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Does waste-recycling really improve Metropolis-Hastings Monte Carlo algorithm?

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

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ABSTRACT. The waste-recycling Monte Carlo (WR) algorithm, introduced by Frenkel, is a modification of the Metropolis-Hastings algorithm, which makes use of all the proposals, whereas the standard Metropolis-Hastings algorithm only uses the accepted proposals. We prove the convergence of the WR algorithm and its asymptotic normality. We give an example which shows that in general the WR algorithm is not asymptotically better than the Metropolis-Hastings algorithm : 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

Let E be a finite or countable set. For $\nu = (\nu(x), x \in E)$ a measure on E and $h = (h(x), x \in E)$ a real function defined on E, we denote $\langle \nu, h\rangle = \sum_{x\in E} \nu(x)h(x)$ when h is non-negative or $\langle \nu, |h|\rangle < +\infty$.

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 s.t. f is non-negative or $\langle \pi, |f|\rangle < +\infty$. 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.

The Markov chain X 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

$$\rho(x, y)\pi(x)Q(x, y) = \rho(y, x)\pi(y)Q(y, x). \tag{1}$$

For example, one gets such a function ρ by setting

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

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 Baker algorithm.

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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

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

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 properties 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 s.t. f is non-negative or $\langle \pi, |f|\rangle$ is finite, the ergodic theorem (see e.g. [5]) implies that a.s.

$$\lim_{n\to\infty} I_n(f) = \langle \pi, f\rangle,$$

where

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

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. Frenkel [3] claims that the efficiency of the estimation can be improved by including these rejected states in the sampling procedure. He suggests to use the so-called waste-recycling Monte Carlo (WR) algorithm, which consists in replacing $f(X_k)$ in $I_n(f)$ by its conditional expectation knowing the previous step and the proposal, that is $(X_{k-1},\tilde{X}_k)$. For any $h : E \to \mathbb{R}$, let h^c denote the real function defined on E^2 by the analytic or equivalent probabilistic formulas

$$\begin{aligned} h^c(x,\tilde{x}) &= \rho(x,\tilde{x})h(\tilde{x}) + (1-\rho(x,\tilde{x}))h(x) \\ &= \mathbb{E}[h(X_1)|X_0 = x, \tilde{X}_1 = \tilde{x}]. \end{aligned} \tag{5}$$

The WR algorithm is then given by the following equivalent formulas:

$$\begin{aligned} I_n^{WR}(f) = \frac{1}{n}\sum_{k=0}^{n-1} f^c(X_k,\tilde{X}_{k+1}) &= \frac{1}{n}\sum_{k=0}^{n-1} \rho(X_k,\tilde{X}_{k+1})f(\tilde{X}_{k+1}) + (1-\rho(X_k,\tilde{X}_{k+1}))f(X_k) \\ &= \frac{1}{n}\sum_{k=0}^{n-1} \mathbb{E}[f(X_{k+1})|X_k,\tilde{X}_{k+1}]. \end{aligned}$$

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 [8] and references therein. In the Rao-Blackwell Metropolis-Hasting algorithm, the weight of $f(\tilde{X}_{k+1})$ depends on all the proposals $\tilde{X}_1,\dots,\tilde{X}_n$.

In Section 2.1, we check that $X^c = (X^c_n = (X_n, \tilde{X}_{n+1}); n \geq 0)$ is a Markov chain on E^2 with invariant probability

$$\pi^c((x,\tilde{x})) = \pi(x)Q(x,\tilde{x}) \quad x,\tilde{x} \in E. \tag{6}$$

For any real function g defined on E^2, we set $\langle \pi^c, g\rangle = \sum_{x,y\in E} \pi(x,y)Q(x,y)g(x,y)$ when g is non-negative or such that $\langle \pi^c, |g|\rangle < +\infty$. We first check that we can apply the ergodic theorem, in order to deduce the convergence of $I_n^{WR}(f)$ to $\langle \pi^c, f^c\rangle$. As remarked by Frenkel in its motivation to introduce the WR algorithm, we have $\langle \pi^c, f^c\rangle = \langle \pi, f\rangle$, see also (11). This gives the convergence of the WR algorithm. The detailed proof of the next Proposition is given in Section 2.2.

Proposition 1.1. *Let f be a real valued function defined on E s.t. f is non-negative or $\langle \pi, |f|\rangle$ is finite.*

- *A.s., $\lim_{n\to\infty} I_n^{WR}(f) = \langle \pi, f\rangle$.*
- *The bias of the WR estimator $I_n^{WR}(f)$ of $\langle \pi, f\rangle$ is the same as the one of the classical Metropolis-Hastings estimator $I_n(f)$: $\mathbb{E}[I_n^{WR}(f)] = \mathbb{E}[I_n(f)]$.*

Let us formally derive the expression of the asymptotic variance of the Metropolis-Hastings algorithm. The variance of $\sqrt{n}I_n(f)$ is equal to

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

Intuitively it converges to $\sigma(f)^2 = \mathrm{Var}_\pi(f(X_0)) + 2\sum_{j\geq 1} \mathrm{Cov}_\pi(f(X_0), f(X_j))$ 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 $R \in \mathbb{R}_+^{E\times E}$ and $x \in E$, we denote $Rh(x) = \sum_{y\in E} R(x,y)h(y)$ when $h : E \to \mathbb{R}$ is non-negative or such that $R|h|(x) < +\infty$. 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

$$\sigma(f)^2 = \langle \pi, (F - PF)^2\rangle + 2\langle \pi, (F - PF)PF\rangle = \langle \pi, F^2\rangle - \langle \pi, (PF)^2\rangle. \tag{7}$$

This intuitive derivation can be made rigorous. We say that a function $F : E \to \mathbb{R}$ is a solution to the Poisson equation with f if

$$\forall x \in E,\ P|F|(x) < +\infty \quad \text{and} \quad F(x) - PF(x) = f(x) - \langle \pi, f\rangle. \tag{8}$$

Notice that if F is a solution to the Poisson equation with f, then so is $F + a$, for any constant $a \in \mathbb{R}$. If E is finite, there exists a unique solution, up to an additive constant, to the Poisson equation (see Remark 4.2, where the finite and infinite case are considered, see also [5] or [4]).

If F is a solution to the Poisson equation with f s.t. $\langle \pi, F^2\rangle < \infty$, then we have the following convergence in distribution (see [2] or [5])

$$\sqrt{n}\left(\frac{1}{n}\sum_{k=1}^{n} f(X_k) - \langle \pi, f\rangle\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0, \sigma(f)^2),$$

where $\mathcal{N}(0,\sigma^2)$ denotes the Gaussian distribution with mean 0 and variance σ^2 and $\sigma(f)^2$ is given by (7). Notice that $\sigma(f)^2$ is well defined as soon as $\langle \pi, F^2\rangle < \infty$. Indeed, Jensen inequality implies $(P|F|)^2 \leq P(F^2)$ which gives $\langle \pi, (P|F|)^2\rangle \leq \langle \pi, P(F)^2\rangle = \langle \pi, F^2\rangle$, where we used that π is invariant for P in the last equality. This implies that $\langle \pi, (PF)^2\rangle$ is well defined and less than $\langle \pi, F^2\rangle$.

The next Theorem gives the asymptotic variance of the WR estimator.

Theorem 1.2. *Let f be a real valued function defined on E s.t. $\langle \pi, |f|\rangle$ is finite and there exists a solution F to the Poisson equation with f s.t. $\langle \pi, F^2\rangle < \infty$. We have $\langle \pi^c, ((PF)^c)^2\rangle \leq \langle \pi^c, (F^c)^2\rangle \leq \langle \pi, F^2\rangle < \infty$ and the following convergence in distribution*

$$\sqrt{n}\left(I_n^{WR}(f) - \langle \pi, f\rangle\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0, \sigma_{WR}(f)^2),$$

where

$$\sigma_{WR}(f)^2 = \langle \pi^c, (F^c)^2\rangle - \langle \pi^c, ((PF)^c)^2\rangle.$$

Remark 1.3. For any real function h defined E, we have from Lemma 2.2 that $\langle \pi^c, (h^c)^2\rangle \leq \langle \pi^c, (h^2)^c\rangle = \langle \pi, h^2\rangle$. Taking $h = F$ then $h = PF$, we get $\langle \pi^c, (F^c)^2\rangle \leq \langle \pi, F^2\rangle$ and $\langle \pi^c, ((PF)^c)^2\rangle \leq \langle \pi, (PF)^2\rangle$. Therefore the comparison of $\sigma_{WR}(f)^2$ with $\sigma(f)^2$ is not obvious.

As noticed by Frenkel in a particular case, 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 $I_n(f)$. This is indeed a consequence of Jensen inequality:

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

with $h = f - \langle \pi, f\rangle$. This and simulations strongly suggest that the variance (resp. asymptotic variance) of I_n^{WR} should be smaller than the variance (resp. asymptotic variance) of I_n.

To study the difference between the asymptotic variances $\sigma(f)^2$ and $\sigma_{WR}(f)^2$ we rewrite it as follows.

Proposition 1.4. *Let f be a real valued function defined on E s.t. $\langle \pi, |f|\rangle$ is finite and there exists a solution F to the Poisson equation with f s.t. $\langle \pi, F^2\rangle < \infty$. We have*

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

where $s(x,y) = \rho(x,y) + \rho(y,x)$ for $(x,y) \in E^2$ and $\mathbb{E}_\pi$ means that X_0 is distributed according to π.

Using the first formula, we give in Section 3 a simple example such that the asymptotic variance of the WR estimation is greater than the one of the standard Metropolis-Hastings algorithm.

Corollary 1.5. *The asymptotic variance of the WR algorithm is not smaller in general than the one of the standard Metropolis-Hastings algorithm.*

Notice the function $s(x,y) = \rho(x,y) + \rho(y,x)$ is symmetric on E^2 and $0 < s(x,y) \le 2$. By (1), if $Q(x,y) > 0$, we have

$$\rho(x,y) = \frac{s(x,y)\pi(y)Q(y,x)}{\pi(x)Q(x,y) + \pi(y)Q(y,x)} \quad \text{and} \quad \rho(y,x) = \frac{s(x,y)\pi(x)Q(x,y)}{\pi(x)Q(x,y) + \pi(y)Q(y,x)}.$$

Since $\max(\rho(x,y), \rho(y,x)) \le 1$, we have $s(x,y) \le 1 + \min\left(\frac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)}, \frac{\pi(x)Q(x,y)}{\pi(y)Q(y,x)}\right)$ with equality obtained when ρ is given by (2) and $\gamma(u) = \min(1,u)$. The Metropolis algorithm ($\gamma(u) = \min(1,u)$) maximizes the acceptance probabilities.

Under some specific assumption on the function s, the asymptotic variance of the WR algorithm is smaller or equal to the one of the standard Metropolis-Hastings algorithm, for all functions f.

Proposition 1.6.

(i) *Let ϕ defined on E be such that $\langle \pi, \phi^2 \rangle < \infty$. We have $\Delta \ge 0$, where*

$$\Delta = \frac{1}{2}\,\mathbb{E}_\pi\Big[(\phi(X_1) - \phi(X_0))^2 - (P\phi(X_1) - P\phi(X_0))^2\Big]. \tag{9}$$

(ii) *We assume there exists $\beta \in (0,2)$ such that*

$$s(x,y) = \beta \quad \textit{for all} \quad x \neq y \in E \quad \textit{s.t.} \quad Q(x,y) > 0. \tag{10}$$

Then for all real valued functions defined on E s.t. $\langle \pi, |f| \rangle$ is finite and there exists a solution F to the Poisson equation with f s.t. $\langle \pi, F^2 \rangle < \infty$, we have

$$\sigma(f)^2 \ge \sigma_{WR}(f)^2,$$

with strict inequality if f is non constant.

We end this section with some comments on hypothesis (10).

(1) If $\beta = 2$, 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 algorithm coincide.
(2) Hypothesis (10) means that (2) holds with $\gamma(u) = \frac{\beta u}{1+u}$. The constant β has to be smaller than $1 + \min_{x \neq y, Q(x,y)>0} \frac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)}$. The so-called Boltzmann algorithm corresponds to $\beta = 1$. In Remark 4.3, we provide formulas for $\sigma(f)^2$ and $\sigma_{WR}(f)^2$. If $\beta = 1$, we also check that P is non-negative (equivalently if E is finite: all the eigenvalues of P belongs to $[0,1]$). Let us however recall that the asymptotic performance of the Boltzmann algorithm is sub-optimal compared to the choice $\gamma(u) = \min(1,u)$, see [6] or [9].
(3) Assume ρ satisfies (2) for some function γ. Hypothesis (10) 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 $x \in E$, $\pi(x) = \mathrm{e}^{-H(x)} / \sum_{y \in E} \mathrm{e}^{-H(y)}$ for some energy function H. Then hypothesis (10) 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 $Q(x,y) > 0$.

Organization of the paper. Section 2 is devoted to the proof of the main results. The counter-example, which provides a proof of Corollary 1.5 is given in Section 3. The proof of Proposition 1.6 is detailed in Section 4. In most of the proofs, we shall give analytical arguments in order to reach non-specialists in probability theory. We sometimes also provide an alternative probabilistic argument.

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2. Proofs

2.1. **Preliminaries.** Notice that $X^c = (X^c_n = (X_n, \tilde{X}_{n+1}); n \geq 0)$ is a Markov chain on E^2. Its transition matrix, P^c, is given by: for $x, \tilde{x}, y, \tilde{y} \in E$

$$P^c((x,\tilde{x}),(y,\tilde{y})) = \left[\mathbf{1}_{\{y=\tilde{x}\}}\rho(x,\tilde{x}) + \mathbf{1}_{\{y=x\}}(1-\rho(x,\tilde{x}))\right] Q(y,\tilde{y}).$$

(If $x = \tilde{x}$, then $P^c((x,\tilde{x}),(y,\tilde{y})) = \mathbf{1}_{\{y=x\}}Q(y,\tilde{y})$.)

Lemma 2.1. *The transition matrix P^c is irreducible on $E^c = \{(x,\tilde{x}) \in E^2; Q(x,\tilde{x}) > 0\}$. The probability measure π^c defined by (6) is invariant for P^c.*

Proof. Let $(x,\tilde{x})$ and $(y,\tilde{y})$ be such that $Q(x,\tilde{x}) > 0$ and $Q(y,\tilde{y}) > 0$. By irreducibility of P, there are $m \in \mathbb{N}^*$ and $x_1, \ldots, x_{m-1} \in E$ with $x_i \neq x_{i+1}$ for $i \in \{1, \ldots, m-2\}$ such that $P(\tilde{x}, x_1)P(x_1,x_2)\cdots P(x_{m-2},x_{m-1})P(x_{m-1},y) > 0$. One has

$$\begin{aligned}
&P^c((\tilde{x},x_1),(x_1,x_2))P^c((x_1,x_2),(x_2,x_3))\ldots P^c((x_{m-1},y),(y,\tilde{y}))\\
&\qquad = \rho(\tilde{x},x_1)Q(x_1,x_2)\rho(x_1,x_2)Q(x_2,x_3)\cdots\rho(x_{m-1},y)Q(y,\tilde{y}).
\end{aligned}$$

Multiplying by $P^c((x,\tilde{x}),(\tilde{x},x_1)) \geq \rho(x,\tilde{x})Q(\tilde{x},x_1) > 0$, one deduces that

$$P^c((x,\tilde{x}),(\tilde{x},x_1))P^c((\tilde{x},x_1),(x_1,x_2))\cdots P^c((x_{m-1},y),(y,\tilde{y})) > 0.$$

Hence P^c is irreducible on E^c.

Let us check that π^c is invariant for P^c. We have

$$\begin{aligned}
&\sum_{x,\tilde{x}\in E} \pi(x)Q(x,\tilde{x})P^c((x,\tilde{x}),(y,\tilde{y}))\\
&= \sum_{x\in E}\pi(x)Q(x,y)\rho(x,y)Q(y,\tilde{y}) + \sum_{\tilde{x}\in E}\pi(y)Q(y,\tilde{x})(1-\rho(y,\tilde{x}))Q(y,\tilde{y})\\
&= \left[\sum_{x\in E, x\neq y}\pi(x)P(x,y) + \pi(y)Q(y,y)\rho(y,y)\right]Q(y,\tilde{y}) + \pi(y)\left[1 - \sum_{\tilde{x}\in E}Q(y,\tilde{x})\rho(y,\tilde{x})\right]Q(y,\tilde{y})\\
&= \left[\sum_{x\in E}\pi(x)P(x,y)\right]Q(y,\tilde{y})\\
&= \pi(y)Q(y,\tilde{y}),
\end{aligned}$$

where we used (3) for the second and third equalities and the invariance of π for P for the last. □

Lemma 2.2. *For any real function h defined on E, we have $\langle \pi^c, |h^c|\rangle \leq \langle \pi, |h|\rangle$. If h is non-negative or if $\langle \pi, |h|\rangle < \infty$, then we have*

$$\langle \pi^c, h^c\rangle = \langle \pi, h\rangle. \tag{11}$$

We have $(h^2)^c - (h^c)^2 \geq 0$ *and*

$$\langle \pi^c, (h^2)^c - (h^c)^2 \rangle = \sum_{(x,\tilde{x}) \in E^2} \pi(x) P(x,\tilde{x})(1-\rho(x,\tilde{x}))(h(\tilde{x}) - h(x))^2 \geq 0. \tag{12}$$

Proof. If h is non-negative, by (3), we have

$$\begin{aligned} Ph(x) &= \sum_{y \neq x} Q(x,y)\rho(x,y)h(y) + \left[Q(x,x) + \sum_{y \neq x} Q(x,y)(1-\rho(x,y)) \right] h(x) \\ &= \sum_{y \in E} Q(x,y) \left[\rho(x,y)h(y) + (1-\rho(x,y))h(x) \right] \\ &= \sum_{y \in E} Q(x,y) h^c(x,y). \end{aligned} \tag{13}$$

Therefore if h is non-negative, since π is invariant for P, we have

$$\langle \pi, h \rangle = \langle \pi, Ph \rangle = \sum_{x \in E} \pi(x) \sum_{y \in E} Q(x,y) h^c(x,y) = \langle \pi^c, h^c \rangle.$$

Use $|h^c| \leq |h|^c$ to deduce $\langle \pi^c, |h^c| \rangle \leq \langle \pi^c, |h|^c \rangle = \langle \pi, |h| \rangle$. Fubini Theorem implies that (13) also holds if $P|h|(x) < +\infty$ and that if $\langle \pi, |h| \rangle < +\infty$, then $\langle \pi, h \rangle = \langle \pi^c, h^c \rangle$.

From a probabilistic point of view, for h non-negative or s.t. $\langle \pi, |h| \rangle < +\infty$, we have

$$\langle \pi^c, h^c \rangle = \mathbb{E}_\pi \left[\mathbb{E}[h(X_1) | X_0, \tilde{X}_1] \right] = \mathbb{E}_\pi[h(X_1)] = \langle \pi, h \rangle,$$

where we used that X_1 is distributed according to π under $\mathbb{E}_\pi$.

By an easy computation,

$$(h^2)^c(x,\tilde{x}) - (h^c)^2(x,\tilde{x}) = \rho(x,\tilde{x})(1-\rho(x,\tilde{x}))(h(\tilde{x}) - h(x))^2.$$

Since $Q(x,\tilde{x})\rho(x,\tilde{x})$ is equal to $P(x,\tilde{x})$ when $\tilde{x} \neq x$ and $h(\tilde{x}) - h(x) = 0$ otherwise, one easily deduces (12). □

2.2. **Proof of Proposition 1.1.** The Markov chain X^c is irreducible with invariant probability measure π^c. Let g defined on E^2 be s.t. g is non-negative or $\langle \pi^c, |g| \rangle < \infty$. The ergodic theorem (see e.g. [5]) implies that a.s. $\lim_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} g(X_k, \tilde{X}_{k+1}) = \langle \pi^c, g \rangle$. The first statement in the Proposition is a consequence of this result for $g = f^c$, since by Lemma 2.2, $\langle \pi^c, |f^c| \rangle < \langle \pi, |f| \rangle$ and for f non-negative or such that $\langle \pi, |f| \rangle < +\infty$, $\langle \pi^c, f^c \rangle = \langle \pi, f \rangle$.

Denoting the distribution of X_j by ν_j, one has using (13) for the second equality

$$\begin{aligned} \mathbb{E}[f^c(X_k, \tilde{X}_{k+1})] &= \sum_{x,y \in E} \nu_k(x) Q(x,y) f^c(x,y) = \sum_{y \in E} \left(\sum_{x \in E} \nu_k(x) P(x,y) \right) f(x) \\ &= \sum_{y \in E} \nu_{k+1}(y) f(y) = \mathbb{E}[f(X_{k+1})]. \end{aligned}$$

We can recover this result using a probabilistic approach:

$$\mathbb{E}\left[\mathbb{E}[f(X_{k+1}) | X_k, \tilde{X}_{k+1}] \right] = \mathbb{E}[f(X_{k+1})].$$

This gives the second statement in the Proposition.

2.3. **Proof of Theorem 1.2.** Let g defined on E^c. If G is a solution of the Poisson equation:

$$\forall (x,\tilde{x}) \in E^c,\ P^c|G|(x,\tilde{x}) < +\infty \quad \text{and} \quad G - P^c G = g - \langle \pi^c, g\rangle, \tag{14}$$

such that $\langle \pi^c, G^2\rangle < +\infty$, then we have the following convergence in distribution (see [2] or [5])

$$\sqrt{n}\left(\frac{1}{n}\sum_{k=0}^{n-1} g(X_k, \tilde{X}_{k+1}) - \langle \pi^c, g\rangle\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0,\sigma^2),$$

with $\sigma^2 = \langle \pi^c, G^2\rangle - \langle \pi^c, (P^c G)^2\rangle$. We have to apply this result for $g = f^c$.

Thus, to complete the proof, it is enough to check that $P^c F^c = (PF)^c$. Indeed, using (8) for the third equality, this ensures that $G = F^c$ solves the Poisson equation (14) with $g = f^c$:

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

Moreover, $\langle \pi, F^2\rangle < \infty$ implies, thanks to (12) and (11), $\langle \pi^c, (F^c)^2\rangle \leq \langle \pi^c, (F^2)^c\rangle = \langle \pi, F^2\rangle$. Last, by Jensen inequality, $(P^c F^c)^2 \leq P^c (F^c)^2$, which combined with the invariance of π^c by P^c, implies $\langle \pi^c, ((PF)^c)^2\rangle = \langle \pi^c, (P^c F^c)^2\rangle \leq \langle \pi^c, (F^c)^2\rangle$. Notice this implies that $\sigma_{WR}(f)^2$ is well defined.

Let us prove that $P^c F^c = (PF)^c$. We have

$$\begin{aligned} P^c F^c(x,\tilde{x}) &= \sum_{y,\tilde{y}\in E^2} \left[\mathbf{1}_{\{y=\tilde{x}\}}\rho(x,\tilde{x}) + \mathbf{1}_{\{y=x\}}(1-\rho(x,\tilde{x}))\right] Q(y,\tilde{y}) F^c(y,\tilde{y}) \\ &= \rho(x,\tilde{x}) \sum_{\tilde{y}\in E} Q(\tilde{x},\tilde{y}) F^c(\tilde{x},\tilde{y}) + (1-\rho(x,\tilde{x})) \sum_{\tilde{y}\in E} Q(x,\tilde{y}) F^c(x,\tilde{y}) \\ &= \rho(x,\tilde{x}) PF(\tilde{x}) + (1-\rho(x,\tilde{x})) PF(x) = (PF)^c(x,\tilde{x}), \end{aligned}$$

where we used (13) for the third equality. From a probabilistic point of view, the fact that F^c solves the Poisson equation (14) with $g = f^c$ comes from

$$\begin{aligned} F^c(x,\tilde{x}) - P^c F^c(x,\tilde{x}) &= \mathbb{E}[F(X_1)|X_0 = x, \tilde{X}_1 = \tilde{x}] - \mathbb{E}[\mathbb{E}[F(X_2)|X_1, \tilde{X}_2]|X_0 = x, \tilde{X}_1 = \tilde{x}] \\ &= \mathbb{E}[F(X_1) - PF(X_1)|X_0 = x, \tilde{X}_1 = \tilde{x}] \\ &= \mathbb{E}[f(X_1)|X_0 = x, \tilde{X}_1 = \tilde{x}] - \langle \pi, f\rangle \\ &= f^c(x,\tilde{x}) - \langle \pi^c, f^c\rangle. \end{aligned}$$

2.4. **Proof of Proposition 1.4.** Since π is reversible with respect to P, when X_0 is distributed according to π, then (X_0, X_1) and (X_1, X_0) have the same distribution. Therefore the second equality of Proposition 1.4 easily follows from the first. Let us now prove this first equality. Using (11), we have

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

Therefore we get

$$\sigma(f)^2 - \sigma_{WR}(f)^2 = \langle \pi^c, (F^2)^c - (F^c)^2\rangle - \langle \pi^c, ((PF)^2)^c - ((PF)^c)^2\rangle.$$

The result is then a consequence of (12). From a probabilistic point of view, we have

$$\begin{aligned} \sigma(f)^2 - \sigma_{WR}(f)^2 &= \mathbb{E}_\pi[F^2(X_1) - (PF)^2(X_1)] - \mathbb{E}_\pi[\mathbb{E}[F(X_1)|X_0, \tilde{X}_1]^2 - \mathbb{E}_\pi[PF(X_1)|X_0, \tilde{X}_1]^2] \\ &= \mathbb{E}_\pi[(F(X_1) - \mathbb{E}[F(X_1)|X_0, \tilde{X}_1])^2] \\ &\qquad - \mathbb{E}_\pi[((PF)(X_1) - \mathbb{E}[PF(X_1)|X_0, \tilde{X}_1])^2] \\ &= \mathbb{E}_\pi[(F(X_1) - F^c(X_0, \tilde{X}_1))^2] - \mathbb{E}_\pi[((PF)(X_1) - (PF)^c(X_0, \tilde{X}_1))^2]. \end{aligned}$$

One concludes by taking $h = F$ and $h = PF$ in the next equality :

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

3. A counter-example

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 (8): $F - PF = f - \langle \pi, f \rangle$.

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

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

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 Proposition 1.4, we have

$$\sigma(f)^2 - \sigma_{WR}(f)^2 = -\pi(a)P(a, b)(1 - \rho)(P(b, c) - P(a, c))^2 < 0.$$

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. $f^c(X_0, \tilde{X}_1)$, instead of $f(X_1)$ is equal to

$$\begin{aligned}
\langle \pi, f^2 \rangle - \langle \pi^c, (f^c)^2 \rangle &= \langle \pi^c, (f^2)^c - (f^c)^2 \rangle \\
&= \mathbb{E}_\pi[(1 - \rho(X_0, X_1))(f(X_1) - f(X_0))^2] \\
&= \pi(a)P(a, b)(1 - \rho)(P(b, c) - P(a, c))^2,
\end{aligned}$$

where we used (12) with $h = f$. 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 $\sigma(f)^2 - \sigma_{WR}(f)^2 = -0.010115$ 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]

4. Proof of Proposition 1.6 and other results

4.1. **Proof of (i) of Proposition 1.6.** Notice that for any real function h defined on E s.t. $\langle \pi, h^2 \rangle < \infty$, we have

$$\begin{aligned}\mathbb{E}_\pi[(h(X_1) - h(X_0))^2] &= \mathbb{E}_\pi[h(X_1)^2 + h(X_0)^2 - 2h(X_1)h(X_0)] \\ &= 2\langle \pi, h^2 \rangle - 2\langle \pi, hPh \rangle,\end{aligned} \tag{15}$$

where we used that X_1 is distributed according to π under $\mathbb{E}_\pi$ for the last equality. Using this result for $h = \phi$ and $h = P\phi$, we get

$$\Delta = \left[\langle \pi, \phi^2 \rangle - \langle \pi, \phi P\phi \rangle - \langle \pi, (P\phi)^2 \rangle + \langle \pi, (P\phi)(P^2\phi) \rangle \right]. \tag{16}$$

Recall that $\pi(x) > 0$ for all $x \in E$. In order to prove the result, we shall use the spectral decomposition associated with the matrix R defined by

$$R(x, y) = \sqrt{\pi(x)} P(x, y) \frac{1}{\sqrt{\pi(y)}}, \quad x, y \in E.$$

Since P is reversible w.r.t. π, R is symmetric. We consider the Hilbert space $\ell^2 = \{g \in \mathbb{R}^E; \| g \| = \sum_{x \in E} g(x)^2 < \infty\}$ with the scalar product $\langle g_1, g_2 \rangle = \sum_{x \in E} g_1(x) g_2(x)$. (Notice this is coherent with the previous definition of $\langle \cdot, \cdot \rangle$.) For any real function g defined on E, we have

$$\begin{aligned}\sum_{x,y \in E} R(x, y)\, |g(x)|\, |g(y)| &= \sum_{x,y \in E} \pi(x) P(x, y) \frac{|g(x)|}{\sqrt{\pi(x)}} \frac{|g(y)|}{\sqrt{\pi(y)}} \\ &\leq \frac{1}{2} \sum_{x,y \in E} \pi(x) P(x, y) \left(\frac{g(x)^2}{\pi(x)} + \frac{g(y)^2}{\pi(y)} \right) \\ &= \| g \|^2.\end{aligned}$$

The operator $g \mapsto Rg$ is bounded and self-adjoint on ℓ^2. As $\langle g, Rg \rangle \leq \| g \|^2$ for all $g \in \ell^2$, this implies that the spectrum of R lies in $[-1, 1]$. Next Lemma implies that 1 is an eigenvalue of R with eigenspace $\{c\sqrt{\pi}, c \in \mathbb{R}\}$.

Lemma 4.1. *The harmonic functions h for P (resp. g for R) i.e. the solutions to $Ph = h$ (resp. $Rg = g$) s.t. $\langle \pi, h^2 \rangle < \infty$ (resp. $g \in \ell_2$) are the constants (resp. the functions $c\sqrt{\pi}$ with $c \in \mathbb{R}$).*

Proof. Notice that any constant function h is harmonic for P and such that $\langle \pi, h^2\rangle < \infty$.

Let now h be an harmonic function for P s.t. $\langle \pi, h^2\rangle < \infty$. We have, using (15),

$$\sum_{x,y\in E} \pi(x)P(x,y)(h(x)-h(y))^2 = \mathbb{E}_\pi[(h(X_0)-h(X_1))^2] = 2\langle \pi, h(h-Ph)\rangle = 0.$$

As P is irreducible, this implies that h is constant.

Since g is harmonic for R if and only if $g = \sqrt{\pi} h$ with h harmonic for P and then $\|g\|^2 = \langle \pi, h^2\rangle$, one easily deduces the statement concerning the harmonic functions for R. $\square$

We first consider the case E finite with cardinal J to get a clear intuition of the result.

Case E finite. The matrix R has J eigenvalues $\lambda_1, \ldots, \lambda_J$, s.t. $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_J \geq -1$. Let $e_1, \ldots, e_J$ be a family of corresponding orthogonal eigenvectors with norm 1.

We set $\varphi = \sqrt{\pi}\phi$. We have $\varphi = \sum_{1\leq j\leq J} \alpha_j e_j$ with $\alpha_j = \langle \varphi, e_j\rangle$ for $1 \leq j \leq J$. We rewrite Δ using (16) and the definition of φ :

$$\Delta = \left[\langle \varphi, \varphi\rangle - \langle \varphi, R\varphi\rangle - \langle R\varphi, R\varphi\rangle + \langle R\varphi, R^2\varphi\rangle\right]. \tag{17}$$

Using the orthonormality of $e_1, \ldots, e_J$, we get $\langle \varphi, \varphi\rangle = \sum_{1\leq j\leq J} \alpha_j^2$, $\langle \varphi, R\varphi\rangle = \sum_{1\leq j\leq J} \lambda_j\alpha_j^2$, $\langle R\varphi, R\varphi\rangle = \sum_{1\leq j\leq J} \lambda_j^2\alpha_j^2$ and $\langle R\varphi, R^2\varphi\rangle = \sum_{1\leq j\leq J} \lambda_j^3\alpha_j^2$. We deduce from (17) and $\lambda_1 = 1$, that

$$\Delta = \sum_{1\leq j\leq J} (1-\lambda_j-\lambda_j^2+\lambda_j^3)\alpha_j^2 = \sum_{2\leq j\leq J} (1-\lambda_j)^2(1+\lambda_j)\alpha_j^2 \geq 0. \tag{18}$$

Case E countable. We shall use the spectral decomposition of R, and we refer to [7] chapter VII and VIII or to [1] chapter VIII. For any $g \in \ell^2$, there exists a bounded non-negative measure μ_g on $[-1,1]$, called the spectral measure associated with g s.t. if ψ is a measurable function defined on $[-1,1]$ and $\int \psi(\lambda)^2\mu_g(d\lambda) < \infty$, then g belongs to the domain of the operator $\psi(R)$, defined by formula VIII-4 in [7] or VIII.3.110 in [1], and $\|\psi(R)g\|^2 = \int_{[-1,1]} \psi(\lambda)^2\mu_g(d\lambda)$. (If E is finite, then we have $\mu_g(d\lambda) = \sum_{1\leq j\leq J}\langle e_j, g\rangle\delta_{\lambda_j}(d\lambda)$.)

Notice that $\varphi = \sqrt{\pi}\phi$ belongs to ℓ^2 and that $\sqrt{\pi}P\phi = R\varphi$ belongs also to ℓ^2. We shall compute all the quantities of the right hand side of (16):

$$\langle \pi, \phi^2\rangle = \langle \varphi, \varphi\rangle = \int_{[-1,1]} \mu_\varphi(d\lambda),$$

$$\langle \pi, (P\phi)^2\rangle = \langle R\varphi, R\varphi\rangle = \int_{[-1,1]} \lambda^2\mu_\varphi(d\lambda).$$

As φ belongs to the domain of $R+I = \psi(R)$, with $\psi(r) = r+1$, we have

$$\langle \pi, \phi P\phi\rangle = \langle \varphi, R\varphi\rangle = \frac{1}{2}\left(\|(R+I)\varphi\|^2 - \|R\varphi\|^2 - \|\varphi\|^2\right) = \int_{[-1,1]} \lambda\mu_\varphi(d\lambda).$$

As φ belongs to the domain of R^2 and of R^2+R, we have

$$\langle \pi, (P\phi)(P^2\phi)\rangle = \langle R\varphi, R^2\varphi\rangle = \frac{1}{2}\left(\|(R^2+R)\varphi\|^2 - \|R^2\varphi\|^2 - \|R\varphi\|^2\right) = \int_{[-1,1]} \lambda^3\mu_\varphi(d\lambda).$$

We deduce from (16), that

$$\Delta = \int_{[-1,1]} (1-\lambda-\lambda^2+\lambda^3)\mu_\varphi(d\lambda) = \int_{[-1,1]} (1-\lambda)^2(1+\lambda)\mu_\varphi(d\lambda) \geq 0. \tag{19}$$

Notice that this last equation replaces (18), but that (17) still holds for E countable.

4.2. **Proof of (ii) of Proposition 1.6.** We have $\sigma(f)^2 - \sigma_{WR}(f)^2 = (2-\beta)\Delta$. So from (i) of the Proposition, it remains to prove that $\Delta = 0$, where $\phi = F$ in (9), if and only if f is a constant.

Since $\beta < 2$, there exists $x, y \in E$ s.t. $Q(x, y) > 0$ and $\rho(x, y) < 1$, and thus $P(x, x) > 0$. It is easy to check that this implies that P^2 is irreducible. Indeed, let $y \in E$. There exist $n \geq 1$, $x_0, \ldots, x_n \in E$ s.t. $x_0 = y$, $x_{n-1} = x_n = x$ and $P(x_i, x_{i+1}) > 0$ for $i \in \{0, \ldots, n-1\}$. We have $P^2(x_{2i}, x_{2i+2}) \geq P(x_{2i}, x_{2i+1})P(x_{2i+1}, x_{2i+2}) > 0$ for $0 \leq i \leq \lfloor n/2 \rfloor - 1$. We deduce that $(P^2)^{\lfloor n/2 \rfloor}(y, x) \geq P^2(x_0, x_2) \cdots P^2(x_{2\lfloor n/2 \rfloor - 2}, x_{2\lfloor n/2 \rfloor}) > 0$. For $z \in E$, one gets similarly the existence of $m \geq 1$ such that $(P^2)^m(x, z) > 0$. Thus P^2 is irreducible.

Then we prove that this implies that -1 is not an eigenvalue for R.

Let $g \in \ell^2$ be s.t. $Rg = -g$. This implies that $R^2 g = g$. We set $h = g/\sqrt{\pi}$ so that we have $Ph = -h$ and $P^2 h = h$, i.e. h is an harmonic function for P^2. The probability measure π is invariant for P^2 and according to Lemma 4.1, the only harmonic functions, h, for P^2 s.t. $\langle \pi, h^2 \rangle < \infty$ are the constants. Hence we get $Ph = h$. As $h = -Ph$, this implies that $h = 0$. Therefore -1 is not an eigenvalue of R.

Case E finite. We use notation of Section 4.1. Since -1 is not an eigenvalue of R, we have $\lambda_j \in (-1, 1)$ and thus $(1-\lambda_j)^2(1+\lambda_j) > 0$ for $2 \leq j \leq J$. Recall that 1 is an eigenvalue of R with eigenspace $\{c\sqrt{\pi}, c \in \mathbb{R}\}$. From (18) we get that $\Delta = 0$ if and only if $\varphi = c\sqrt{\pi}$ for some $c \in \mathbb{R}$, i.e. $F = \varphi/\sqrt{\pi}$ and therefore $f = F - PF + \langle \pi, f \rangle$ are constant functions.

Case E countable. Since -1 is not an eigenvalue of R, the spectral measure associated with an element of ℓ^2 does not put a mass on $\{-1\}$, see Theorem 8 ii) of chapter VIII in [1]. Hence, we deduce from (19) that $\Delta = 0$ implies the support of μ_φ, with $\varphi = \sqrt{\pi}F$, is reduced to $\{1\}$. This implies $\|\varphi - R\varphi\|^2 = \int (1-\lambda)^2 \mu_\varphi(d\lambda) = 0$, that is $\varphi = R\varphi$ or equivalently $F = PF$. From Lemma 4.1, we get that F is constant.

4.3. **Other results.** We make some comments on existence and uniqueness for the Poisson equation (8) in Remark 4.2 and prove in Remark 4.3 that, under assumption (10) with $\beta = 1$, R is non-negative .

Remark 4.2. Let f be a real function defined on E s.t. $\langle \pi, |f| \rangle < \infty$. This last condition is automatically satisfied if E is finite. We set $g = \sqrt{\pi}(f - \langle \pi, f \rangle)$.

Case E finite. Recall that the eigenvalues of R are such that $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_J \geq -1$ and let $e_1, \ldots, e_J$ be a family of corresponding orthogonal eigenvector with norm 1. We choose $e_1 = \sqrt{\pi}$. We have $\langle e_1, g \rangle = 0$. There exists $\alpha_j \in \mathbb{R}$, $2 \leq j \leq J$ s.t. $g = \sum_{2 \leq j \leq J} \alpha_j (1-\lambda_j) e_j$ or equivalently $f = \langle \pi, f \rangle + \sum_{2 \leq j \leq J} \alpha_j (1-\lambda_j) f_j$, where $f_j = e_j/\sqrt{\pi}$.

The function $\varphi = \sum_{2 \leq j \leq J} \alpha_j e_j$ solves $\varphi - R\varphi = g$ and the function $F = \varphi/\sqrt{\pi} = \sum_{2 \leq j \leq J} \alpha_j f_j$ is a solution to the Poisson equation (8). If F' is another solution, then $F - F'$ is harmonic, and thanks to Lemma 4.1, $F - F'$ is constant. Hence there exists, up to an additive constant, a unique solution to the Poisson equation (8).

Case E countable. Assume that there exists a solution, F, to the Poisson equation (8) s.t. $\langle \pi, F^2 \rangle < \infty$. By Jensen inequality, we have $\langle \pi, (PF)^2 \rangle < \infty$ and $\langle \pi, f^2 \rangle < \infty$. Notice that g belongs to ℓ^2 as well as $\varphi = \sqrt{\pi}F$. We have $\varphi - R\varphi = g$, which implies that g belongs to the domain of $(I-R)^{-1}$. Thus the spectral measure μ_g on $[-1, 1]$ associated with g is s.t. $\int_{[-1,1]} (1-\lambda)^{-2} \mu_g(d\lambda) < \infty$. Notice the converse is also true: if $\langle \pi, f^2 \rangle < \infty$ (so that $g \in \ell^2$)

and the spectral measure associated with g, μ_g, is s.t. $\int_{[-1,1]}(1-\lambda)^{-2}\mu_g(d\lambda) < \infty$, then g belongs to the domain of $(I-R)^{-1}$ and if we set $F = \varphi/\sqrt{\pi}$ with $\varphi = (I-R)^{-1}g$, then F is a solution of the Poisson equation (8) s.t. $\langle \pi, F^2\rangle < \infty$.

Notice that the first statement in Lemma 4.1 implies that 1 is an eigenvalue of R and that any eigenvector associated with 1 is equal to $\sqrt{\pi}$ up to a multiplicative constant. Then $P_1 = \mathbf{1}_{\{1\}}(R)$, defined by equation (3.20) in chapter VIII of [1], see also section VIII.4 of [7], is the orthogonal projector on $\{c\sqrt{\pi}, c \in \mathbb{R}\}$. As $\langle g, \sqrt{\pi}\rangle = \langle \pi, f\rangle - \langle \pi, f\rangle = 0$, we have $0 = \langle g, \sqrt{\pi}\rangle^2 = \| P_1 g\|^2 = \mu_g(\{1\})$ that is $\mu_g(\{1\}) = 0$. In particular, if 1 is an isolated point of the spectrum of R, then the support of μ_g is a closed subset of $[-1,1)$ and $\int_{[-1,1]}(1-\lambda)^{-2}\mu_g(d\lambda) < \infty$. Thus if 1 is an isolated point of the spectrum of R, then condition $\langle \pi, f^2\rangle < \infty$ implies the existence of a solution, F, to the Poisson equation (8) s.t. $\langle \pi, F^2\rangle < \infty$.

If F' be another solution s.t. $\langle \pi, F'^2\rangle < \infty$, then $F - F'$ is harmonic for P, and thanks to Lemma 4.1 , $F - F'$ is a constant. Hence, if there exists a solution to the Poisson equation (8) s.t. $\langle \pi, F^2\rangle < \infty$, then this solution is unique up to an additive constant.

Remark 4.3. We keep the notation of the previous Remark and assume (10). We give formulas for $\sigma(f)^2$, $\sigma_{WR}(f)^2$ and prove that R is non-negative if $\beta = 1$.

We have

$$\sigma(f)^2 = \langle \pi, F^2\rangle - \langle \pi, (PF)^2\rangle = \langle \varphi, \varphi\rangle - \langle R\varphi, R\varphi\rangle = \int_{[-1,1]} (1-\lambda^2)\mu_\varphi(d\lambda)$$

and, if E is finite, $\sigma(f)^2 = \sum_{2\le j\le J}(1-\lambda_j^2)\alpha_j^2$. It is then easy to compute $\sigma_{WR}(f)^2$. Using (19), we have

$$\sigma_{WR}(f)^2 = \sigma(f)^2 - (2-\beta)\Delta = \int_{[-1,1]} (1-\lambda^2)(\beta - 1 + \lambda(2-\beta))\mu_\varphi(d\lambda),$$

and, if E is finite, $\sigma_{WR}(f)^2 = \sum_{2\le j\le J}(1-\lambda_j^2)(\beta-1+\lambda_j(2-\beta))\alpha_j^2$.

For the particular case $\beta = 1$, which corresponds to $\gamma(u) = u/(1+u)$ in (2), we get

$$\sigma_{WR}(f)^2 = \int_{[-1,1]} (1-\lambda^2)\lambda\mu_\varphi(d\lambda),$$

and, if E is finite, $\sigma_{WR}(f)^2 = \sum_{2\le j\le J}(1-\lambda_j^2)\lambda_j\alpha_j^2$. Since this quantity is non-negative for the spectral measure μ_φ associated with any function φ such that $\varphi/\sqrt{\pi}$ is a solution to the Poisson equation, this suggests that R is non-negative.

We shall prove directly that R is non-negative when $\beta = 1$. As $\beta = 1$, for $x \neq y$ and $Q(x,y) > 0$, we have

$$R(x,y) = \frac{\sqrt{\pi(x)\pi(y)}Q(x,y)Q(y,x)}{\pi(x)Q(x,y) + \pi(y)Q(y,x)}.$$

Notice that $R(x,y)=0$ if $Q(x,y)=0$ and $x\neq y$. We also have, using (3),

$$\begin{aligned} R(x,x)=P(x,x) &= Q(x,x)+\sum_{y\neq x, Q(x,y)>0} Q(x,y)\left[1-\frac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)+\pi(y)Q(y,x)}\right] \\ &= Q(x,x)+\sum_{y\neq x, Q(x,y)>0} \frac{\pi(x)Q(x,y)^2}{\pi(x)Q(x,y)+\pi(y)Q(y,x)}. \end{aligned}$$

We deduce that for any function $g\in\ell^2$,

$$\begin{aligned} \sum_{x,y\in E} g(x)g(y)R(x,y) &= \sum_{x\in E} g(x)^2 Q(x,x) + \sum_{y\neq x, Q(x,y)>0} \frac{[g(x)\sqrt{\pi(x)}Q(x,y)]^2}{\pi(x)Q(x,y)+\pi(y)Q(y,x)} \\ &\quad + \sum_{y\neq x, Q(x,y)>0} \frac{[g(x)\sqrt{\pi(x)}Q(x,y)][g(y)\sqrt{\pi(y)}Q(y,x)]}{\pi(x)Q(x,y)+\pi(y)Q(y,x)} \\ &= \sum_{x\in E} g(x)^2 Q(x,x) \\ &\quad + \frac{1}{2}\sum_{y\neq x, Q(x,y)>0} \frac{[g(x)\sqrt{\pi(x)}Q(x,y)+g(y)\sqrt{\pi(y)}Q(y,x)]^2}{\pi(x)Q(x,y)+\pi(y)Q(y,x)} \\ &\geq 0. \end{aligned}$$

This implies that R is non-negative. In particular the spectrum of R lies in $[0,1]$, that is the support of any spectral measure lies in $[0,1]$.

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