in the first term of the r.h.s. of (7) is replaced by the conditional expectation of $\psi(X_k)$ given (X_{k-1}, \tilde{X}_k) which can always be easily computed. From this perspective, the minimality of the asymptotic variance of $I_n(f, \psi)$ for $\psi = F$ is not a surprise.

The comparison between $\sigma(f, \psi)^2$ and $\sigma(f - \psi + P\psi)^2$ can be deduced from Remark 3.5 which is stated in the more general multiproposal framework introduced in the next

paragraph. Since $\sigma(f, -F)^2 - \sigma(f + F - PF)^2 = -3(\sigma(f, F)^2 - \sigma(f - F + PF)^2)$, the sign of $\sigma(f, \psi)^2 - \sigma(f - \psi + P\psi)^2$ depends on ψ .

2.3. Multiproposal WR algorithm. In the classical Metropolis Hasting algorithm, there is only one proposal \tilde{X}_{n+1} at step $n + 1$. Around 1990, some extensions where only one state among multiple proposals is accepted have been proposed in order to speed up the exploration of E . According to Frenkel [5], the waste recycling can be particularly useful for these algorithms where many states are rejected.

To formalize these algorithms, we introduce a proposition kernel $\mathcal{Q} : E \times \mathcal{P}(E) \rightarrow [0, 1]$, where $\mathcal{P}(E)$ denotes the set of parts of E , which describes how to randomly choose the set of proposals:

$$(8) \quad \forall x \in E, \mathcal{Q}(x, A) = 0 \text{ if } x \notin A \quad \text{and} \quad \sum_{A \in \mathcal{P}(E)} \mathcal{Q}(x, A) = 1.$$

The second condition says that $\mathcal{Q}(x, \cdot)$ is a probability on $\mathcal{P}(E)$. The first one insure that the starting point is among the proposals. This last convention will allow us to transform the rejection/acceptation procedure into a selection procedure among the proposals.

The selection procedure is described by a probability κ . For $(x, A) \in E \times \mathcal{P}(E)$, let $\kappa(x, A, \tilde{x}) \in [0, 1]$ denote the probability of choosing $\tilde{x} \in A$ as the next state when the proposal set A has been chosen. We assume that $\sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) = 1$ (that is $\kappa(x, A, \cdot)$ is a probability measure) and that the following condition holds :

$$(9) \quad \forall A \in \mathcal{P}(E), \forall x, \tilde{x} \in A, \pi(x)\mathcal{Q}(x, A)\kappa(x, A, \tilde{x}) = \pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)\kappa(\tilde{x}, A, x).$$

This condition is the analog of (1) for a multiproposal setting. For examples of non-trivial selection probability κ , see after Proposition 2.6 .

The Markov chain $X = (X_n, n \geq 0)$ is now defined inductively in the following way. Let X_0 be a random variable taking values in E with probability distribution ν_0 . At step n , X_0, \dots, X_n are given. The proposal set at step $n + 1$, A_{n+1} , is distributed according to $\mathcal{Q}(X_n, \cdot)$. Then X_{n+1} is chosen distributed according to $\kappa(X_n, A_{n+1}, \cdot)$. It is easy to check that X is a Markov chain with transition matrix

$$(10) \quad P(x, y) = \sum_{A \in \mathcal{P}(E): x, y \in A} \mathcal{Q}(x, A)\kappa(x, A, y).$$

Condition (9) ensures that X is reversible w.r.t. the probability measure $\pi : \pi(x)P(x, y) = \pi(y)P(y, x)$. We also assume that P is irreducible (easy to check sufficient conditions are given in Section 3.2). This dynamics generalizes the previous Metropolis-Hastings algorithm which can be recovered for the particular choice $\mathcal{Q}(x, \{x, y\}) = Q(x, y)$ and for $y \neq x$, $\kappa(x, \{x, y\}, y) = 1 - \kappa(x, \{x, y\}, x) = \rho(x, y)$.

We keep the definition (4) of $I_n(f)$ but adapt the ones of $J_n(\psi)$ and $I_n(f, \psi)$ as follows :

$$(11) \quad \mathcal{J}_n(\psi) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\tilde{x} \in A_{k+1}} (\kappa(X_k, A_{k+1}, \tilde{x}) - \mathbf{1}_{\{X_{k+1}=\tilde{x}\}}) \psi(\tilde{x})$$

and $\mathcal{I}_n(f, \psi) = I_n(f) + \mathcal{J}_n(\psi)$. The Waste Recycling estimator of $\langle \pi, f \rangle$ studied by Frenkel in [5] is given by $\mathcal{I}_n^{WR}(f) = \mathcal{I}_n(f, f)$. It turns out that Propositions 2.1, 2.2 and 2.3 remain true in this multiproposal framework (see Theorem 3.3).

Proposition 2.6. *For any real functions ψ and f defined on E , we have:*

- *The bias of the estimator $\mathcal{I}_n(f, \psi)$ does not depend on ψ (i.e. $\mathbb{E}[\mathcal{I}_n(f, \psi)] = \mathbb{E}[I_n(f)]$).*
- *The estimator $\mathcal{I}_n(f, \psi)$ of $\langle \pi, f \rangle$ is consistent: a.s. $\lim_{n \rightarrow \infty} \mathcal{I}_n(f, \psi) = \langle \pi, f \rangle$.*

- The estimator $\mathcal{I}_n(f, \psi)$ of $\langle \pi, f \rangle$ is asymptotically normal with asymptotic variance (still denoted by) $\sigma(f, \psi)^2$:

$$\sqrt{n} (I_n(f, \psi) - \langle \pi, f \rangle) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma(f, \psi)^2).$$

- Moreover, for fixed f , the asymptotic variance $\sigma(f, \psi)^2$ is minimal for $\psi = F$ where F solves the Poisson equation (6). In particular, this choice achieves variance reduction : $\sigma(f, F)^2 \leq \sigma(f)^2$.

We now give two examples of non-trivial selection probability κ which satisfies condition (9). The first one, κ^M , defined by (12)

$$\kappa^M(x, A, \tilde{x}) = \begin{cases} \frac{\pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)}{\max(\pi(\tilde{x})\mathcal{Q}(\tilde{x}, A), \pi(x)\mathcal{Q}(x, A)) + \sum_{z \in A \setminus \{x, \tilde{x}\}} \pi(z)\mathcal{Q}(z, A)} & \text{if } \tilde{x} \neq x, \\ 1 - \sum_{z \in A \setminus \{x\}} \kappa^M(x, A, z) & \text{if } \tilde{x} = x, \end{cases}$$

generalizes the Metropolis selection given by (2) with $\gamma(u) = \min(1, u)$. (Notice that for $x \neq \tilde{x}$ one has $\kappa^M(x, A, \tilde{x}) \leq \frac{\pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)}{\sum_{z \in A \setminus \{x\}} \pi(z)\mathcal{Q}(z, A)}$, which implies that $1 - \sum_{z \in A \setminus \{x\}} \kappa^M(x, A, z)$ is indeed non-negative.) The second one, κ^B , which does not depend on the initial point x , is defined by

$$(13) \quad \kappa^B(x, A, \tilde{x}) = \kappa^B(A, \tilde{x}) = \frac{\pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)}{\sum_{z \in A} \pi(z)\mathcal{Q}(z, A)},$$

generalizes the Boltzmann (or Barker) selection given by (2) with $\gamma(u) = \frac{u}{1+u}$.

For those two particular cases of selection probability, we can extend the result of Proposition 2.3.

Proposition 2.7.

- When $\kappa = \kappa^M$ is given by (12) (Metropolis case), then it may happen that $\sigma^2(f, f) > \sigma^2(f)$.
- When $\kappa = \kappa^B$ is given by (13) (Boltzmann or Barker case), then we have $\sigma^2(f, f) \leq \sigma^2(f)$.

Of course, the counter-example (see Section 3.4.2 and equation (27)) such that $\sigma^2(f, f) > \sigma^2(f)$ in the single proposal Metropolis case, still provides a counter-example in the more general multi-proposal framework and provides the first result of Proposition 2.7. Moreover, since for $\tilde{x} \neq x \in A$, $\kappa^M(x, A, \tilde{x}) > \kappa^B(A, \tilde{x})$, according to [9], the asymptotic variance $\sigma^2(f)$ remains smaller in the Metropolis case than in the Boltzmann one. Nethertheless, it is likely that the difference decreases when the cardinality of the proposal sets increases.

3. CASE OF A FINITE STATE SPACE E

After giving some preliminary results, we state our main Theorem which implies Propositions 2.1, 2.2 and 2.6. Then we give a counter-example such that $\sigma^2(f, f) > \sigma^2(f)$ in the single proposal Metropolis case. Last, by considering the Boltzmann case, we complete the proofs of Propositions 2.3 and 2.7.

Let π be a positive probability on a finite space E . We consider a proposition kernel $\mathcal{Q} : E \times \mathcal{P}(E) \rightarrow [0, 1]$ s.t. (8) holds. We also consider a selection procedure $\kappa : E \times \mathcal{P}(E) \times E \rightarrow [0, 1]$ s.t. for all $x \in E$, $A \in \mathcal{P}(E)$, $\kappa(x, A, \cdot)$ is a probability and (9) holds.

Consider the Markov chain $X = (X_n, n \geq 0)$ defined inductively as follow. Let X_0 be a random variable taking values in E with probability distribution ν_0 . At step n , X_0, \dots, X_n are given. The proposal set at step $n + 1$, A_{n+1} , is distributed according to $\mathcal{Q}(X_n, \cdot)$. Then X_{n+1} is chosen distributed according to $\kappa(X_n, A_{n+1}, \cdot)$. The transition matrix of X , P , is given by (10): $P(x, y) = \sum_{A \in \mathcal{P}(E): x, y \in A} p(x, A, y)$ where

$$p(x, A, y) = \mathcal{Q}(x, A)\kappa(x, A, y).$$

Condition (9) ensures that X is reversible w.r.t. the probability measure $\pi : \pi(x)P(x, y) = \pi(y)P(y, x)$, and therefore that π is invariant for P : $\pi P = \pi$.

3.1. Preliminaries. One easily checks that $((X_n, A_{n+1}, X_{n+1}), n \geq 0)$ is itself a Markov chain on $E^c = E \times \mathcal{P}(E) \times E$ with transition matrix

$$P^c((x, A, y), (x', A', y')) = \mathbf{1}_{\{x'=y\}}p(x', A', y').$$

Let us also introduce the following probability measure on E^c : $\pi^c(x, A, y) = \pi(x)p(x, A, y)$. For β a real valued function defined on E^c , we set for $w^c \in E^c$

$$P^c\beta(w^c) = \sum_{u^c \in E^c} P^c(w^c, u^c)\beta(u^c) \quad \text{and} \quad \langle \pi^c, \beta \rangle = \sum_{u^c \in E^c} \pi^c(u^c)\beta(u^c).$$

Lemma 3.1.

- The probability measure π^c is invariant for P^c .
- In the particular case of a function β which depends only on the last variable, for all $(x, A, y) \in E^c$, $\beta(x, A, y) = \psi(y)$ with ψ a real valued function defined on E , we have

$$(14) \quad P^c\psi(x, A, y) = P\psi(y) \quad \text{and} \quad \langle \pi^c, \psi \rangle = \langle \pi, \psi \rangle,$$

where we write $P^c\psi$ for $P^c\beta$, $\langle \pi^c, \psi \rangle$ for $\langle \pi^c, \beta \rangle$ and use the notation $P\psi(y) = \sum_{y' \in E} P(y, y')\psi(y')$.

Proof. Using the invariance of π for P in the last equality, we get

$$\begin{aligned} \sum_{(x, A, y) \in E^c} \pi^c(x, A, y)P^c((x, A, y), (x', A', y')) &= p(x', A', y') \sum_{x \in E} \pi(x) \left(\sum_{A \in \mathcal{P}(E)} p(x, A, x') \right) \\ &= p(x', A', y') \sum_{x \in E} \pi(x)P(x, x') \\ &= \pi^c(x', A', y'). \end{aligned}$$

We have

$$\begin{aligned} P^c\psi(x, A, y) &= \sum_{y' \in E} \left(\sum_{A' \in \mathcal{P}(E)} p(y, A', y') \right) \psi(y') = \sum_{y' \in E} P(y, y')\psi(y') = P\psi(y), \\ \langle \pi^c, \psi \rangle &= \sum_{y \in E} \left(\sum_{x \in E} \pi(x) \left(\sum_{A \in \mathcal{P}(E)} p(x, A, y) \right) \right) \psi(y) = \sum_{y \in E} \pi(y)\psi(y) = \langle \pi, \psi \rangle, \end{aligned}$$

where we used the invariance of π for P in the last but one equality. \square

3.2. Irreducibility of P and P^c . By definition, P is irreducible if and only if for all $x' \neq y \in E$, there exist $m \geq 1$, distinct $x_0 = y, x_1, x_2, \dots, x_m = x' \in E$ and $A_1, A_k \dots, A_m \in \mathcal{P}(E)$ such that for all $k \in \{1, \dots, m\}$, $x_{k-1}, x_k \in A_k$ and

$$(15) \quad \prod_{k=1}^m p(x_{k-1}, A_k, x_k) > 0.$$

For both the Metropolis (12) and Boltzmann (13) choices for κ the last condition can be expressed only in terms of \mathcal{Q} :

$$(16) \quad \prod_{k=1}^m \mathcal{Q}(x_{k-1}, A_k) \mathcal{Q}(x_k, A_k) > 0.$$

Lemma 3.2. *If P is irreducible, then the transition matrix P^c is irreducible on $\bar{E}^c = \{(x, A, y) \in E^c; p(x, A, y) > 0\}$.*

Proof. Let (x, A, y) and (x', A', y') be distinct elements of \bar{E}^c . By assumption, there exist $m \geq 0$, distinct $x_0 = y, x_1, x_2, \dots, x_m = x' \in E$ and $A_1, A_k \dots, A_m \in \mathcal{P}(E)$ such that for all $k \in \{1, \dots, m\}$, $x_{k-1}, x_k \in A_k$ and (15) holds. We also set $A_{m+1} = A'$ and $x_{m+1} = y'$. This ensures the positivity of the product

$$P^c((x, A, y), (y, A_1, x_1)) \prod_{k=1}^m P^c((x_{k-1}, A_k, x_k), (x_k, A_{k+1}, x_{k+1}))$$

which is equal to $(\prod_{k=1}^m p(x_{k-1}, A_k, x_k)) p(x', A', y')$. This gives the desired irreducibility property. \square

3.3. Main result. We keep notations of Section 3.1 and we assume that P is irreducible. We consider the functional \mathcal{J}_n defined as follows: for β a real valued function defined on E^c ,

$$(17) \quad \mathcal{J}_n(\beta) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\tilde{x} \in A_{k+1}} (\kappa(X_k, A_{k+1}, \tilde{x}) - \mathbf{1}_{\{X_{k+1}=\tilde{x}\}}) \beta(X_k, A_{k+1}, \tilde{x}).$$

We set $\mathcal{I}_n(f, \beta) = I_n(f) + \mathcal{J}_n(\beta)$, where $I_n(f)$ is given by (4).

Theorem 3.3. *For any real functions f defined on E and β defined on E^c , we have:*

- (1) *The bias of the estimator $\mathcal{I}_n(f, \beta)$ does not depend on β (i.e. $\mathbb{E}[\mathcal{I}_n(f, \beta)] = \mathbb{E}[I_n(f)]$).*
- (2) *The estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f \rangle$ is consistent: a.s. $\lim_{n \rightarrow \infty} \mathcal{I}_n(f, \beta) = \langle \pi, f \rangle$.*
- (3) *The estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f \rangle$ is asymptotically normal with asymptotic variance $\sigma(f, \beta)^2$:*

$$\sqrt{n}(I_n(f, \beta) - \langle \pi, f \rangle) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma(f, \beta)^2),$$

where

$$(18) \quad \sigma(f, \beta)^2 = \sigma(f)^2 + \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) [2((\kappa F)(\kappa \beta) - \kappa(\beta F)) + \kappa(\beta^2) - (\kappa \beta)^2] (x, A),$$

with

$$\begin{aligned}\kappa F(x, A) &= \sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) F(\tilde{x}), \\ \kappa \beta(x, A) &= \sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) \beta(x, A, \tilde{x}), \\ \kappa(\beta F)(x, A) &= \sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) \beta(x, A, \tilde{x}) F(\tilde{x}), \\ \kappa(\beta^2)(x, A) &= \sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) \beta^2(x, A, \tilde{x}).\end{aligned}$$

There is a nice way to rewrite $\sigma(f, \beta)^2$ which leads to the optimal choice of β in terms of variance reduction. Let us introduce a simple notation. For a probability measure ν on E and real valued functions h and g defined on E , we denote by

$$\text{Cov}_\nu(h, g) = \langle \nu, gh \rangle - \langle \nu, g \rangle \langle \nu, h \rangle \quad \text{and} \quad \text{Var}_\nu(h) = \langle \nu, h^2 \rangle - \langle \nu, h \rangle^2$$

respectively the covariance of g and h and the variance of h w.r.t. to the probability measure ν . Then, we notice that

$$(19) \quad \sigma(f, \beta)^2 = \sigma(f)^2 + \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) \left[-2 \text{Cov}_{\kappa(x, A, \cdot)}(\beta_{x, A}, F) + \text{Var}_{\kappa(x, A, \cdot)}(\beta_{x, A}) \right],$$

where $\beta_{x, A}$ is the real valued function defined on E by $\beta_{x, A}(y) = \beta(x, A, y)$.

Proof. Let us introduce

$$\eta(x, A, y) = \sum_{\tilde{x} \in A} (\kappa(x, A, \tilde{x}) - \mathbf{1}_{\{y=\tilde{x}\}}) \beta(x, A, \tilde{x}),$$

and $f^c(x, A, y) = f(y) + \eta(x, A, y)$ so that $\mathcal{I}_n(f, \beta) = \frac{1}{n} \sum_{k=0}^{n-1} f^c(X_k, A_{k+1}, X_{k+1})$. Notice that $\eta(x, A, y) = (\kappa \beta)(x, A) - \beta(x, A, y)$.

We will use the notation $\mathbb{E}_\nu[h] = \langle \nu, h \rangle$, where ν is a probability measure on E and h a real valued function defined on E for the expectation of h w.r.t. ν . We write $\eta_{x, A}$ for the real valued function defined on E by $\eta_{x, A}(y) = \eta(x, A, y)$. Notice that

$$\begin{aligned}\mathbb{E}_{\kappa(x, A, \cdot)}[\eta_{x, A}] &= \sum_{y \in A} \kappa(x, A, y) \sum_{\tilde{x} \in A} (\kappa(x, A, \tilde{x}) - \mathbf{1}_{\{y=\tilde{x}\}}) \beta(x, A, \tilde{x}) \\ &= \sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) \beta(x, A, \tilde{x}) - \sum_{y \in A} \kappa(x, A, y) \beta(x, A, y) \\ (20) \quad &= 0.\end{aligned}$$

We deduce that

$$\mathbb{E}[\eta(X_k, A_{k+1}, X_{k+1})] = \mathbb{E}[\mathbb{E}[\eta(X_k, A_{k+1}, X_{k+1}) | X_k, A_{k+1}]] = \mathbb{E}[\mathbb{E}_{\kappa(X_k, A_{k+1}, \cdot)}[\eta_{X_k, A_{k+1}}]] = 0,$$

and thus $\mathbb{E}[\mathcal{I}_n(f, \beta)] = \mathbb{E}[I_n(f)]$. This proves (1).

By Lemma 3.2, and since P is assumed to be irreducible, we have that P^c is irreducible. By Lemma 3.1, π^c is an invariant probability measure for P^c . The ergodic theorem (see e.g. [7]) ensures that a.s. $\mathcal{I}_n(f, \beta)$ converges to

$$(21) \quad \langle \pi^c, f^c \rangle = \langle \pi, f \rangle + \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) \mathbb{E}_{\kappa(x, A, \cdot)}[\eta_{x, A}] = \langle \pi, f \rangle,$$

thanks to (14) for the first equality and (20) for the second. This proves (2).

The central limit theorem for Markov chains, see [4] or [7], gives the following convergence in distribution

$$\sqrt{n}(\mathcal{I}_n(f, \beta) - \langle \pi, f \rangle) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma(f, \beta)^2),$$

with $\sigma(f, \beta)^2 = \langle \pi^c, (F^c)^2 \rangle - \langle \pi^c, (P^c F^c)^2 \rangle$, where F^c solves the Poisson equation on E^c :

$$(22) \quad F^c - P^c F^c = f^c - \langle \pi^c, f^c \rangle.$$

Let us check that F^c defined by $F^c(x, A, y) = F(y) + \eta(x, A, y)$ for $(x, A, y) \in E^c$, with F solution to the Poisson equation (6), solves the Poisson equation (22). We have

$$(23) \quad P^c F^c(x, A, y) = P^c F(x, A, y) + P^c \eta(x, A, y) = P F(y),$$

where we used for the last equality (14) for the first term and for the second that

$$(24) \quad P^c \eta(x, A, y) = \sum_{A' \in \mathcal{P}(E)} \mathcal{Q}(y, A') \mathbb{E}_{\kappa(y, A', \cdot)}[\eta_{y, A'}] = 0,$$

thanks to (20). Therefore, as F solves (6), we have

$$\begin{aligned} F^c(x, A, y) - P^c F^c(x, A, y) &= F(y) - P F(y) + \eta(x, A, y) \\ &= f(y) + \eta(x, A, y) - \langle \pi, f \rangle \\ &= f^c(y) - \langle \pi^c, f^c \rangle, \end{aligned}$$

thanks to (21). Thus F^c solves the Poisson equation (22).

We have, thanks to (23) and (14) for the second term of $\sigma(f, \beta)^2$ that $\langle \pi^c, (P^c F^c)^2 \rangle = \langle \pi^c, (P F)^2 \rangle = \langle \pi, (P F)^2 \rangle$. As $F^c = F + \eta$, we get, using (14) with $\psi = F$, that

$$\sigma(f, \beta)^2 - \sigma(f)^2 = \langle \pi^c, (F^c)^2 - F^2 \rangle = \langle \pi^c, (F + \eta)^2 - F^2 \rangle = \langle \pi^c, 2F\eta + \eta^2 \rangle.$$

One easily concludes as $\eta(x, A, y) = (\kappa\beta)(x, A) - \beta(x, A, y)$ and thus

$$\begin{aligned} &(2F\eta + \eta^2)(x, A, y) \\ &= 2F(y)\kappa\beta(x, A) - 2F(y)\beta(x, A, y) + (\kappa\beta)^2(x, A) - 2\beta(x, A, y)\kappa\beta(x, A) + \beta^2(x, A, y). \end{aligned}$$

□

Remark 3.4. In fact, to guess the solution to the Poisson equation (22), we used the formal formula $F^c = \sum_{n=0}^{\infty} (P^c)^n (f^c - \langle \pi^c, f^c \rangle)$. Notice that thanks to (24) and (14), we have $(P^c)^n f^c = (P^c)^{n-1} (P f) = P^n f$ for $n \geq 1$. Using (21), we get

$$\sum_{n=0}^{\infty} (P^c)^n (f^c - \langle \pi^c, f^c \rangle) = f^c - f + \sum_{n=0}^{\infty} P^n (f - \langle \pi, f \rangle) = \eta + F,$$

and guess that $F + \eta$ has to solve the Poisson equation (22).

Remark 3.5. Motivated by Remark 2.5 on the study of $I_n(f + P\psi - \psi)$, we compute the asymptotic variance $\tilde{\sigma}(f, \beta)^2$ of

$$I_n(f) + \frac{1}{n} \sum_{k=0}^{n-1} \sum_{A, \tilde{x}} (\mathcal{Q}(X_k, A) \kappa(X_k, A, \tilde{x}) - \mathbf{1}_{\{A_{k+1}=A, X_{k+1}=\tilde{x}\}}) \beta(X_k, A, \tilde{x}).$$

Like in the previous proof, one obtains

$$\tilde{\sigma}(f, \beta)^2 = \sigma(f, \beta)^2 + \sum_x \pi(x) [-2\text{Cov}_{\mathcal{Q}(x, \cdot)}(\kappa\beta(x, \cdot), \kappa F(x, \cdot)) + \text{Var}_{\mathcal{Q}(x, \cdot)}(\kappa\beta(x, \cdot))].$$

Notice the sign of $\tilde{\sigma}(f, \beta)^2 - \sigma(f, \beta)^2$ depends on β (see the end of Remark 2.5).

Remark 3.6. Let $\kappa' \neq \kappa$ be such that (9) still holds when κ is replaced by κ' and $\mathcal{J}'_n(\psi)$ and $\mathcal{J}'_n(\beta)$ be defined like $\mathcal{J}_n(\psi)$ and $\mathcal{J}_n(\beta)$ with the chain X unchanged but with $\kappa(X_k, A_{k+1}, \tilde{x})$ replaced by $\kappa'(X_k, A_{k+1}, \tilde{x})$ in (11) and (17). In the single proposal case, Frenkel [6] suggests that $\mathcal{J}'_n(f)$ can also be used as a control variate. It turns out that for any real valued function ψ defined on E , a.s. $\lim_{n \rightarrow +\infty} \mathcal{J}'_n(\psi) = 0$. Indeed, since π is reversible for $P'(x, \tilde{x}) = \sum_A \mathcal{Q}(x, A) \kappa'(x, A, \tilde{x})$ and by (14),

$$\begin{aligned} & \sum_{(x,A,y) \in E^c} \pi^c(x, A, y) \sum_{\tilde{x} \in E} (\kappa'(x, A, \tilde{x}) - \mathbf{1}_{\{\tilde{x}=y\}}) \psi(\tilde{x}) \\ &= \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) \left(\sum_{y \in E} \kappa(x, A, y) \right) \left(\sum_{\tilde{x} \in E} \kappa'(x, A, \tilde{x}) \psi(\tilde{x}) \right) - \langle \pi^c, \psi \rangle \\ &= \sum_{\tilde{x} \in E} \left(\sum_{x \in E} \pi(x) P'(x, \tilde{x}) \right) \psi(\tilde{x}) - \langle \pi, \psi \rangle = 0. \end{aligned}$$

But in general $\mathbb{E}[\mathcal{J}'_n(\psi)] \neq 0$ and, for a real valued function β defined on E^c , the almost sure limit of $\mathcal{J}'_n(\beta)$ and $\mathbb{E}[\mathcal{J}'_n(\beta)]$ are different from zero. It is possible to compute the asymptotic variance of $I_n(f) + \mathcal{J}'_n(\psi)$ but we have not been able to compare it with $\sigma(f)^2$, the one of the original estimator $I_n(f)$.

Using the expression (18) of the asymptotic variance $\sigma(f, \beta)^2$, it is easy to find the choice of β which minimizes this variance.

Corollary 3.7. *The asymptotic variance $\sigma(f, \beta)^2$ is minimal for $\beta(x, A, y) = F(y)$ and*

$$\sigma(f, F)^2 = \sum_{x \in E} \pi(x) \left(\sum_A \mathcal{Q}(x, A) (\kappa F)^2(x, A) - \left(\sum_A \mathcal{Q}(x, A) \kappa F(x, A) \right)^2 \right) \leq \sigma(f)^2.$$

Proof. Setting $\delta_{x,A}(y) = \beta(x, A, y) - F(y)$ and using (19), we get

$$\begin{aligned} \sigma(f, \beta)^2 &= \sigma(f)^2 + \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) [-2\text{Cov}_{\kappa(x,A,\cdot)}(\delta_{x,A} + F, F) + \text{Var}_{\kappa(x,A,\cdot)}(\delta_{x,A} + F)] \\ (25) \quad &= \sigma(f)^2 + \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) [\text{Var}_{\kappa(x,A,\cdot)}(\delta_{x,A}) - \text{Var}_{\kappa(x,A,\cdot)}(F)]. \end{aligned}$$

As the variance $\text{Var}_{\kappa(x,A,\cdot)}(\delta_{x,A})$ is non-negative and zero if δ is constant, this implies that $\sigma(f, \beta)^2$ is minimal for $\beta(x, A, y) = F(y)$. Of course, $\sigma(f, F)^2 \leq \sigma(f, 0)^2 = \sigma(f)^2$.

As by (14),

$$\begin{aligned} \sigma(f)^2 &= \langle \pi, F^2 \rangle - \langle \pi, (PF)^2 \rangle \\ &= \sum_{x,A} \pi(x) \mathcal{Q}(x, A) \kappa(F^2)(x, A) - \sum_x \pi(x) \left(\sum_A \mathcal{Q}(x, A) \kappa F(x, A) \right)^2, \end{aligned}$$

the expression of $\sigma(f, F)^2$ follows from (18). \square

3.4. Further results in the single proposal framework.

3.4.1. *Another expression of the asymptotic variances for $\psi = f$ and $\psi = F$.* Motivated by the study of the WR algorithm which corresponds to $\psi = f$ and of the optimal choice $\psi = F$, let us now derive more convenient expressions of $\sigma(f, f)^2$ and $\sigma^2(f, F)$ in the single proposal framework described in Section 2.1. Notice that P is irreducible as Q is assumed to be irreducible.

Corollary 3.8. *In the single proposal case, we have*

$$\sigma(f, F)^2 - \sigma(f)^2 = -\mathbb{E}_\pi [(1 - \rho(X_0, X_1))(F(X_1) - F(X_0))^2]$$

and

$$\begin{aligned} & \sigma(f, f)^2 - \sigma(f)^2 \\ &= -\mathbb{E}_\pi [(1 - \rho(X_0, X_1)) [(F(X_1) - F(X_0))^2 - (PF(X_1) - PF(X_0))^2]] \\ &= -\mathbb{E}_\pi \left[\left(1 - \frac{\rho(X_0, X_1) + \rho(X_1, X_0)}{2} \right) [(F(X_1) - F(X_0))^2 - (PF(X_1) - PF(X_0))^2] \right] \end{aligned}$$

where the subscript π means that X_0 is distributed according to π .

Proof. In the single proposal case, $\kappa(x, \{x, y\}, y) = 1 - \kappa(x, \{x, y\}, x) = \rho(x, y)$ for $x \neq y$. Therefore, for real valued functions g and h defined on E , we have

$$(26) \quad \begin{aligned} & \kappa g(x, \{x, y\}) = \rho(x, y)g(y) + (1 - \rho(x, y))g(x) \\ & [\kappa(gh) - (\kappa g)(\kappa h)](x, \{x, y\}) = \rho(x, y)(1 - \rho(x, y))(g(y) - g(x))(h(y) - h(x)). \end{aligned}$$

Inserting this equality with $g = h = F$ in (25), one obtains

$$\begin{aligned} \sigma(f, F)^2 - \sigma(f)^2 &= - \sum_{x \neq y \in E} \pi(x)Q(x, y)\rho(x, y)(1 - \rho(x, y))(F(y) - F(x))^2 \\ &= - \sum_{x \neq y \in E} \pi(x)P(x, y)(1 - \rho(x, y))(F(y) - F(x))^2 \\ &= -\mathbb{E}_\pi [(1 - \rho(X_0, X_1))(F(X_1) - F(X_0))^2], \end{aligned}$$

where we used the definition (3) of P in the single proposal case, for the second equality. Now, inserting equality (26) for $g = h = f$ and for $g = F, h = f$ in the expression of $\sigma(f, f)^2 - \sigma(f)^2$ given by (18), one obtains

$$\begin{aligned} & \sigma(f, f)^2 - \sigma(f)^2 \\ &= \sum_{x, y \in E} \pi(x)Q(x, y)\rho(x, y)(1 - \rho(x, y))(f(y) - f(x))[f(y) - f(x) - 2(F(y) - F(x))]. \end{aligned}$$

Notice that, by the Poisson equation (6), $f = F - PF - \langle \pi, f \rangle$, a computation similar to the one made for $\sigma(f, F)^2 - \sigma(f)^2$ leads to

$$\sigma(f, f)^2 - \sigma(f)^2 = -\mathbb{E}_\pi [(1 - \rho(X_0, X_1)) [(F(X_1) - F(X_0))^2 - (PF(X_1) - PF(X_0))^2]].$$

By reversibility of π with respect to P , $\sigma(f, f)^2 - \sigma(f)^2$ is also equal to

$$-\mathbb{E}_\pi [(1 - \rho(X_1, X_0)) [(F(X_1) - F(X_0))^2 - (PF(X_1) - PF(X_0))^2]].$$

The last equality of the Corollary follows. \square

3.4.2. *A counter-example.* We are going to construct a counter-example such that $\sigma^2(f, f) > \sigma^2(f)$ in the Metropolis case, thus proving the statements concerning this case in Propositions 2.3 and 2.7. This counter-example is also such that the optimal choice $\psi = F$ does not achieve variance reduction : $\sigma(f, F)^2 = \sigma(f)^2$. Let P be an irreducible transition matrix on $E = \{a, b, c\}$, with invariant probability measure π s.t. P is reversible w.r.t. π ,

$$P(a, b) > 0, P(a, a) > 0 \text{ and } P(a, c) \neq P(b, c).$$

Let f be defined by $f(x) = \mathbf{1}_{\{x=c\}} - P(x, c)$ for $x \in E$. We have

$$\langle \pi, f \rangle = \pi(c) - \sum_{x \in E} \pi(x)P(x, c) = 0.$$

The function $F(x) = \mathbf{1}_{\{x=c\}}$ solves the Poisson equation (6): $F - PF = f - \langle \pi, f \rangle$.

Let $\rho \in \left(\frac{P(a, b)}{P(a, a) + P(a, b)}, 1 \right)$. We set

$$Q(x, y) = \begin{cases} \frac{P(a, b)}{\rho} & \text{if } (x, y) = (a, b), \\ P(a, a) - P(a, b)\left(\frac{1}{\rho} - 1\right) & \text{if } (x, y) = (a, a), \\ P(x, y) & \text{otherwise.} \end{cases}$$

We choose

$$\rho(x, y) = \begin{cases} \rho & \text{if } (x, y) = (a, b), \\ 1 & \text{otherwise.} \end{cases}$$

Since $\rho(a, b)\pi(a)Q(a, b) = \rho\pi(a)P(a, b)/\rho$, we have $\rho(x, y)\pi(x)Q(x, y) = \pi(x)P(x, y)$ for all $x, y \in E$. Equation (1) follows from the reversibility of π for P . Notice also that (2) holds with $\gamma(u) = \min(1, u)$.

By construction, the matrix P satisfies (3). By Corollary 3.8, we have $\sigma(f, F)^2 - \sigma(f)^2 = 0$ and

$$(27) \quad \sigma(f, f)^2 - \sigma(f)^2 = \pi(a)P(a, b)(1 - \rho)(P(b, c) - P(a, c))^2 > 0.$$

Notice that when X_0 is distributed according to π and $n = 1$ (independent drawings case), then the variance reduction obtained by using the WR conditional expectation, i.e. $\rho(X_0, \tilde{X}_1)f(X_1) + (1 - \rho(X_0, \tilde{X}_1))f(X_0)$, instead of $f(X_1)$ is equal to

$$\begin{aligned} & \mathbb{E}_\pi[\mathbb{E}[f^2(X_1)|(X_0, \tilde{X}_1)] - \{\rho(X_0, \tilde{X}_1)f(\tilde{X}_1) + (1 - \rho(X_0, \tilde{X}_1))f(X_0)\}^2] \\ &= \mathbb{E}_\pi[\rho(X_0, \tilde{X}_1)(1 - \rho(X_0, \tilde{X}_1))(f(\tilde{X}_1) - f(X_0))^2] = \mathbb{E}_\pi[(1 - \rho(X_0, X_1))(f(X_1) - f(X_0))^2] \\ &= \pi(a)P(a, b)(1 - \rho)(P(b, c) - P(a, c))^2. \end{aligned}$$

In this particular case, this quantity is equal to the variance augmentation in the asymptotic n goes to infinity.

Let us illustrate these results by simulation for the following specific choice

$$\pi = \frac{1}{10} \begin{pmatrix} 6 \\ 3 \\ 1 \end{pmatrix}, P = \frac{1}{60} \begin{pmatrix} 38 & 21 & 1 \\ 42 & 0 & 18 \\ 6 & 54 & 0 \end{pmatrix}, \rho = \frac{4}{10} \text{ and } Q = \frac{1}{120} \begin{pmatrix} 13 & 105 & 2 \\ 84 & 0 & 36 \\ 12 & 108 & 0 \end{pmatrix}.$$

Then $\sigma(f)^2 - \sigma(f, f)^2 = -0.010115$ amounts to 14% of $\sigma(f)^2 \simeq 0.0728333$.

Using $N = 10\,000$ simulations, we give estimations of the variances σ_n^2 of $I_n(f)$, $\sigma_{WR, n}^2$ of $I_n^c(f)$ and of the difference $\sigma_n^2 - \sigma_{WR, n}^2$ with asymptotic confidence intervals at level 95%. The initial variable X_0 is generated according to the reversible probability measure π .

n	σ_n^2	$\sigma_{WR,n}^2$	$\sigma_n^2 - \sigma_{WR,n}^2$
1	[0.1213 , 0.1339]	[0.1116 , 0.1241]	[0.0091 , 0.0104]
2	[0.0728 , 0.0779]	[0.0758 , 0.0815]	[-0.0041 , -0.0025]
5	[0.0733 , 0.0791]	[0.0798 , 0.0859]	[-0.0075 , -0.0058]
10	[0.0718 , 0.0772]	[0.0800 , 0.0859]	[-0.0094 , -0.0074]
100	[0.0702 , 0.0751]	[0.0803 , 0.0858]	[-0.0114 , -0.0092]
1000	[0.0719 , 0.0769]	[0.0811 , 0.0867]	[-0.0105 , -0.0083]

3.5. The Boltzmann case. The next proposition completes the proof of Propositions 2.3 and 2.7 by ensuring that the asymptotic variance of the waste recycling algorithm $\sigma(f, f)^2$ is smaller than the one $\sigma(f)^2$ of the standard Metropolis Hastings algorithm in the Boltzmann case. In the same time, we show that this variance $\sigma(f)^2$ is at least divided by two for the optimal choice $\beta(x, A, y) = F(y)$ in our control variate approach. We assume that P is irreducible.

Proposition 3.9. *In the Boltzmann case, when κ is given by (12), for $\beta(x, A, y)$ respectively equal to $F(y)$ and $f(y)$, one has*

$$\sigma(f, F)^2 = \frac{1}{2}(\sigma(f)^2 - \langle \pi, f_0^2 \rangle) \text{ and } \sigma(f, f)^2 = \sigma(f)^2 - \Delta(f)$$

where $f_0 = f - \langle \pi, f \rangle$ and $\Delta(f) = \frac{1}{2} \sum_{x,y \in E} \pi(x)P(x,y)(f_0(x) + f_0(y))^2$. And the non-negative terms $\langle \pi, f_0^2 \rangle$ and $\Delta(f)$ are positive when f is non constant.

Proof. For g and h real valued functions defined on E , we have

$$\begin{aligned}
(28) \quad & \sum_{x \in E, A \in \mathcal{P}(E)} \pi(x) \mathcal{Q}(x, A) [(\kappa^B g)(\kappa^B h)](A) \\
&= \sum_{A \in \mathcal{P}(E)} \left(\sum_{x \in A} \pi(x) \mathcal{Q}(x, A) \right) \sum_{y \in A} \frac{\pi(y) \mathcal{Q}(y, A)}{\sum_{z \in A} \pi(z) \mathcal{Q}(z, A)} g(y) \sum_{\tilde{x} \in A} \kappa^B(A, \tilde{x}) h(\tilde{x}) \\
&= \sum_{y \in E} \pi(y) g(y) \sum_{\tilde{x} \in E} \left(\sum_{A: y, \tilde{x} \in A} \mathcal{Q}(y, A) \kappa^B(A, \tilde{x}) \right) h(\tilde{x}) \\
&= \sum_{y \in E} \pi(y) g(y) Ph(y) = \langle \pi, gPh \rangle.
\end{aligned}$$

Using this equality with $h = g = F$ in the first term of the expression of $\sigma(f, F)^2$ given in Corollary 3.7, we obtain

$$\sigma(f, F)^2 = \langle \pi, FPF - (PF)^2 \rangle = \frac{1}{2} \langle \pi, F^2 - (PF)^2 - (F - PF)^2 \rangle = \frac{1}{2} (\sigma(f)^2 - \langle \pi, f_0^2 \rangle).$$

We deduce from (18) and (28) that

$$\sigma(f, f)^2 - \sigma(f)^2 = \langle \pi, 2fPF - 2fF + f^2 - fPf \rangle = 2\langle \pi, f \rangle^2 - \langle \pi, f(f + Pf) \rangle,$$

where we used (6) for the last equality. So, this gives $\Delta(f) = \langle \pi, f(f + Pf) \rangle - 2\langle \pi, f \rangle^2$. Let $f_0 = f - \langle \pi, f \rangle$. We have

$$(29) \quad \Delta(f) = \langle \pi, f_0(f_0 + Pf_0) \rangle = \frac{1}{2} \sum_{x,y \in E} \pi(x)P(x,y)(f_0(x) + f_0(y))^2,$$

where we used that π is invariant for P . We deduce that $\Delta(f) \geq 0$. Since $\Delta(f) = \langle \pi, f_0^2 \rangle + \langle \pi, f_0 P f_0 \rangle$ and $\langle \pi, f_0^2 \rangle > 0$ if f is non constant, the proof will be completed as soon as we check that $\langle \pi, h P h \rangle \geq 0$, for any real valued function h defined on E .

We have

$$\begin{aligned} \langle \pi, h P h \rangle &= \sum_{x \in E} \pi(x) P(x, y) h(x) h(y) \\ &= \sum_{(x, A, y) \in E^c} \frac{\pi(x) \mathcal{Q}(x, A) \pi(y) \mathcal{Q}(y, A)}{\sum_{z \in A} \pi(z) \mathcal{Q}(z, A)} h(x) h(y) \\ &= \sum_{A \in \mathcal{P}(E)} \frac{[\sum_{x \in A} \pi(x) \mathcal{Q}(x, A) h(x)]^2}{\sum_{z \in A} \pi(z) \mathcal{Q}(z, A)} \geq 0. \end{aligned}$$

□

In the single proposal case, the use of Boltzmann function $\gamma(u) = \frac{u}{1+u}$ ensures that $\rho(x, y) + \rho(y, x) = 1$. It turns out that we are still able to prove that the asymptotic variance $\sigma(f, f)^2$ of $I_n^{WR}(f) = I_n(f, f)$ is smaller than the one $\sigma(f)^2$ of $I_n(f)$ as soon as $\rho(x, y) + \rho(y, x)$ is constant. (Recall that P is irreducible as Q is assumed to be irreducible.)

Proposition 3.10. *In the single proposal case, if there exists $\alpha \in (0, 2)$ such that*

$$(30) \quad \rho(x, y) + \rho(y, x) = \alpha \quad \text{for all } x \neq y \in E \quad \text{s.t. } Q(x, y) > 0,$$

then $\sigma(f, f)^2 - \sigma(f)^2 = -(2 - \alpha)\Delta(f)$, where $\Delta(f)$ given in Proposition 3.9 is non-negative and positive if f is non constant.

Let us make some comments on hypothesis (30).

- (1) If $\alpha = 2$, then $\rho(x, y) = 1$ for $x \neq y$. Thus all the proposals are accepted that is $P = Q$. In this case, WR and Metropolis-Hastings algorithms coincide.
- (2) By (1), Hypothesis (30) means that (2) holds with $\gamma(u) = \frac{\alpha u}{1+u}$. The constant α has to be smaller than $1 + \min_{x \neq y, Q(x, y) > 0} \frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}$.
- (3) Assume ρ satisfies (2) for some function γ . Hypothesis (30) is satisfied if there exists a constant $c > 0$ s.t. for all distinct $x, y \in E$ s.t. $Q(x, y) > 0$, the quantity $\frac{\pi(x)Q(x, y)}{\pi(y)Q(y, x)}$ is equal to c or $1/c$. For example assume that the transition matrix Q is symmetric and that π is written as a Gibbs distribution: for all $x \in E$, $\pi(x) = e^{-H(x)} / \sum_{y \in E} e^{-H(y)}$ for some energy function H . Then hypothesis (30) is satisfied if the energy increases or decreases by the same amount for all the authorized transitions: $|H(x) - H(y)|$ is constant for all distinct x, y such that $Q(x, y) > 0$.

Proof. For the first part of the Proposition, thanks to (29), it is enough to check that

$$\frac{1}{2} \mathbb{E}_\pi [(F(X_1) - F(X_0))^2 - (PF(X_1) - PF(X_0))^2] = \langle \pi, f_0(f_0 + P f_0) \rangle,$$

where F solves the Poisson equation (6) and $f_0 = f - \langle \pi, f \rangle$.

We have, using that π is invariant for P and that P is reversible with respect to π , that

$$\begin{aligned} \frac{1}{2} \mathbb{E}_\pi [(F(X_1) - F(X_0))^2 - (PF(X_1) - PF(X_0))^2] &= \langle \pi, F^2 - FPF - (PF)^2 + (PF)(P^2F) \rangle \\ &= \langle \pi, F(F - PF) - (PF)(PF - P^2F) \rangle \\ &= \langle \pi, f_0(F - P^2F) \rangle \\ &= \langle \pi, f_0(f_0 + Pf_0) \rangle. \end{aligned}$$

To conclude the proof, we shall check that $\langle \pi, hPh \rangle \geq (1 - \alpha)\langle \pi, h \rangle^2$ for any real valued function h defined on E .

Since $\rho(x, y) + \rho(y, x) = \alpha$ for $x \neq y$, we deduce from (1), that for $x \neq y$,

$$\rho(x, y) = \alpha \frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y) + \pi(y)Q(y, x)}.$$

We have

$$\begin{aligned} \langle \pi, hPh \rangle + (\alpha - 1)\langle \pi, h \rangle^2 &= \sum_{x, y \in E} \pi(x)P(x, y)h(x)h(y) + (\alpha - 1) \sum_{x \in E} \pi(x)h(x)^2 \\ &= \sum_{x \in E} \pi(x)(P(x, x) + \alpha - 1)h(x)^2 + \sum_{x \neq y \in E} \pi(x)P(x, y)h(x)h(y). \end{aligned}$$

Using (3), we get

$$\begin{aligned} P(x, x) + \alpha - 1 &= \alpha \left(1 - \sum_{y \neq x} Q(x, y)\rho(x, y) \right) \\ &= \alpha \left(Q(x, x) + \sum_{y \neq x} Q(x, y)(1 - \rho(x, y)) \right) \\ &= \alpha Q(x, x) + \alpha \sum_{y \neq x} \frac{\pi(x)Q(x, y)^2}{\pi(x)Q(x, y) + \pi(y)Q(y, x)}. \end{aligned}$$

This implies that, using (3), that

$$\begin{aligned} \langle \pi, hPh \rangle + (\alpha - 1)\langle \pi, h \rangle^2 &= \alpha \sum_{x \in E} \pi(x)Q(x, x)h(x)^2 + \frac{\alpha}{2} \sum_{y \neq x} \frac{[\pi(x)Q(x, y)h(x) + \pi(y)Q(y, x)h(y)]^2}{\pi(x)Q(x, y) + \pi(y)Q(y, x)} \geq 0. \end{aligned}$$

□

4. RESULTS FOR GENERAL STATE SPACE

Let (E, \mathcal{F}_E) be a measurable space s.t. $\{x\} \in \mathcal{F}_E$ for all $x \in E$, and π be a probability measure on E . Let $\mathcal{P} = \cup_{n \geq 1} E^n$ be the set of finite subsets of E and $\mathcal{F}_{\mathcal{P}}$ be the smallest σ -field on \mathcal{P} which contains $A_1 \times \cdots \times A_n$ for all $A_i \in \mathcal{F}_E$ and $n \geq 1$. We consider a measurable proposition probability kernel $\mathcal{Q} : E \times \mathcal{F}_{\mathcal{P}} \rightarrow [0, 1]$ s.t.

$$\int_{\mathcal{P}} \mathcal{Q}(x, dA) = 1 \quad \text{and} \quad \int_{\mathcal{P}} \mathcal{Q}(x, dA) \mathbf{1}_{\{x \notin A\}} = 0$$

(this is the analogue of (8)) and a measurable selection probability kernel $\kappa : E \times \mathcal{P} \times \mathcal{F}_E \rightarrow [0, 1]$ s.t. for $x \in A$ we have $\kappa(x, A, A) = 1$. Let δ_y be the Dirac mass at point y . In

particular, since A is finite, with a slight abuse of notation, we shall also write $\kappa(x, A, d\tilde{x}) = \sum_{y \in A} \kappa(x, A, y) \delta_y(d\tilde{x})$ and so $\sum_{y \in A} \kappa(x, A, y) = 1$.

We assume that the analogue of (9) holds, that is

$$(31) \quad \pi(dx) \mathcal{Q}(x, dA) \kappa(x, A, d\tilde{x}) = \pi(d\tilde{x}) \mathcal{Q}(\tilde{x}, dA) \kappa(\tilde{x}, A, dx).$$

Remark 4.1. Let us give a natural example. Let ν be a reference measure on E with no atoms, π a probability measure on E with density w.r.t. ν which we still denote by π , a selection procedure given by $\mathcal{Q}(x, \mathcal{A}) = \mathbb{P}_x(\{x, Y_1, \dots, Y_n\} \subset \mathcal{A})$ for $\mathcal{A} \in \mathcal{F}_{\mathcal{P}}$, where Y_1, \dots, Y_n are E -valued independent random variables with density w.r.t. ν given by $q(x, \cdot)$ under \mathbb{P}_x and $n \geq 1$ is fixed. Now (31) is satisfied for the two selection procedures:

$$\kappa_k^B(x, A, y) = \mathbf{1}_{\{x, y \in A\}} \frac{\pi(y) \prod_{z \in A \setminus \{y\}} q(y, z)}{\sum_{\tilde{x} \in A} \pi(\tilde{x}) \prod_{z \in A \setminus \{\tilde{x}\}} q(\tilde{x}, z)},$$

as well as

$$\kappa_k^M(x, A, y) = \frac{\mathbf{1}_{\{x, y \in A\}} \pi(y) \prod_{z \in A \setminus \{y\}} q(y, z)}{\max \left(\pi(y) \prod_{z \in A \setminus \{y\}} q(y, z), \pi(x) \prod_{z \in A \setminus \{x\}} q(x, z) \right) + \sum_{\tilde{x} \in A \setminus \{x, y\}} \pi(\tilde{x}) \prod_{z \in A \setminus \{\tilde{x}\}} q(\tilde{x}, z)}$$

if $x \neq y$ and $\kappa_k^M(x, A, x) = 1 - \sum_{y \in A \setminus \{x\}} \kappa_k^M(x, A, y)$.

The Markov chain $X = (X_n, n \geq 0)$ is defined inductively in the following way. Let X_0 be a random variable taking values in E with probability distribution ν_0 . At step n , X_0, \dots, X_n are given. The proposal set at step $n+1$, A_{n+1} , is distributed according to $\mathcal{Q}(X_n, \cdot)$. Then X_{n+1} is chosen distributed according to $\kappa(X_n, A_{n+1}, \cdot)$. It is easy to check that X is a Markov chain with transition matrix

$$P(x, dy) = \int_{\mathcal{P}} \mathcal{Q}(x, dA) \kappa(x, A, dy).$$

Condition (31) ensures that X is reversible w.r.t. the probability measure $\pi : \pi(dx) P(x, dy) = \pi(dy) P(y, dx)$. We also assume that X is Harris recurrent (see [7] section 9). This is equivalent to assume that for all $B \in \mathcal{F}_E$ s.t. $\pi(B) > 0$ we have $\mathbb{P}(\text{Card} \{n \geq 0; X_n \in B\} = \infty | X_0 = x) = 1$ for all $x \in E$. It is easy to check for the example of Remark 4.1 that X is Harris recurrent if the random walk with transition kernel q is itself Harris recurrent.

Let f be a real-valued measurable function defined on E s.t. $\langle \pi, |f| \rangle < \infty$, where $\langle \pi, g \rangle = \int g(x) \pi(dx)$. Theorem 17.3.2 in [7] asserts that a.s. $\lim_{n \rightarrow \infty} I_n(f) = \langle \pi, f \rangle$, with $I_n(f)$ defined by (4).

We consider the functional \mathcal{J}_n defined by (17) for β any real-valued measurable function defined on $E \times \mathcal{P} \times E$. We set $\mathcal{I}_n(f, \beta) = I_n(f) + \mathcal{J}_n(\beta)$. To prove the analogue of Theorem 3.3, we shall use a martingale approach and shall assume there exists F a solution to the Poisson equation $F - PF = f - \langle \pi, f \rangle$ s.t. $\langle \pi, F^2 \rangle < \infty$ (see theorem 17.4.2 and condition (V.3) p.341 in [7] to ensure the existence of such a solution).

Theorem 4.2. *We assume X is Harris recurrent, $\langle \pi, |f| \rangle < \infty$, there exists a solution F to the Poisson equation $F - PF = f - \langle \pi, f \rangle$ such that $\langle \pi, F^2 \rangle < \infty$, and β is square integrable: $\int \pi(dx) \mathcal{Q}(x, dA) \kappa(x, A, dy) \beta(x, A, y)^2 < \infty$. Under those assumptions, we have:*

- (1) *The estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f \rangle$ is consistent: a.s. $\lim_{n \rightarrow \infty} \mathcal{I}_n(f, \beta) = \langle \pi, f \rangle$.*

- (2) The estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f \rangle$ is asymptotically normal with asymptotic variance $\sigma(f, \beta)^2$:

$$\sqrt{n}(\mathcal{I}_n(f, \beta) - \langle \pi, f \rangle) \xrightarrow[n \rightarrow \infty]{(d)} \mathcal{N}(0, \sigma(f, \beta)^2),$$

and $\sigma(f, \beta)^2$ is given by (18) (or (19)) where the sums are replaced by integrals.

Proof. We shall prove the Theorem when X_0 is distributed according to π . The general case follows from proposition 17.1.6 in [7], since X is Harris recurrent.

We set, for $n \geq 1$,

$$\Delta M_n = F(X_n) - PF(X_{n-1}) + \eta(X_{n-1}, A_n, X_n),$$

where $\eta(x, A, y) = \sum_{\tilde{x} \in A} (\kappa(x, A, \tilde{x}) - \mathbf{1}_{\{y=\tilde{x}\}}) \beta(x, A, \tilde{x})$. Notice that ΔM_n is square integrable and that $\mathbb{E}[\Delta M_{n+1} | \mathcal{G}_n] = 0$, where \mathcal{G}_n is the σ -field generated by X_0 and (A_i, X_i) for $1 \leq i \leq n$. In particular $M = (M_n, n \geq 0)$ with $M_n = \sum_{k=1}^n \Delta M_k$ is a martingale w.r.t. to the filtration $(\mathcal{G}_n, n \geq 0)$. Using that F solves the Poisson equation, we also have that

$$(32) \quad \mathcal{I}_n(f, \beta) = \frac{1}{n} M_n - \frac{1}{n} PF(X_n) + \frac{1}{n} PF(X_0) + \langle \pi, f \rangle.$$

As $\langle \pi, F^2 \rangle < \infty$ implies that $\langle \pi, |PF| \rangle < \infty$, we deduce from theorem 17.3.3 in [7] that a.s. $\lim_{n \rightarrow \infty} \frac{1}{n} PF(X_{n+1}) = 0$. In particular part (1) of the Theorem will be proved as soon as we check that $\lim_{n \rightarrow \infty} \frac{1}{n} M_n = 0$. For a probability measure ν on E and real valued functions h and g defined on E , we denote, when well defined, by $\langle \nu, h \rangle = \int h(x) \nu(dx)$ the expectation of h w.r.t. ν and

$$\text{Cov}_\nu(h, g) = \langle \nu, gh \rangle - \langle \nu, g \rangle \langle \nu, h \rangle \quad \text{and} \quad \text{Var}_\nu(h) = \langle \nu, h^2 \rangle - \langle \nu, h \rangle^2$$

respectively the covariance of g and h and the variance of h w.r.t. ν . we easily compute the bracket of M_n :

$$\langle M \rangle_n = \sum_{k=1}^n \mathbb{E}[\Delta M_k^2 | \mathcal{G}_{k-1}] = \sum_{k=1}^n h(X_{k-1}),$$

with

$$h(x) = P(F^2)(x) - (PF(x))^2 + \int \mathcal{Q}(x, dA) [-2\text{Cov}_{\kappa(x, A, \cdot)}(\beta_{x, A}, F) + \text{Var}_{\kappa(x, A, \cdot)}(\beta_{x, A})]$$

and $\beta_{x, A}(\cdot) = \beta(x, A, \cdot)$. Notice that $\langle \pi, |h| \rangle < \infty$ and that $\langle \pi, h \rangle$ is given by the right-hand side of (19), with $\sigma(f)^2 = \langle \pi, F^2 \rangle - \langle \pi, (PF)^2 \rangle$, and the sum replaced by an integral. Generalizing (19) (and (18)), we set $\sigma(f, \beta)^2 = \langle \pi, h \rangle$. Theorem 17.3.2 in [7] asserts that a.s. $\lim_{n \rightarrow \infty} \frac{1}{n} \langle M \rangle_n = \langle \pi, h \rangle$. Then theorem 1.3.15 in [4] implies that a.s. $\lim_{n \rightarrow \infty} \frac{1}{n} M_n = 0$. This ends the proof of part (1).

The proof of part (2) relies on the central limit theorem for martingales, see theorem 2.1.9 in [4]. We have already proved that a.s. $\lim_{n \rightarrow \infty} \frac{1}{n} \langle M \rangle_n = \sigma(f, \beta)^2$. Let us now check the Lindeberg's condition. Notice that theorem 17.3.2 in [7] implies that for any $a > 0$, we have

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n \mathbb{E}[\Delta M_k^2 \mathbf{1}_{\{|\Delta M_k^2| > a\}} | \mathcal{G}_{k-1}] = \langle \pi, h_a \rangle,$$

where $h_a(x) = \mathbb{E}[\Delta M_1^2 \mathbf{1}_{\{|\Delta M_1^2| > a\}} | X_0 = x]$. Notice that $0 \leq h_a \leq h$ and that $(h_a, a > 0)$ decreases to 0 as a goes to infinity. We deduce that a.s.

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n \mathbb{E}[\Delta M_k^2 \mathbf{1}_{\{|\Delta M_k^2| > \sqrt{n}\}} | \mathcal{G}_{k-1}] \leq \limsup_{a \rightarrow \infty} \langle \pi, h_a \rangle = 0,$$

which gives the Lindeberg's condition. We deduce then that $(\frac{1}{\sqrt{n}} M_n, n \geq 1)$ converges in distribution to $\mathcal{N}(0, \sigma(f, \beta)^2)$. Then use (32) and that a.s. $\lim_{n \rightarrow \infty} \frac{1}{n} (PF(X_{n+1}))^2 = 0$ (thanks to theorem 17.3.3 in [7]) to get part (2). \square

Under the assumptions of Theorem 4.2, it is easy to check that Corollaries 3.7 and 3.8 hold, as soon as the sums are replaced by integrals. For the single proposal case, then $\mathcal{Q}(x, d\{x, y\}) = Q(x, dy)$ for some kernel Q . Then Propositions 3.9 and 3.10 can also be proved if for example $\pi(dx) = \pi(x)\nu(dx)$ and $Q(x, dy) = q(x, y)\nu(dy)$ for a given reference measure ν .

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