

Improving the convergence of Markov chains via permutations and projections

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Abstract

This paper aims at improving the convergence to equilibrium of finite ergodic Markov chains via permutations and projections. First, we prove that a specific mixture of permuted Markov chains arises naturally as a projection under the KL divergence or the squared-Frobenius norm. We then compare various mixing properties of the mixture with other competing Markov chain samplers and demonstrate that it enjoys improved convergence. This geometric perspective motivates us to propose samplers based on alternating projections to combine different permutations and to analyze their rate of convergence. We give necessary, and under some additional assumptions also sufficient, conditions for the projection to achieve stationarity in the limit in terms of the trace of the transition matrix. We proceed to discuss tuning strategies of the projection samplers when these permutations are viewed as parameters. Along the way, we reveal connections between the mixture and a Markov chain Sylvester's equation as well as assignment problems, and highlight how these can be used to understand and improve Markov chain mixing. We provide two examples as illustrations. In the first example, the projection sampler (with a suitable choice of the permutation) improves upon Metropolis-Hastings in a discrete bimodal distribution with a reduced relaxation time from exponential to polynomial in the system size, while in the second example,

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the mixture of permuted Markov chain yields a mixing time that is logarithmic in system size (with high probability under random permutation), compared to a linear mixing time in the Diaconis-Holmes-Neal sampler.

Keywords: Markov chains, Kullback-Leibler divergence, Markov chain Monte Carlo, Metropolis-Hastings, alternating projections, isometric involution, permutation, Sylvester’s equation, assignment problems, Dobrushin coefficient

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1 Introduction

Given an ergodic discrete-time Markov chain with transition matrix P and stationary distribution π , in this paper we focus on improving the convergence of the Markov chain towards π via permutations and projections. In the literature, a wide variety of tools and methods have been developed to improve mixing of finite Markov chains. This includes techniques such as lifting [Apers et al. \(2021\)](#), non-reversible Markov chain Monte Carlo (MCMC) [Diaconis et al. \(2000\)](#); [Rey-Bellet and Spiliopoulos \(2016\)](#), to name but a few. More recently, there is growing interests in using permutations as a promising technique to accelerate Markov chains, see for example [Ben-Hamou and Peres \(2023\)](#); [Chatterjee and Diaconis \(2020\)](#); [Dubail \(2024a,b\)](#).

This manuscript proposes samplers based on projections to improve mixing over the original P . These projection samplers depend on some underlying permutation matrices that can be understood as tuning parameters of the algorithms. We summarize several key contributions of the paper as follows.

First, we seek to understand new projections of transition matrices. It is shown in [Andrieu and Livingstone \(2021\)](#) that some state-of-the-art non-reversible MCMC samplers are in fact (π, Q) -self-adjoint, where Q is an isometric involution matrix. These notions are to be properly recalled in Section 2 below. When Q is further assumed to be a permutation matrix, a natural question to ask is, what is the projection of P onto the set of (π, Q) -self-adjoint transition matrices? We prove that, the unique closest (π, Q) -self-adjoint transition matrix, under the Kullback-Leibler divergence or the squared-Frobenius norm (when P is π -reversible), is given by

$$\frac{1}{2}(P + QP^*Q). \tag{1}$$

This is also known in the literature as a specific mixture of permuted Markov chains in the sense of [Dubail \(2024b\)](#). In Section 2, we offer geometric interpretations and related Pythagorean-type results of the mixture in this setting, thus continuing the line of work in [Billera and Diaconis \(2001\)](#); [Diaconis and Miclo \(2009\)](#). These results are interesting since this projection can be non-reversible. This is unlike earlier results in the literature where the projections possess nice mathematical structure such as symmetry or reversibility [Choi and Wolfer \(2024\)](#); [Wolfer and Watanabe \(2021\)](#).

Second, we compare the projection sampler (1) with other competing samplers, such as

P, QP, PQ, QPQ or the mixture $\alpha P + (1 - \alpha)QP^*Q$ for $\alpha \in [0, 1]$. In Section 3 we prove that, for a host of mixing parameters such as the Dobrushin coefficient, asymptotic variances, spectral gap and the average hitting time, (1) enjoys improved performance on these metrics compared with its counterparts. This justifies the decision to focus on investigating transition matrices of the form (1) in subsequent sections.

Third, we propose and analyze an alternating projection procedure to combine a sequence of isometric involution permutation matrices Q_0, \dots, Q_{m-1} in Section 4. Specifically, we first project P onto the space of (π, Q_0) -self-adjoint matrices, followed by (π, Q_1) , and so on. If we denote the projection sampler after n steps of alternating projections to be R_n , then we prove that a limit R_∞ exists and we give a rate of convergence of R_n towards R_∞ via an application of the theory of alternating projections in Hilbert space.

Fourth, we give necessary, and under some additional assumptions also sufficient, condition characterizing the ideal situations where R_n or R_∞ equals to Π , the transition matrix where each row equals to π . We manage to relate this property to the trace of P , and more generally to the spectrum of P or R_n via a Sylvester equation. This is discussed in Section 5.

Fifth, we discuss tuning strategies when Q is viewed as a tuning parameter of the sampler in Section 6. Interestingly, one strategy lies in finding an optimal Q that solves a Markov chain assignment problem. We also make connections with the equi-energy sampler [Kou et al. \(2006\)](#).

Sixth, as a case-study and illustration we apply the theory developed to consider projection samplers where the original P is the Metropolis-Hastings (MH) chain in Section 7. We show that using (1) is equivalent to either a proposal chain with increased connections or a landscape with reduced energy barrier. We give an example where the target distribution is a discrete bimodal distribution. In this example, upon suitable tuning of Q , the projection sampler enjoys polynomial relaxation time while the original MH chain exhibits exponential (in the system size) relaxation time.

Finally, we relax the assumption to consider Q being a general permutation matrix (instead of an isometric involution transition matrix) when P admits the discrete uniform stationary distribution in Section 8. We show that many of the earlier results carry over to this setting. In particular, when Q is drawn uniformly at random from the set of permutation matrices, we show that the total variation mixing time of the mixture of permuted chain is, with high probability, at most logarithmic in the system size, while the competing sampler of Diaconis-Holmes-Neal has a linear mixing time.

2 Two types of deformed information divergences and the induced information projections onto the set of (π, Q) -self-adjoint transition matrices

Let \mathcal{X} be a finite state space and we denote by $\mathcal{L} = \mathcal{L}(\mathcal{X})$ to be the set of transition matrices on \mathcal{X} . Analogously we write $\mathcal{P}(\mathcal{X})$ to be the set of probability masses with full support on \mathcal{X} , that is, $\min_x \pi(x) > 0$ for $\pi \in \mathcal{P}(\mathcal{X})$. For $m, n \in \mathbb{Z}$ with $m \leq n$, we write $\llbracket m, n \rrbracket := \{m, m+1, \dots, n-1, n\}$. In particular, when $m = 1$ we write $\llbracket n \rrbracket := \llbracket 1, n \rrbracket$.

Let $\ell^2(\pi)$ be the Hilbert space weighted by π endowed with the inner product, for $f, g : \mathcal{X} \rightarrow \mathbb{R}$,

$$\langle f, g \rangle_\pi := \sum_{x \in \mathcal{X}} f(x)g(x)\pi(x).$$

The $\ell^2(\pi)$ -norm of f is defined to be $\|f\|_\pi^2 = \langle f, f \rangle_\pi$. We also define $\ell_0^2(\pi) := \{f \in \ell^2(\pi); \pi(f) = 0\}$.

Given a probability mass $\pi \in \mathcal{P}(\mathcal{X})$, we write $\mathcal{S}(\pi) \subseteq \mathcal{L}$ to be the set of π -stationary transition matrices, that is, $P \in \mathcal{S}(\pi)$ satisfies $\pi P = \pi$. We also denote by $\mathcal{L}(\pi) \subseteq \mathcal{L}$ to be the set of π -reversible transition matrices, that is, $P \in \mathcal{L}(\pi)$ satisfies the detailed balance condition with $\pi(x)P(x, y) = \pi(y)P(y, x)$ for all $x, y \in \mathcal{X}$. For $P \in \mathcal{S}(\pi)$, we write $P^* \in \mathcal{S}(\pi)$ to be the time-reversal or the $\ell^2(\pi)$ -adjoint of P . Thus, $P \in \mathcal{L}(\pi)$ if and only if $P = P^*$.

Let $Q : \ell^2(\pi) \rightarrow \ell^2(\pi)$ be an isometric involution on \mathcal{X} with respect to π as in [Andrieu and Livingstone \(2021\)](#), that is, Q satisfies $Q^2 = I$ and $Q^* = Q$. We write $\mathcal{I}(\pi) = \mathcal{I}(\pi, \mathcal{X})$ to be the set of isometric involution matrices on \mathcal{X} with respect to π . $L \in \mathcal{S}(\pi)$ is said to be (π, Q) -self-adjoint if and only if $L^* = QLQ$. This is also equivalent to say that QL is $\ell^2(\pi)$ -self-adjoint, and when Q is also a Markov kernel, $QL \in \mathcal{L}(\pi)$. We write $\mathcal{L}(\pi, Q) \subseteq \mathcal{L}$ to be the set of (π, Q) -self-adjoint transition matrices. In the special case of $Q = I$, we recover that $\mathcal{L}(\pi, I) = \mathcal{L}(\pi)$.

We now characterize $\mathcal{I}(\pi) \cap \mathcal{L}$ in the finite state space setting. Let \mathbf{P} be the set of permutations on \mathcal{X} . Let $\psi \in \mathbf{P}$ be a permutation, and Q_ψ be the induced permutation matrix with entries $Q_\psi(x, y) := \delta_{y=\psi(x)}$ for all $x, y \in \mathcal{X}$, where δ is the Dirac mass function. Define a set of permutations with respect to π to be

$$\Psi(\pi) := \{\psi \in \mathbf{P}; \forall x \in \mathcal{X}, \psi(\psi(x)) = x, \pi(x) = \pi(\psi(x))\}.$$

Proposition 2.1.

$$\mathcal{I}(\pi) \cap \mathcal{L} = \{Q_\psi; \psi \in \Psi(\pi)\}.$$

Proof. We first prove that $\{Q_\psi; \psi \in \Psi(\pi)\} \subseteq \mathcal{I}(\pi) \cap \mathcal{L}$. We check that $Q_\psi^2(x, y) = \delta_{y=x}$ and hence $Q_\psi^2 = I$. The detailed balance condition is also satisfied since $\pi(x)Q_\psi(x, y) = \pi(x)\delta_{y=\psi(x)} = \pi(\psi(x))\delta_{x=\psi(y)} = \pi(y)Q_\psi(y, x)$. This shows $Q_\psi \in \mathcal{I}(\pi) \cap \mathcal{L}$.

Next, we prove the opposite direction. Precisely, if $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$, then by (Miclo, 2018, Remark 4(a)) $Q = Q_\sigma$ where σ is a permutation such that $\sigma^{-1} = \sigma$. Since Q_σ is π -reversible, we check that $\pi(x) = \pi(x)Q_\sigma(x, \sigma(x)) = \pi(\sigma(x))Q_\sigma(\sigma(x), x) = \pi(\sigma(x))$. This verifies that $\sigma \in \Psi(\pi)$, which completes the proof. \square

Note that since the identity mapping $\psi(x) = x$ belongs to $\Psi(\pi)$ for all $\pi \in \mathcal{P}(\mathcal{X})$, $I = Q_\psi \in \mathcal{I}(\pi) \cap \mathcal{L}$, and hence the set $\mathcal{I}(\pi) \cap \mathcal{L}$ is non-empty. We also note that $\pm(2\Pi - I) \in \mathcal{I}(\pi)$ but these are not transition matrices, where Π is the matrix with each row equals to π .

Another remark is that, for $\psi \in \Psi(\pi)$, this is an ‘‘equi-probability’’ permutation with respect to π since we require $\pi(x) = \pi(\psi(x))$ for all x . This connection with the equi-energy sampler Kou et al. (2006) is further highlighted in Section 6.

As another important point to note, QP or PQ have been proposed and analyzed in the literature as promising samplers over the original P , see for example Ben-Hamou and Peres (2023); Chatterjee and Diaconis (2020) and the references therein. In the special case of $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$, we see that

$$(QP)^* = Q(QP)Q, \quad (PQ)^* = Q(PQ)Q,$$

and hence both $QP, PQ \in \mathcal{L}(\pi, Q)$. That is, they are (π, Q) -self-adjoint transition matrices, even if they are non-reversible with respect to π .

We now introduce two types of deformed Kullback-Leibler (KL) divergences that depend on Q .

Definition 2.1 (Q -left-deformed and Q -right-deformed KL divergences). *Let $\pi \in \mathcal{P}(\mathcal{X})$. Let $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix, $P, L \in \mathcal{L}$. The Q -left-deformed KL divergence from L to P with respect to π is defined to be*

$${}^Q D_{KL}(P||L) := D_{KL}^\pi(QP||QL) := \sum_x \pi(x) \sum_y QP(x, y) \ln \left(\frac{QP(x, y)}{QL(x, y)} \right),$$

where the usual conventions of $0 \ln(0/0) := 0$ and $0 \cdot \infty := 0$ applies. Note that the dependency on π of ${}^Q D_{KL}$ is suppressed.

Similarly, we define the Q -right-deformed KL divergence from L to P with respect to π to be

$$D_{KL}^Q(P||L) := D_{KL}^\pi(PQ||LQ).$$

Note that in the special case of $Q = I$, ${}^I D_{KL} = D_{KL}^I$ is the classical KL divergence rate from L to P when $P \in \mathcal{S}(\pi)$.

In the next proposition, we summarize a few properties of D_{KL}^Q and ${}^Q D_{KL}$:

Proposition 2.2. *Let $\pi \in \mathcal{P}(\mathcal{X})$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. For $P, L \in \mathcal{L}$, we have the following:*

1. (Non-negativity)

$${}^Q D_{KL}(P\|L) \geq 0.$$

Equality holds if and only if $QP = QL$ if and only if $P = L$. Similarly,

$$D_{KL}^Q(P\|L) \geq 0.$$

Equality holds if and only if $PQ = LQ$ if and only if $P = L$.

2. (Duality) Let $P, L \in \mathcal{S}(\pi)$.

$${}^Q D_{KL}(P\|L) = D_{KL}^Q(P^*\|L^*).$$

Proof. First, we prove non-negativity.

$${}^Q D_{KL}(P\|L) = D_{KL}^\pi(QP\|QL) \geq 0,$$

and the equality holds, by (Wang and Choi, 2023, Proposition 3.1), if and only if $QP = QL$ if and only if $P = L$. The proof for D_{KL}^Q is similar and hence omitted.

Next, we prove duality. We see that,

$${}^Q D_{KL}(P\|L) = D_{KL}^\pi(QP\|QL) = D_{KL}^\pi(P^*Q\|L^*Q) = D_{KL}^Q(P^*\|L^*),$$

where the second equality follows from the bisection property (Choi and Wolfer, 2024, Theorem III.1). \square

For $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ being an isometric involution transition matrix, we define

$$\bar{P} = \bar{P}(Q) := \frac{1}{2}(P + QP^*Q). \quad (2)$$

It can readily be seen that $Q\bar{P}Q = \bar{P}^*$, and hence $\bar{P} \in \mathcal{L}(\pi, Q)$. In the special case of $Q = I$, we recover that $\bar{P}(I)$ is the additive reversibilization of P . We also note that $\bar{P}(Q)$ can be interpreted as a specific mixture of permuted Markov chains in the sense of Dubail (2024b).

The next result presents a Pythagorean identity, which can be interpreted as the property that \bar{P} is the closest (π, Q) -self-adjoint transition matrix to a given P :

Proposition 2.3. *Let $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. For $L \in \mathcal{L}(\pi, Q)$, we then have*

$${}^Q D_{KL}(P\|L) = {}^Q D_{KL}(P\|\bar{P}) + {}^Q D_{KL}(\bar{P}\|L), \quad (3)$$

$$D_{KL}^Q(P\|L) = D_{KL}^Q(P\|\bar{P}) + D_{KL}^Q(\bar{P}\|L). \quad (4)$$

Proof. First, we prove (3). It is easy to see that

$${}^Q D_{KL}(P\|L) = {}^Q D_{KL}(P\|\bar{P}) + \sum_x \pi(x) \sum_y QP(x, y) \ln \left(\frac{Q\bar{P}(x, y)}{QL(x, y)} \right),$$

thus it suffices to show that the second term on the right hand side can be expressed as

$$\sum_x \pi(x) \sum_y QP(x, y) \ln \left(\frac{Q\bar{P}(x, y)}{QL(x, y)} \right) = \sum_x \pi(x) \sum_y P^*Q(x, y) \ln \left(\frac{Q\bar{P}(x, y)}{QL(x, y)} \right). \quad (5)$$

To see (5), we compute that

$$\sum_x \sum_y \pi(x) QP(x, y) \ln \left(\frac{Q\bar{P}(x, y)}{QL(x, y)} \right) = \sum_x \sum_y \pi(y) P^*Q(y, x) \ln \left(\frac{Q\bar{P}(y, x)}{QL(y, x)} \right),$$

where the equality uses the fact that $L, \bar{P} \in \mathcal{L}(\pi, Q)$.

Next, we prove (4). Applying (3) to (P^*, L^*) and using the duality formula in Proposition 2.3, we note that

$$\begin{aligned} D_{KL}^Q(P\|L) &= {}^Q D_{KL}(P^*\|L^*) \\ &= {}^Q D_{KL}(P^*\|\bar{P}^*) + {}^Q D_{KL}(\bar{P}^*\|L^*) \\ &= D_{KL}^Q(P\|\bar{P}) + D_{KL}^Q(\bar{P}\|L), \end{aligned}$$

where we use that $\bar{P}^{**} = \bar{P}$. □

2.1 Projection under the squared-Frobenius norm

In this subsection, we consider projection of P under the squared-Frobenius norm. Let $n = |\mathcal{X}|$ and we write \mathcal{M} to be the set of real-valued matrices on \mathcal{X} , that is,

$$\mathcal{M} = \mathcal{M}(\mathcal{X}) := \{M \in \mathbb{R}^{n \times n}\},$$

equipped with the Frobenius inner product defined to be, for $M, N \in \mathcal{M}$,

$$\langle M, N \rangle_F := \text{Tr}(M^*N)$$

and the induced Frobenius norm $\|A\|_F := \sqrt{\langle A, A \rangle_F}$, where $\text{Tr}(M)$ is the trace of M and $M^*(x, y) := \frac{\pi(y)}{\pi(x)} M(y, x)$ for all x, y is the $\ell^2(\pi)$ -adjoint of M . Define for $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$,

$$\mathcal{M}(\pi, Q) := \{M \in \mathcal{M}; M = QMQ\}.$$

We also define

$$\bar{M}(Q) := \frac{1}{2}(M + QMQ).$$

Note that $\overline{M}(Q)$ is a projection in the functional analytic sense, since it can be checked that for all $M \in \mathcal{M}$,

$$\overline{\overline{M}(Q)}(Q) = \overline{M}(Q).$$

In fact, it is an orthogonal projection. To see that, we observe that

$$\begin{aligned} \langle \overline{M}(Q), N \rangle_F &= \frac{1}{2} \langle M, N \rangle_F + \frac{1}{2} \text{Tr}(N^* Q M Q) = \frac{1}{2} \langle M, N \rangle_F + \frac{1}{2} \text{Tr}(Q N^* Q M) \\ &= \langle M, \overline{N}(Q) \rangle_F, \end{aligned}$$

where the second equality follows from the cyclic property of trace and $Q^* = Q$. Note that $\mathcal{M}(\pi, Q)$ is a subspace of the Hilbert space $(\mathcal{M}, \langle \cdot, \cdot \rangle_F)$. However, $\mathcal{L}(\pi, Q)$ is not a subspace since it is not closed under scalar multiplication. For example, if $P \in \mathcal{L}(\pi, Q)$ and $\alpha < 0$, then $\alpha P \notin \mathcal{L}(\pi, Q)$.

We now state that $\overline{M}(Q)$ is the unique orthogonal projection of M onto $\mathcal{M}(\pi, Q)$ under the squared-Frobenius norm:

Proposition 2.4 (Pythagorean identity under squared-Frobenius norm). *Let $M \in \mathcal{M}$, $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ and $N \in \mathcal{M}(\pi, Q)$. We have*

$$\|M - N\|_F^2 = \|M - \overline{M}(Q)\|_F^2 + \|\overline{M}(Q) - N\|_F^2.$$

In particular, this yields $\overline{M}(Q)$ is the unique projection of M onto $\mathcal{M}(\pi, Q)$.

Proof.

$$\begin{aligned} \|M - N\|_F^2 &= \langle M - N, M - N \rangle_F \\ &= \left\langle \frac{M - Q M Q}{2} + \frac{M + Q M Q}{2} - N, \frac{M - Q M Q}{2} + \frac{M + Q M Q}{2} - N \right\rangle_F \\ &= \|M - \overline{M}(Q)\|_F^2 + \|\overline{M}(Q) - N\|_F^2 + 2 \left\langle \frac{M - Q M Q}{2}, \frac{M + Q M Q}{2} - N \right\rangle_F, \end{aligned}$$

and it suffices to show that the rightmost inner product equals to zero, that is,

$$\left\langle \frac{M - Q M Q}{2}, \frac{M + Q M Q}{2} - N \right\rangle_F = \text{Tr} \left(\left(\frac{M - Q M Q}{2} \right)^* \left(\frac{M + Q M Q}{2} - N \right) \right) = 0.$$

To see that, we shall prove that $\text{Tr}(A) = \text{Tr}(-A)$ with $A = \left(\frac{M - Q M Q}{2} \right)^* \left(\frac{M + Q M Q}{2} - N \right)$. We calculate that

$$\begin{aligned} \text{Tr} \left(\left(\frac{M - Q M Q}{2} \right)^* \left(\frac{M + Q M Q}{2} - N \right) \right) &= \text{Tr} \left(\left(\frac{M + Q M Q}{2} - N \right)^* \left(\frac{M - Q M Q}{2} \right) \right) \\ &= \text{Tr} \left(Q^2 \left(\frac{M^* + Q M^* Q}{2} - N^* \right) \left(\frac{M - Q M Q}{2} \right) \right) \end{aligned}$$

$$\begin{aligned}
&= \text{Tr} \left(Q \left(\frac{M^* + QM^*Q}{2} - N^* \right) \left(\frac{M - QMQ}{2} \right) Q \right) \\
&= \text{Tr} \left(\left(\frac{QM^* + M^*Q}{2} - QN^* \right) \left(\frac{MQ - QM}{2} \right) \right) \\
&= \text{Tr} \left(\left(\frac{QM^*Q + M^*}{2} - N^* \right) \left(\frac{QMQ - M}{2} \right) \right) \\
&= \text{Tr} \left(\left(\frac{QMQ - M}{2} \right)^* \left(\frac{QMQ + M}{2} - N \right) \right),
\end{aligned}$$

where the third equality follows from the cyclic property of the trace and the fifth equality makes use of $N^* = QN^*Q$. This completes the proof. \square

Using both Proposition 2.3 and 2.4, we see that, for a given $P \in \mathcal{L}(\pi)$, not only $\bar{P}(Q)$ is the unique information projection of P onto $\mathcal{L}(\pi, Q)$ under the deformed divergences D_{KL}^Q and ${}^QD_{KL}$, it is also the unique orthogonal projection of P onto $\mathcal{M}(\pi, Q)$ under the squared-Frobenius norm.

3 Comparisons of some samplers

Given $\pi \in \mathcal{P}(\mathcal{X})$, $P \in \mathcal{S}(\pi)$ and Q being an isometric involution transition matrix, the aim of this section is to compare the convergence of various natural samplers associated with these matrices, such as P , QP , PQ , QPQ , $\bar{P}(Q)$ or more generally the mixture $\alpha P + (1 - \alpha)QPQ$ for $\alpha \in [0, 1]$.

3.1 Comparisons of entropic parameters

In this section, we compare parameters related to the KL divergence and entropy.

To this end, let us recall that the KL-divergence Dobrushin coefficient (Wang and Choi, 2023, Definition 2.7) is defined to be

Definition 3.1. *Let $\pi \in \mathcal{P}(\mathcal{X})$, $P \in \mathcal{S}(\pi)$. Then the KL-divergence Dobrushin coefficient of P , $c_{KL}(P)$, is defined to be*

$$c_{KL}(P) := \max_{M, N \in \mathcal{S}(\pi), M \neq N} \frac{D_{KL}^\pi(MP \| NP)}{D_{KL}^\pi(M \| N)} \in [0, 1].$$

Making use of the KL-divergence Dobrushin coefficient, we first show that, for π -stationary transition matrices, the original π -weighted KL divergence in fact coincides with the deformed KL divergences that we introduce earlier in Section 2.

Proposition 3.1. *Let $\pi \in \mathcal{P}(\mathcal{X})$, $M, N \in \mathcal{L}$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$. We have*

$$D_{KL}^\pi(M\|N) = D_{KL}^Q(M\|N).$$

If $M, N \in \mathcal{S}(\pi)$, then

$$D_{KL}^\pi(M\|N) = {}^Q D_{KL}(M\|N).$$

Proof. If $M = N$, then the equalities obviously hold and the values are all zeros. For $M \neq N$, we note that

$$\begin{aligned} D_{KL}^\pi(M\|N) &= D_{KL}^\pi((MQ)Q\|(NQ)Q) \\ &\leq c_{KL}(Q)D_{KL}^\pi(MQ\|NQ) \\ &\leq D_{KL}^\pi(MQ\|NQ) \\ &\leq c_{KL}(Q)D_{KL}^\pi(M\|N) \leq D_{KL}^\pi(M\|N). \end{aligned}$$

The equalities hold and hence $D_{KL}^\pi(MQ\|NQ) = D_{KL}^\pi(M\|N)$.

Using the duality in Proposition 2.2 and the bisection property (Choi and Wolfer, 2024, Theorem III.1), we note that

$${}^Q D_{KL}(M\|N) = D_{KL}^Q(M^*\|N^*) = D_{KL}^\pi(M^*\|N^*) = D_{KL}^\pi(M\|N).$$

□

Our second result states that, when measured by D_{KL}^π , the KL divergence from Π to any of P, PQ, QP, QPQ are all the same. Analogous results hold for the KL-divergence Dobrushin coefficient. We also demonstrate that the projection is trace-preserving in the sense that $\text{Tr}(P) = \text{Tr}(\overline{P}(Q))$, a property that we shall utilize in Section 5 below.

Proposition 3.2. *Let $\pi \in \mathcal{P}(\mathcal{X})$, $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ to be an isometric involution transition matrix. Let Π be the matrix where each row equals to π . We have*

- (One-step contraction measured by D_{KL}^π)

$$D_{KL}^\pi(P\|\Pi) = D_{KL}^\pi(PQ\|\Pi) = D_{KL}^\pi(QP\|\Pi) = D_{KL}^\pi(QPQ\|\Pi). \quad (6)$$

- (KL-divergence Dobrushin coefficient)

$$c_{KL}(P) = c_{KL}(PQ) = c_{KL}(QP) = c_{KL}(QPQ). \quad (7)$$

- (Projection is trace-preserving)

$$\text{Tr}(P) = \text{Tr}(QP^*Q) = \text{Tr}(\overline{P}(Q)). \quad (8)$$

Proof. (6) can readily be seen from (3.1). We replace P above in this proof by QP to yield the rightmost equality of (6).

Next, we prove (7). Using submultiplicativity of c_{KL} (Wang and Choi, 2023, Proposition 3.9), we see that

$$c_{KL}(P) = c_{KL}((PQ)Q) \leq c_{KL}(PQ)c_{KL}(Q) \leq c_{KL}(PQ).$$

Replacing P by PQ in the equations above yields

$$c_{KL}(PQ) \leq c_{KL}(PQ^2) = c_{KL}(P).$$

Similarly, $c_{KL}(P) = c_{KL}(QP)$ can be shown. Replacing P by QP in the expressions above leads us to $c_{KL}(QP) = c_{KL}(QPQ)$.

Finally, we prove (8), which follows from the linearity and cyclic property of trace, $Q^2 = I$ and $\text{Tr}(P) = \text{Tr}(P^*)$. \square

Our next result states that, the KL-divergence from Π to $\bar{P}(Q)$ is at least smaller than that to P .

Proposition 3.3 (Pythagorean identity). *Let $\pi \in \mathcal{P}(\mathcal{X})$, $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ to be an isometric involution transition matrix. Let Π be the matrix where each row equals to π . We have*

$$D_{KL}^\pi(\bar{P}\|\Pi) \leq D_{KL}^\pi(P\|\bar{P}) + D_{KL}^\pi(\bar{P}\|\Pi) = D_{KL}^\pi(P\|\Pi),$$

and the equality holds if and only if $P \in \mathcal{L}(\pi, Q)$ so that $\bar{P}(Q) = P$.

Similarly, if P is further assumed to be π -reversible, then

$$c_{KL}(\bar{P}(Q)) \leq c_{KL}(P).$$

Remark 3.1. *Note that by Proposition 3.2, we have*

$$D_{KL}^\pi(\bar{P}(Q)\|\Pi) = D_{KL}^\pi((1/2)(PQ + QP^*)\|\Pi).$$

Proof. By taking $L = \Pi$ in Proposition 2.3, we see that

$$D_{KL}^Q(P\|\Pi) = D_{KL}^Q(P\|\bar{P}) + D_{KL}^Q(\bar{P}\|\Pi)$$

In view of Proposition 3.1 and 3.2, we arrive at

$$\begin{aligned} D_{KL}^\pi(P\|\Pi) &= D_{KL}^Q(P\|\Pi) \\ &= D_{KL}^Q(P\|\bar{P}) + D_{KL}^Q(\bar{P}\|\Pi) \\ &= D_{KL}^\pi(PQ\|\bar{P}Q) + D_{KL}^\pi(\bar{P}Q\|\Pi) \\ &= D_{KL}^\pi(P\|\bar{P}) + D_{KL}^\pi(\bar{P}\|\Pi) \end{aligned}$$

$$\geq D_{KL}^\pi(\bar{P} \parallel \Pi),$$

where the equality holds if and only if $P = \bar{P}$ if and only if P is itself (π, Q) -self-adjoint.

Using the convexity of c_{KL} (Wang and Choi, 2023, Proposition 3.9), we see that

$$c_{KL}(\bar{P}) \leq \frac{1}{2}(c_{KL}(P) + c_{KL}(QPQ)) = c_{KL}(P),$$

which the last equality follows from Proposition 3.2. \square

In view of Proposition 3.2 and 3.3, given an arbitrary π -stationary P , it is thus advantageous to use the transition matrix $\bar{P}^n(Q)$ over other competing samplers such as P^n, QP^n, P^nQ, QP^nQ , when measured by D_{KL}^π .

For $\alpha \in [0, 1]$, we define $\bar{P}_\alpha(Q) := \alpha P + (1 - \alpha)QPQ$. In the special case of $\alpha = 1/2$, we recover $\bar{P}_{1/2}(Q) = \bar{P}(Q)$ when $P \in \mathcal{L}(\pi)$. Also, we compute that

$$\overline{\alpha P + (1 - \alpha)QPQ}(Q) = \bar{P}(Q). \quad (9)$$

An interesting consequence of Proposition 3.3 is that the choice of $\alpha = 1/2$ is optimal within the family $(\bar{P}_\alpha(Q))_{\alpha \in [0,1]}$ in the sense that it minimizes the KL divergence D_{KL}^π and the KL-divergence Dobrushin coefficient when P is π -reversible:

Corollary 3.1 (Optimality of $\alpha = 1/2$). *Let $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. We have*

$$\begin{aligned} \min_{\alpha \in [0,1]} D_{KL}^\pi(\bar{P}_\alpha(Q) \parallel \Pi) &= D_{KL}^\pi(\bar{P}(Q) \parallel \Pi), \\ \min_{\alpha \in [0,1]} c_{KL}(\bar{P}_\alpha(Q)) &= c_{KL}(\bar{P}(Q)). \end{aligned}$$

The proof can readily be seen from Proposition 3.3 by replacing P therein by $\bar{P}_\alpha(Q)$ and using (9). It is interesting to note that P and QPQ are “equivalent” in terms of their one-step contraction and Dobrushin coefficient, but randomly choosing to move according to P or QPQ at each step using a fair coin (i.e. using $(1/2)(P + QPQ)$) improves the performance.

3.2 Comparisons of spectral parameters

The aim of this subsection is to compare spectral parameters of various Markov chains. To this end, let us now fix a few notations.

For a matrix $M \in \mathcal{M}$, we write $\lambda(M)$ to be the set of eigenvalues of M counted with multiplicities. For a self-adjoint M , we denote by $\lambda_1(M) \geq \lambda_2(M) \geq \dots \lambda_{|\mathcal{X}|}(M)$ to be its eigenvalues arranged in non-increasing order. The right spectral gap $\gamma(P)$ of $P \in \mathcal{L}(\pi)$ is

defined to be $\gamma(P) := 1 - \lambda_2(P)$, while the second largest eigenvalue in modulus $\text{SLEM}(P)$ of P is defined to be $\text{SLEM}(P) := \max\{\lambda_2(P), |\lambda_{|\mathcal{X}|}(P)|\}$.

We shall be interested in several hitting and mixing time parameters that are related to the spectrum of ergodic $P \in \mathcal{L}(\pi)$. Let $\tau_A = \tau_A(P) := \inf\{n \in \mathbb{N}; X_n \in A\}$ be the first hitting time of the set A of the Markov chain $(X_n)_{n \in \mathbb{N}}$ associated with P , where the usual convention of $\inf \emptyset := \infty$ applies. We write $\tau_x := \tau_{\{x\}}$ for $x \in \mathcal{X}$. The average hitting time $t_{av}(P)$ of P is defined to be

$$t_{av}(P) := \sum_{x,y} \pi(x)\pi(y)\mathbb{E}_x(\tau_y).$$

The eigentime identity [Aldous and Fill \(2002\)](#) relates $t_{av}(P)$ to the spectrum of P via

$$t_{av}(P) = \sum_{i=2}^{|\mathcal{X}|} \frac{1}{1 - \lambda_i(P)}.$$

The relaxation time of P is given by

$$t_{rel}(P) := \frac{1}{\gamma(P)}.$$

Under the assumptions that $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ is an isometric involution transition matrix, QPQ is a similarity transformation of P and hence various spectral parameters between these two coincide.

Proposition 3.4. *Let $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ is an isometric involution transition matrix. We have*

$$\lambda(QPQ) = \lambda(P).$$

Consequently, this leads to

$$t_{av}(QPQ) = t_{av}(P), \quad t_{rel}(QPQ) = t_{rel}(P).$$

In the next results, we compare the eigenvalues of $\alpha P + (1 - \alpha)QPQ$ for $\alpha \in (0, 1)$ with that of P (or QPQ). A natural tool to utilize in this context is the Weyl's inequality.

Proposition 3.5. *Let $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ is an isometric involution transition matrix. Fix $\alpha \in (0, 1)$ and recall that $\bar{P}_\alpha(Q) = \alpha P + (1 - \alpha)QPQ$. Let $n := |\mathcal{X}|$. We have*

- $\lambda_2(\bar{P}_\alpha(Q)) \leq \lambda_2(P)$, where the equality holds if and only if there exists a common eigenvector f such that $\bar{P}_\alpha(Q)f = \lambda_2(\bar{P}_\alpha(Q))f$, $Pf = \lambda_2(P)f$ and $QPQf = \lambda_2(QPQ)f$.
- $\lambda_n(P) \leq \lambda_n(\bar{P}_\alpha(Q))$, where the equality holds if and only if there exists a common eigenvector g such that $\bar{P}_\alpha(Q)g = \lambda_n(\bar{P}_\alpha(Q))g$, $Pg = \lambda_n(P)g$ and $QPQg = \lambda_n(QPQ)g$.

Consequently, this leads to

$$\text{SLEM}(\bar{P}_\alpha(Q)) \leq \text{SLEM}(P).$$

If P (and hence QPQ) is further assumed to be positive-semi-definite, then

$$\begin{aligned} \max\{\alpha, 1 - \alpha\}\lambda_2(P) &\leq \lambda_2(\bar{P}_\alpha(Q)) \leq \lambda_2(P), \\ \max\{\alpha, 1 - \alpha\}\text{SLEM}(P) &\leq \text{SLEM}(\bar{P}_\alpha(Q)) \leq \text{SLEM}(P). \end{aligned}$$

Proof. This proposition is mainly a consequence of the Weyl's inequality (So, 1994, Theorem 1.3). Specifically, in view of Proposition 3.4, we note that

$$\lambda_2(\bar{P}_\alpha(Q)) = \lambda_1(\bar{P}_\alpha(Q) - \Pi) \leq \lambda_1(\alpha(P - \Pi)) + \lambda_1((1 - \alpha)(QPQ - \Pi)) = \lambda_2(P),$$

where the equality holds in the Weyl's inequality if and only if there exists a common eigenvector f .

Similarly, applying the Weyl's inequality again leads to

$$\lambda_n(\bar{P}_\alpha(Q)) \geq \lambda_n(\alpha P) + \lambda_n((1 - \alpha)QPQ) = \lambda_n(P),$$

where the equality holds in the Weyl's inequality if and only if there exists a common eigenvector g .

In the positive-semi-definite setting, we note that by Weyl's inequality

$$\begin{aligned} \alpha\lambda_2(P) &\leq \alpha\lambda_2(P) + (1 - \alpha)\lambda_n(QPQ) \leq \lambda_2(\bar{P}_\alpha(Q)), \\ (1 - \alpha)\lambda_2(QPQ) &\leq (1 - \alpha)\lambda_2(QPQ) + \alpha\lambda_n(P) \leq \lambda_2(\bar{P}_\alpha(Q)), \end{aligned}$$

and the desired result follows from Proposition 3.4. \square

In view of Proposition 3.5, it is advantageous to consider the family of samplers $(\bar{P}_\alpha(Q))_{\alpha \in [0,1]}$ over the original P . Within this family and in the positive-semi-definite case, we see that the speedup measured in terms of λ_2 is at most one half, and as such one may seek to find an optimal Q that minimizes $\lambda_2(\bar{P}_\alpha(Q))$ subject to the constraints $Q^* = Q$ and $Q^2 = I$. We shall discuss tuning strategies of Q in Section 6.

Another interesting consequence of Proposition 3.5 lies in the equality characterizations. Under what situation(s) are we guaranteed to have $\lambda_2(\bar{P}_\alpha(Q)) < \lambda_2(P)$? Suppose that P is ergodic, π -reversible with distinct eigenvalues (such as birth-death processes), and hence both the algebraic and geometric multiplicity equal to 1 for each eigenvalue of P . Suppose that there exists $x \neq y$ such that $\pi(x) = \pi(y)$. We define $\phi(x) := y, \phi(y) := x, \phi(z) := z$ for all $z \in \mathcal{X} \setminus \{x, y\}$. Define $Q_\phi(x, y) = \delta_{y=\phi(x)}$, the Dirac mass of the set $\{y = \phi(x)\}$. Then, a necessary condition for $\lambda_2(\bar{P}_\alpha(Q_\phi)) = \lambda_2(P)$ is that the common eigenvector f satisfies $f(x) = \pm f(y)$. Thus, under these assumptions of Q_ϕ , if the eigenvector of P has distinct absolute values such that $|f(x)| \neq |f(y)|$ for all $x \neq y$, the Weyl's inequality is strict and

hence $\lambda_2(\overline{P}_\alpha(Q_\phi)) < \lambda_2(P)$. Similar analysis can be done to give a sufficient condition for $\lambda_n(P) < \lambda_n(\overline{P}_\alpha(Q_\phi))$.

Analogous to Corollary 3.1, an interesting corollary of Proposition 3.5 is that the choice of $\alpha = 1/2$ is optimal within the family $(\overline{P}_\alpha(Q))_{\alpha \in [0,1]}$ in the sense that it minimizes SLEM and λ_2 when P is π -reversible:

Corollary 3.2 (Optimality of $\alpha = 1/2$). *Let $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. We have*

$$\begin{aligned} \min_{\alpha \in [0,1]} \text{SLEM}(\overline{P}_\alpha(Q)) &= \text{SLEM}(\overline{P}(Q)), \\ \min_{\alpha \in [0,1]} \lambda_2(\overline{P}_\alpha(Q)) &= \lambda_2(\overline{P}(Q)). \end{aligned}$$

The proof can readily be seen from Proposition 3.5 by replacing P therein by $\overline{P}_\alpha(Q)$ as well as (9).

3.3 Comparisons of asymptotic variances

In addition to entropic and spectral parameters, another commonly used parameter to assess the convergence of Markov chain samplers is asymptotic variance. In this subsection, we compare the asymptotic variances of various Markov chains. We first fix a few notations.

For an ergodic $P \in \mathcal{S}(\pi)$, its fundamental matrix $Z(P)$, see for example (Brémaud, 1999, Chapter 6), is defined to be

$$Z(P) := (I - (P - \Pi))^{-1},$$

where we recall that Π is the matrix where each row equals to π . Note that the above inverse always exists for ergodic P . For $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$, we see that

$$Z(QPQ) = QZ(P)Q.$$

Let $(X_n)_{n \geq 0}$ be the Markov chain with ergodic transition matrix P . Its asymptotic variance of $f \in \ell_0^2(\pi)$ is, for any initial distribution μ ,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \text{Var}_\mu \left(\sum_{i=1}^n f(X_i) \right) = 2 \langle f, Z(P)f \rangle_\pi - \langle f, f \rangle_\pi =: v(f, P).$$

For a proof of the above expression one can consult (Brémaud, 1999, Theorem 6.5). From this definition we readily check that

$$v(f, P) = v(Qf, QPQ). \tag{10}$$

A useful variational characterization of asymptotic variance for $P \in \mathcal{L}(\pi)$ [Sherlock \(2018\)](#) is given by

$$v(f, P) = \sup_{g \in \ell_0^2(\pi)} 4\langle f, g \rangle_\pi - 2\langle (I - P)g, g \rangle_\pi - \langle f, f \rangle_\pi. \quad (11)$$

The worst-case asymptotic variance, studied for example in [Frigessi et al. \(1993\)](#), is

$$V(P) := \sup_{f \in \ell_0^2(\pi), \|f\|_\pi=1} v(f, P) = \frac{1 + \lambda_2(P)}{1 - \lambda_2(P)}, \quad (12)$$

while the average-case asymptotic variance, investigated in [Chen et al. \(2012\)](#), is

$$\bar{v}(P) := \int_{f \in \ell_0^2(\pi), \|f\|_\pi=1} v(f, P) dS(f), \quad (13)$$

where $dS(f)$ is the uniform measure on the normalized surface area.

Our first proposition compares the asymptotic variances between $\bar{P}_\alpha(Q)$ and P .

Proposition 3.6. *Let $P \in \mathcal{L}(\pi)$ be ergodic and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. For $\alpha \in [0, 1]$, recall that $\bar{P}_\alpha(Q) = \alpha P + (1 - \alpha)QPQ$. For any $f \in \ell_0^2(\pi)$, we have*

$$v(f, \bar{P}_\alpha(Q)) \leq \alpha v(f, P) + (1 - \alpha)v(Qf, P).$$

In particular, if f satisfies $Qf = \pm f$, it leads to

$$v(f, \bar{P}_\alpha(Q)) \leq v(f, P),$$

and hence

$$\min_{\alpha \in [0, 1]} v(f, \bar{P}_\alpha(Q)) = v(f, \bar{P}(Q)).$$

Proof. First, we calculate that

$$\begin{aligned} & 4\langle f, g \rangle_\pi - 2\langle (I - \bar{P}_\alpha(Q))g, g \rangle_\pi - \langle f, f \rangle_\pi \\ &= \alpha (4\langle f, g \rangle_\pi - 2\langle (I - P)g, g \rangle_\pi - \langle f, f \rangle_\pi) + (1 - \alpha) (4\langle f, g \rangle_\pi - 2\langle (I - QPQ)g, g \rangle_\pi - \langle f, f \rangle_\pi). \end{aligned}$$

Taking the sup over $g \in \ell_0^2(\pi)$ and using (11) leads to

$$\begin{aligned} v(f, \bar{P}_\alpha(Q)) &\leq \alpha v(f, P) + (1 - \alpha)v(f, QPQ) \\ &= \alpha v(f, P) + (1 - \alpha)v(Qf, P), \end{aligned}$$

where the last equality follows from (10).

Finally, when $Qf = \pm f$ and P is π -reversible, by replacing P with $\bar{P}_\alpha(Q)$ above and recalling (9) earlier, we arrive at

$$\min_{\alpha \in [0, 1]} v(f, \bar{P}_\alpha(Q)) = v(f, \bar{P}(Q)).$$

□

Our second result compares the worst-case and average-case asymptotic variance between $\bar{P}_\alpha(Q)$ and P , and demonstrates the optimality of $\alpha = 1/2$.

Proposition 3.7. *Let $P \in \mathcal{L}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. Fix $\alpha \in (0, 1)$ and recall that $\bar{P}_\alpha(Q) = \alpha P + (1 - \alpha)QPQ$. We have*

- (worst-case asymptotic variance)

$$V(\bar{P}_\alpha(Q)) \leq V(P),$$

where the equality holds if and only if $\lambda_2(\bar{P}_\alpha(Q)) = \lambda_2(P)$ if and only if there exists a common eigenvector g such that $\bar{P}_\alpha(Q)g = \lambda_2(\bar{P}_\alpha(Q))g$, $Pg = \lambda_2(P)g$ and $QPQg = \lambda_2(QPQ)g$.

If P is further assumed to be positive-semi-definite, then

$$\max\{\alpha, 1 - \alpha\}V(P) \leq V(\bar{P}_\alpha(Q)) \leq V(P).$$

- (average-case asymptotic variance)

$$\bar{v}(\bar{P}_\alpha(Q)) \leq \bar{v}(P).$$

Consequently, this leads to

$$\begin{aligned} \min_{\alpha \in [0,1]} V(\bar{P}_\alpha(Q)) &= V(\bar{P}(Q)), \\ \min_{\alpha \in [0,1]} \bar{v}(\bar{P}_\alpha(Q)) &= \bar{v}(\bar{P}(Q)). \end{aligned}$$

Proof. We first handle the results for worst-case asymptotic variance. Using (12), Proposition 3.5 and the fact that the mapping $0 < c \mapsto \frac{1+c}{1-c}$ is strictly increasing, we have

$$V(\bar{P}_\alpha(Q)) = \frac{1 + \lambda_2(\bar{P}_\alpha(Q))}{1 - \lambda_2(\bar{P}_\alpha(Q))} \leq \frac{1 + \lambda_2(P)}{1 - \lambda_2(P)} = V(P),$$

and so the equality holds if and only if $\lambda_2(\bar{P}_\alpha(Q)) = \lambda_2(P)$. If P is positive-semi-definite, using the inequality that, for $a \in (0, 1)$ and $c > 0$,

$$a \frac{1 + c}{1 - c} \leq \frac{1 + ac}{1 - ac},$$

we arrive at

$$\max\{\alpha, 1 - \alpha\}V(P) \leq \frac{1 + \max\{\alpha, 1 - \alpha\}\lambda_2(P)}{1 - \max\{\alpha, 1 - \alpha\}\lambda_2(P)} \leq \frac{1 + \lambda_2(\bar{P}_\alpha(Q))}{1 - \lambda_2(\bar{P}_\alpha(Q))} = V(\bar{P}_\alpha(Q)),$$

where the second inequality above follows from Proposition 3.5.

Next, we proceed to show the results for average-case asymptotic variance. In view of Proposition 3.6, it suffices to show that

$$\bar{v}(P) = \int_{f \in \ell_0^2(\pi), \|f\|_\pi=1} v(Qf, P) dS(f),$$

which is indeed true since

$$\begin{aligned} \int_{f \in \ell_0^2(\pi), \|f\|_\pi=1} v(Qf, P) dS(f) &= \int_{f \in \ell_0^2(\pi), \|f\|_\pi=1} v(f, QPQ) dS(f) \\ &= \frac{2}{|\mathcal{X}| - 1} \text{Tr}(Z(QPQ)) - 1 \\ &= \frac{2}{|\mathcal{X}| - 1} \text{Tr}(Z(P)) - 1 \\ &= \bar{v}(P), \end{aligned}$$

where the first equality uses (10), the second equality comes from (Chen et al., 2012, Theorem 2.1), the third equality uses $\lambda(P) = \lambda(QPQ)$, and the last equality uses again (Chen et al., 2012, Theorem 2.1).

Finally, the optimality of $\alpha = 1/2$ can be seen by replacing P with $\bar{P}_\alpha(Q)$ above and recalling (9) earlier. \square

When will there be no improvement in the worst-case asymptotic variance, i.e. $V(\bar{P}_\alpha(Q)) = V(P)$? One interesting consequence of Proposition 3.7 is that, there is no improvement if and only if $\lambda_2(P) = \lambda_2(\bar{P}_\alpha(Q))$ and by the Weyl's inequality if and only if there exists a common eigenvector.

4 Alternating projections to combine Q s

Let $m \in \mathbb{N}$ and suppose that we have a sequence of isometric involution matrices $Q_i \in \mathcal{I}(\pi) \cap \mathcal{L}$ for $i \in \llbracket 0, m-1 \rrbracket$. Is there a way to combine these Q_i to further improve the convergence to equilibrium?

One natural idea in this context is alternating projections. Specifically, given a $P \in \mathcal{L}(\pi)$, we first project it onto the space $\mathcal{L}(\pi, Q_0)$ to obtain $R_1 = R_1(Q_0, \dots, Q_{m-1}, P) := \bar{P}(Q_0)$. Second, we project R_1 onto the space $\mathcal{L}(\pi, Q_1)$ to obtain $R_2 = R_2(Q_0, \dots, Q_{m-1}, P) := \overline{R_1}(Q_1)$. Third, we project R_2 onto the space $\mathcal{L}(\pi, Q_2)$ to obtain $R_3 = R_3(Q_0, \dots, Q_{m-1}, P) := \overline{R_2}(Q_2)$. We proceed iteratively and the projection order is deterministic in a cycle in the order of Q_0, \dots, Q_{m-1} . Precisely, for $n \in \mathbb{N}$, we define

$$R_n = R_n(Q_0, \dots, Q_{m-1}, P) := \overline{R_{n-1}}(Q_{(n-1) \bmod m}) \quad (14)$$

with the initial condition $R_0 := P$.

We remark that, in the context of MCMC, alternating projections have appeared in the analysis of Gibbs samplers in [Diaconis et al. \(2010\)](#); [Qin \(2024\)](#).

The sequence of alternating projections $(R_i)_{i \in \mathbb{N}}$ yields a monotone sequence of mixing time parameters:

Proposition 4.1. *Let $P \in \mathcal{L}(\pi)$ and $Q_i \in \mathcal{I}(\pi) \cap \mathcal{L}$ for $i \in \llbracket 0, m-1 \rrbracket$ be a sequence of isometric involution transition matrices. Define R_n as in (14). The sequences $(D_{KL}^\pi(R_n \| \Pi))_{n \in \mathbb{N}}$, $(c_{KL}(R_n))_{n \in \mathbb{N}}$, $(\text{SLEM}(R_n))_{n \in \mathbb{N}}$, $(V(R_n))_{n \in \mathbb{N}}$ and $(\bar{v}(R_n))_{n \in \mathbb{N}}$ are monotonically non-increasing in n with limits*

$$\begin{aligned} \lim_{n \rightarrow \infty} D_{KL}^\pi(R_n \| \Pi) &= \inf_{n \in \mathbb{N}} D_{KL}^\pi(R_n \| \Pi), \\ \lim_{n \rightarrow \infty} c_{KL}(R_n) &= \inf_{n \in \mathbb{N}} c_{KL}(R_n), \\ \lim_{n \rightarrow \infty} \text{SLEM}(R_n) &= \inf_{n \in \mathbb{N}} \text{SLEM}(R_n), \\ \lim_{n \rightarrow \infty} V(R_n) &= \inf_{n \in \mathbb{N}} V(R_n), \\ \lim_{n \rightarrow \infty} \bar{v}(R_n) &= \inf_{n \in \mathbb{N}} \bar{v}(R_n). \end{aligned}$$

Proof. Using the monotone convergence theorem, the desired results can readily be seen by recursive application of Proposition 3.3, 3.5, 3.7 and noting a lower bound of zero on these quantities. \square

Denote the intersections of $\mathcal{L}(\pi, Q_0), \dots, \mathcal{L}(\pi, Q_{m-1})$ to be

$$\mathcal{E} = \mathcal{E}(\pi, Q_0, \dots, Q_{m-1}) := \bigcap_{k=0}^{m-1} \mathcal{L}(\pi, Q_k).$$

Note that since $\Pi \in \mathcal{L}(\pi, Q_k)$ for all $k \in \llbracket 0, m-1 \rrbracket$, $\Pi \in \mathcal{E}$ and hence $\mathcal{E} \neq \emptyset$. Since $\mathcal{L}(\pi, Q_k)$ is a convex and compact set and intersections preserve convexity and compactness, \mathcal{E} is also a convex and compact set. Let R_∞ be an information projection of $P \in \mathcal{L}(\pi)$ onto \mathcal{E} , that is,

$$R_\infty = R_\infty(Q_0, \dots, Q_{m-1}, P) := \arg \min_{N \in \mathcal{E}} D_{KL}^\pi(P \| N).$$

Observe that since for fixed P the mapping $N \mapsto D_{KL}^\pi(P \| N)$ is convex (see e.g. [Melbourne \(2020\)](#)) and the above minimization is taken over a convex and compact set \mathcal{E} , a unique minimizer R_∞ exists owing to the Pythagorean theorem (see e.g. ([Brémaud, 2017](#), Lemma 13.2.3)).

We state a decomposition of the KL divergence and squared-Frobenius norm, and use it to show that the information projection of any R_k onto \mathcal{E} coincides and are equal to R_∞ :

Proposition 4.2. *Let $l, m, n \in \mathbb{N} \cup \{0\}$ with $l > n \geq 0$ and $m \geq 1$. Let $P \in \mathcal{L}(\pi)$ and $Q_i \in \mathcal{I}(\pi) \cap \mathcal{L}$ for $i \in \llbracket 0, m-1 \rrbracket$ be a sequence of isometric involution transition matrices. Define R_n as in (14).*

- For $E \in \mathcal{E}$, we have

$$D_{KL}^\pi(R_n \| E) = \sum_{j=n}^{l-1} D_{KL}^\pi(R_j \| R_{j+1}) + D_{KL}^\pi(R_l \| E).$$

- For $E \in \mathcal{E}$, we have

$$\|R_n - E\|_F^2 = \sum_{j=n}^{l-1} \|R_j - R_{j+1}\|_F^2 + \|R_l - E\|_F^2.$$

- We have

$$R_\infty(Q_0, \dots, Q_{m-1}, P) = R_\infty(Q_0, \dots, Q_{m-1}, R_l).$$

- (Projection is trace-preserving)

$$\text{Tr}(R_n) = \text{Tr}(P).$$

Proof. Let $Q = Q_{n \bmod m}$. For the first item, we repeatedly apply Proposition 3.1 and the Pythagorean identity in Proposition 2.3 to obtain

$$\begin{aligned} D_{KL}^\pi(R_n \| E) &= D_{KL}^Q(R_n \| E) \\ &= D_{KL}^Q(R_n \| R_{n+1}) + D_{KL}^Q(R_{n+1} \| E) \\ &= D_{KL}^\pi(R_n \| R_{n+1}) + D_{KL}^\pi(R_{n+1} \| E) \\ &= D_{KL}^\pi(R_n \| R_{n+1}) + D_{KL}^\pi(R_{n+1} \| R_{n+2}) + D_{KL}^\pi(R_{n+2} \| E) \\ &= \vdots \\ &= \sum_{j=n}^{l-1} D_{KL}^\pi(R_j \| R_{j+1}) + D_{KL}^\pi(R_l \| E). \end{aligned}$$

Now, we take $n = 0$ above and since $D_{KL}^\pi(R_0 \| E) \geq D_{KL}^\pi(R_0 \| R_\infty)$, we are led to $D_{KL}^\pi(R_l \| E) \geq D_{KL}^\pi(R_l \| R_\infty)$, and hence $R_\infty(Q_0, \dots, Q_{m-1}, P) = R_\infty(Q_0, \dots, Q_{m-1}, R_l)$, which proves the third item.

For the second item, we repeatedly apply Proposition 2.4 to obtain

$$\begin{aligned} \|R_n - E\|_F^2 &= \|R_n - R_{n+1}\|_F^2 + \|R_{n+1} - E\|_F^2 \\ &= \|R_n - R_{n+1}\|_F^2 + \|R_{n+1} - R_{n+2}\|_F^2 + \|R_{n+2} - E\|_F^2 \\ &= \vdots \\ &= \sum_{j=n}^{l-1} \|R_j - R_{j+1}\|_F^2 + \|R_l - E\|_F^2. \end{aligned}$$

Finally, we apply Proposition 3.2 repeatedly to yield $\text{Tr}(R_n) = \text{Tr}(P)$. □

Our main result shows that the limit of R_n exists and is given by R_∞ .

Theorem 4.1. *Let $m, n \in \mathbb{N}$. Let $P \in \mathcal{L}(\pi)$ and $Q_i \in \mathcal{I}(\pi) \cap \mathcal{L}$ for $i \in \llbracket 0, m-1 \rrbracket$ be a sequence of isometric involution transition matrices. Define R_n as in (14). The following limit exists (pointwise or in total variation):*

$$\lim_{n \rightarrow \infty} R_n = R_\infty,$$

and

$$R_\infty \in \mathcal{L}(\pi) \cap \mathcal{E}, \quad \text{Tr}(R_\infty) = \text{Tr}(P).$$

Proof. The proof is inspired by that of (Csiszár, 1975, Theorem 3.2). On a finite state space \mathcal{X} , it suffices to show that for every converging subsequence $(R_{n_k})_{k \geq 1}$ such that $R_{n_k} \rightarrow R'$, we have $R' = R_\infty$.

For $M, N \in \mathcal{L}$ and $\pi \in \mathcal{P}(\mathcal{X})$, we define the π -weighted total variation distance between M and N to be

$$D_{TV}^\pi(M, N) := \sum_x \pi(x) \sum_y |M(x, y) - N(x, y)|.$$

First, we show that $R' \in \mathcal{E}$. Taking $n = 0$ in Proposition 4.2 and using Proposition 4.1 give us that

$$\lim_{l \rightarrow \infty} \sum_{j=0}^{l-1} D_{KL}^\pi(R_j \| R_{j+1}) = \lim_{l \rightarrow \infty} D_{KL}^\pi(P \| E) - D_{KL}^\pi(R_l \| E) = D_{KL}^\pi(P \| E) - \inf_{l \in \mathbb{N}} D_{KL}^\pi(R_l \| E) < \infty,$$

and hence $\lim_{l \rightarrow \infty} D_{KL}^\pi(R_l \| R_{l+1}) = 0$. By the Markov chain Pinsker's inequality (Wang and Choi, 2023, Proposition 3.5), we thus have $\lim_{l \rightarrow \infty} D_{TV}^\pi(R_l, R_{l+1}) = 0$. By the triangle inequality, the subsequences $(R_{n_k})_{k \geq 1}$, $(R_{n_k+1})_{k \geq 1}$, $(R_{n_k+2})_{k \geq 1}$ up to $(R_{n_k+m})_{k \geq 1}$ all converge to R' . Since the spaces $\mathcal{L}(\pi, Q_0), \dots, \mathcal{L}(\pi, Q_{m-1})$ are closed, $R' \in \mathcal{E}$. It is also obvious to note that $R' \in \mathcal{L}(\pi)$ since $P \in \mathcal{L}(\pi)$.

By the definition of R_∞ and Proposition 4.2, we have

$$D_{KL}^\pi(R_{n_k} \| R') \geq D_{KL}^\pi(R_{n_k} \| R_\infty).$$

Taking $k \rightarrow \infty$ yields

$$\lim_{k \rightarrow \infty} D_{KL}^\pi(R_{n_k} \| R_\infty) = D_{KL}^\pi(R' \| R_\infty) = 0,$$

and hence $R' = R_\infty$.

Finally, to prove that $\text{Tr}(R_\infty) = \text{Tr}(P)$, we take the limit $n \rightarrow \infty$ in item 3 of Proposition 4.2. Since \mathcal{X} is finite and R_n converges to R_∞ pointwise, this completes the proof. \square

R_∞ can therefore be interpreted as an “optimal” transition matrix that combines Q_0, \dots, Q_{m-1} .

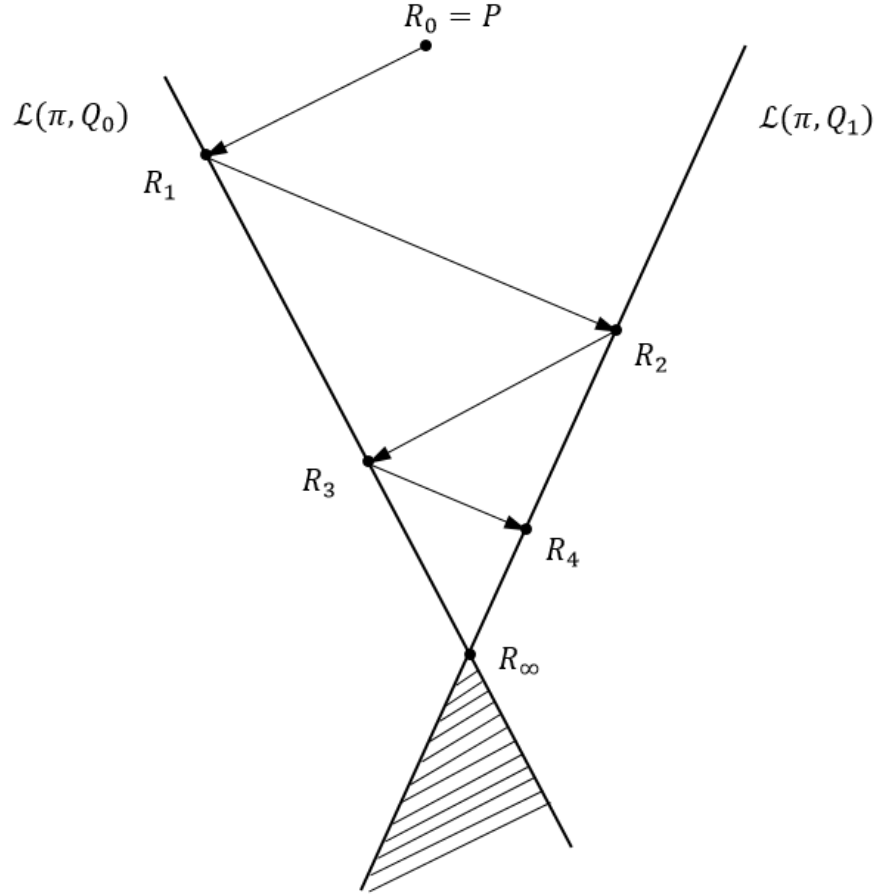


Figure 1: Improving the mixing of P via alternating projections with $m = 1$. The intersection $\mathcal{E} = \bigcap_{i=0}^1 \mathcal{L}(\pi, Q_i)$ is the striped region in the bottom, and R_∞ is the projection of $R_0 = P$ onto \mathcal{E} under D_{KL}^π .

In using these alternating projections to improve mixing, the worst possible case that can happen is that $P = R_\infty$, that is, using these alternating projections have no effect on the original P . This happens if and only if $P \in \mathcal{E}$, that is, the original P is (π, Q_i) -self-adjoint for all $i \in \llbracket 0, m-1 \rrbracket$.

On the other hand, an ideal scenario is that $R_\infty = \Pi$, and by Proposition 4.2 that happens if and only if

$$D_{KL}^\pi(P \parallel \Pi) = \sum_{j=0}^{\infty} D_{KL}^\pi(R_j \parallel R_{j+1}).$$

We shall investigate some other necessary conditions of $R_\infty = \Pi$ in Section 5.

A special case appears when $(Q_i)_{i=0}^{m-1}$ is pairwise commutative, that is, $Q_i Q_j = Q_j Q_i$ for all $i \neq j, i, j \in \llbracket 0, m-1 \rrbracket$. Define the product to be

$$\mathbf{Q} = \mathbf{Q}(\pi, Q_0, \dots, Q_{m-1}) := \prod_{i=0}^{m-1} Q_i.$$

Using the pairwise commutative property one can verify that $\mathbf{Q}^2 = I$, $\mathbf{Q}^* = \mathbf{Q}$ and $R_n = R_m$ for all $n \geq m$. It can also be seen that

$$\mathcal{E} = \mathcal{L}(\pi, \mathbf{Q}),$$

and hence

$$R_\infty = \overline{P}(\mathbf{Q}) = \frac{1}{2}(P + \mathbf{Q}P\mathbf{Q}) = R_m.$$

4.1 A recursive simulation procedure for $(R_n)_{n \in \mathbb{N}}$

In view of Proposition 2.1, let $(\psi_i)_{i=0}^{m-1}$ be a sequence of permutations with $\psi_i \in \Psi(\pi)$ and we take $Q_i = Q_{\psi_i}$ to be the induced permutation matrices. In this subsection, we devise a recursive simulation procedure for R_n assuming $R_0 = P \in \mathcal{L}(\pi)$.

First, to simulate $R_1 = (1/2)(P + Q_0 P Q_0)$ is straightforward: with probability 1/2 we either use P or $Q_0 P Q_0$. Let σ_1 be a random permutation defined to be either the identity map \mathbf{i} or ψ_0 with equal probability. That is,

$$\sigma_1 := \begin{cases} \mathbf{i}, & \text{with probability } 1/2, \\ \psi_0, & \text{with probability } 1/2. \end{cases}$$

Thus, to simulate one step of R_1 with an initial state x to a state y , it is equivalent to simulate $y' \sim P(\sigma_1(x), \cdot)$ followed by setting $y = \sigma_1(y')$.

Building upon R_1 , we simulate $R_2 = (1/2)(R_1 + Q_1 \text{ mod } m R_1 Q_1 \text{ mod } m)$. Let σ_2 be a random permutation defined to be either the identity map \mathbf{i} or $\psi_1 \text{ mod } m$ with equal probability. That is,

$$\sigma_2 := \begin{cases} \mathbf{i}, & \text{with probability } 1/2, \\ \psi_1 \text{ mod } m, & \text{with probability } 1/2. \end{cases}$$

Thus, to simulate one step of R_2 with an initial state x to a state y , it is equivalent to simulate $y' \sim P(\sigma_1(\sigma_2(x)), \cdot)$ followed by setting $y = \sigma_2(\sigma_1(y'))$.

Continuing the above construction recursively or by induction, we simulate $R_n = (1/2)(R_{n-1} + Q_{n-1 \text{ mod } m} R_{n-1} Q_{n-1 \text{ mod } m})$. Let σ_n be a random permutation defined to be either the identity map \mathbf{i} or $\psi_{n-1 \text{ mod } m}$ with equal probability. That is,

$$\sigma_n := \begin{cases} \mathbf{i}, & \text{with probability } 1/2, \\ \psi_{n-1 \text{ mod } m}, & \text{with probability } 1/2. \end{cases}$$

Thus, to simulate one step of R_n with an initial state x to a state y , it is equivalent to simulate $y' \sim P(\sigma_1 \circ \dots \circ \sigma_n(x), \cdot)$ followed by setting $y = \sigma_n \circ \dots \circ \sigma_1(y')$.

In summary, we first simulate realizations of the permutations $\sigma_1, \dots, \sigma_n$. Starting from an initial state x , we draw a random $y' \sim P(\sigma_1 \circ \dots \circ \sigma_n(x), \cdot)$, then we set $y = \sigma_n \circ \dots \circ \sigma_1(y')$. This simulates a move from x to y using R_n .

4.2 Angle between subspaces and the rate of convergence of R_n towards R_∞

In practice, to compute R_∞ , we can only run the alternating projections up to a finite time n and arrive at R_n . How far away is R_n from R_∞ ? One way to measure this is, by Proposition 4.2,

$$D_{KL}^\pi(R_n \| R_\infty) = \sum_{j=n}^{\infty} D_{KL}^\pi(R_j \| R_{j+1}).$$

We now apply the theory of alternating projections to obtain a rate of convergence. First, we recall the notation of Section 2.1, where we have m closed subspaces $(\mathcal{M}(\pi, Q_i))_{i=0}^{m-1}$ of the Hilbert space $(\mathcal{M}, \langle \cdot, \cdot \rangle_F)$. Denote the intersection to be $\mathcal{F} = \mathcal{F}(\pi, Q_0, \dots, Q_{m-1}) := \bigcap_{i=0}^{m-1} \mathcal{M}(\pi, Q_i)$.

For any two closed subspace $(\mathcal{M}_i)_{i=1}^2$ of \mathcal{M} , we define the cosine of the angle between these two subspaces (Deutsch, 2001, Definition 9.4) to be

$$\alpha(\mathcal{M}_1, \mathcal{M}_2) := \sup\{|\langle M_1, M_2 \rangle_F|; M_i \in \mathcal{M}_i \cap (\mathcal{M}_1 \cap \mathcal{M}_2)^\perp, \|M_i\|_F \leq 1, i \in \{1, 2\}\}.$$

Consider $\alpha(\mathcal{M}(\pi, Q_i), \mathcal{M}(\pi, Q_j))$ for $i \neq j$. If Q_i is different from (resp. similar to) Q_j , we expect the angle between the two subspaces to be large (resp. small), leading to a small (resp. large) α . Thus, α in our context can be broadly understood as a measure of dissimilarity between two permutations.

Let $P \in \mathcal{L}(\pi) \subseteq \mathcal{M}$ and consider the sequence (R_n) defined in (14). Define the projection of P onto \mathcal{F} under the Frobenius norm to be

$$R'_\infty = \arg \min_{M \in \mathcal{F}} \|P - M\|_F.$$

According to (Deutsch, 2001, Corollary 9.28), we have

$$\lim_{n \rightarrow \infty} \|R_{mn} - R'_\infty\|_F = 0.$$

Since $R_n \rightarrow R_\infty$ pointwise as shown in Theorem 4.1, we thus have $R_\infty = R'_\infty$.

Define for $i \in \{0, 1, \dots, r-2\}$

$$\alpha_i := \alpha(\mathcal{M}(\pi, Q_i), \bigcap_{j=i+1}^{m-1} \mathcal{M}(\pi, Q_j)),$$

$$\alpha := \sqrt{1 - \prod_{i=0}^{r-2} (1 - \alpha_i^2)}. \quad (15)$$

Using (Deutsch, 2001, Theorem 9.33) we arrive at

Corollary 4.1. *Let $P \in \mathcal{L}(\pi) \subseteq \mathcal{M}$ and consider the sequence (R_n) defined in (14), where $Q_i \in \mathcal{I}(\pi) \cap \mathcal{L}$ for $i \in \llbracket 0, m-1 \rrbracket$ is a sequence of isometric involution transition matrices. We have*

$$\|R_{mn} - R_\infty\|_F \leq \alpha^n \|P\|_F,$$

where α is given by (15).

An implication of the above Corollary allows us to answer the following question: how many alternating projection steps t one need to run until we are guaranteed that $\|R_t - R_\infty\|_F \leq \varepsilon$ for a given error $\varepsilon > 0$? Using the crude bound that $\|P\|_F \leq \sqrt{|\mathcal{X}|}$, we see that one can set

$$t = m \frac{\log(\sqrt{|\mathcal{X}|}/\varepsilon)}{\log(1/\alpha)}.$$

5 The “maximum speed limit” of projection samplers

In this section, we explore necessary conditions of achieving $R_n = \Pi$ or $R_\infty = \Pi$.

5.1 A simple three-point example that achieves $\overline{P}(Q) = \Pi$

In this subsection, we let \mathcal{X} be a three-point state space. The aim of this subsection is to provide a non-trivial example that achieves $\overline{P}(Q) = \Pi$. For $P \in \mathcal{L}(\mathcal{X})$, recall that $\lambda(P)$ is the set of eigenvalues of P . Let P be a transition matrix given by

$$P = \begin{bmatrix} \frac{1}{2} & \frac{1}{3} & \frac{1}{6} \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{2} \\ \frac{1}{6} & \frac{1}{2} & \frac{1}{3} \end{bmatrix}, \quad \lambda(P) = \left\{ 1, \pm \frac{1}{2\sqrt{3}} \right\}.$$

Clearly, $\pi = (1/3, 1/3, 1/3)$ and $P^* = P$. We take Q to be

$$Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \lambda(Q) = \{1, 1, -1\}.$$

It can easily be seen that $Q^* = Q$ and $Q^2 = I$. We compute that

$$QP = \begin{bmatrix} \frac{1}{3} & \frac{1}{6} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{2} & \frac{1}{3} \end{bmatrix}, \quad \lambda(QP) = \left\{ 1, \pm \frac{\sqrt{-3}}{6} \right\},$$

$$\begin{aligned}
PQ &= \begin{bmatrix} \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{3} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} \end{bmatrix}, & \lambda(PQ) &= \left\{ 1, \pm \frac{\sqrt{-3}}{6} \right\}, \\
QPQ &= \begin{bmatrix} \frac{1}{6} & \frac{1}{3} & \frac{1}{2} \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} \end{bmatrix}, & \lambda(QPQ) &= \left\{ 1, \pm \frac{1}{2\sqrt{3}} \right\}, \\
\bar{P}(Q) &= \frac{1}{2}(P + QPQ) = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}, & \lambda(\bar{P}(Q)) &= \{1, 0, 0\}, \\
\frac{1}{2}(PQ + QP) &= \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}, & \lambda\left(\frac{1}{2}(PQ + QP)\right) &= \{1, 0, 0\}.
\end{aligned}$$

We see that there are two interesting properties of P : it satisfies $\text{Tr}(P) = 1$ and $\lambda(P) \cap \lambda(-P) \neq \emptyset$. This motivates our investigations in the following subsections.

5.2 A necessary condition of $R_n = \Pi$ in terms of trace

In view of Proposition 4.2 and 3.2, we recall that the projections are trace-preserving and hence

$$\text{Tr}(R_n) = \text{Tr}(P).$$

Thus, if for some $n \in \mathbb{N} \cup \{\infty\}$ such that $R_n = \Pi$, this implies $\text{Tr}(P) = 1$. We record this as a Corollary:

Corollary 5.1. *Let $P \in \mathcal{S}(\pi)$ and consider the sequence (R_n) defined in (14), where $Q_i \in \mathcal{I}(\pi) \cap \mathcal{L}$ for $i \in \llbracket 0, m-1 \rrbracket$ is a sequence of isometric involution transition matrices. If $R_n = \Pi$ for some $n \in \mathbb{N} \cup \{\infty\}$, then*

$$\text{Tr}(P) = 1.$$

Consequently, this implies that if P is positive-definite so that $\text{Tr}(P) > 1$, then for any sequence of $(Q_i)_{i=0}^{m-1}$, $R_n \neq \Pi$ for all $n \in \mathbb{N} \cup \{\infty\}$.

5.3 A necessary condition of $\bar{P}(Q) = \Pi$ via the Sylvester's equation

Let us first briefly recall the Sylvester's equation. It is a linear matrix equation in $X \in \mathcal{M}$ of the form, for given $A, B, C \in \mathcal{M}$,

$$AX + XB = C.$$

The Sylvester's theorem (Horn and Johnson, 2013, Theorem 2.4.4.1) gives a necessary and sufficient condition for the above Sylvester's equation to admit a unique solution in $X \in \mathcal{M}$

for each given C : X is unique if and only if $\lambda(A) \cap \lambda(-B) = \emptyset$, that is, A and $-B$ have no eigenvalue in common.

In our setting, we specialize into $A = P, B = P^*$ and $C = 2\Pi$ with $P \in \mathcal{S}(\pi)$. We note that $X = \Pi$ is always a solution. Thus, if $\overline{P}(Q) = \Pi$, the Sylvester's equation has at least two solutions $X \in \{\Pi, Q\}$, and hence by the Sylvester's theorem we have $\lambda(P) \cap \lambda(-P^*) \neq \emptyset$. We record this as a Corollary:

Corollary 5.2. *Let $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ be an isometric involution transition matrix. If $\overline{P}(Q) = \Pi$, then*

$$\lambda(P) \cap \lambda(-P^*) \neq \emptyset,$$

that is, P and $-P^$ have at least one common eigenvalue.*

Consequently, the above result implies that, for π -reversible $P \in \mathcal{L}(\pi)$, if it is positive-definite or if $|\lambda_i(P)| \neq |\lambda_j(P)|$ for all $i \neq j$, then P and $-P^* = -P$ have no common eigenvalue, and hence $\overline{P}(Q) \neq \Pi$.

5.4 Characterization of R_∞ when π is the discrete uniform distribution, and a necessary and sufficient condition of $R_\infty = \Pi$

In this subsection, we let $n = |\mathcal{X}|$ and consider π to be the discrete uniform distribution with $P = P^T \in \mathcal{L}(\pi)$. Without loss of generality we assume the state space is of the form $\mathcal{X} = \llbracket n \rrbracket$. For $j \in \llbracket 2, n \rrbracket$, we define the permutations $(\psi_{1,j})_{j=2}^n$ to be $\psi_{1,j}(1) = j$, $\psi_{1,j}(j) = 1$ and $\psi_{1,j}(x) = x$ for all $x \in \mathcal{X} \setminus \{1, j\}$, and denote the induced permutation matrices by $(Q_{1,j})_{j=2}^n$. Clearly, $Q_{1,j} \in \mathcal{I}(\pi) \cap \mathcal{L}$, and we recall that the intersection of $(\mathcal{L}(\pi, Q_{1,j}))_{j=2}^n$ is written as

$$\mathcal{E} = \bigcap_{j=2}^n \mathcal{L}(\pi, Q_{1,j}).$$

In the above setting, the main result of this subsection characterizes R_∞ and demonstrates that R_∞ is a linear combination of Π and I . It also proves that, under the choices of the permutation matrices $(Q_{1,j})_{j=2}^n$, $\text{Tr}(P) = 1$ is necessary and sufficient to achieve $R_\infty = \Pi$:

Theorem 5.1. *Let π be the discrete uniform distribution on \mathcal{X} and $P = P^T \in \mathcal{L}(\pi)$. Denote the sequence of isometric involution transition matrices to be $Q_{1,j}$ as in this subsection, and define the sequence of projections $(R_l)_{l \in \mathbb{N}}$ as in (14). The limit R_∞ is given by*

$$R_\infty = (nb)\Pi + (a-b)I = \begin{bmatrix} a & b & \dots & b \\ b & a & \ddots & \vdots \\ \vdots & \ddots & \ddots & b \\ b & \dots & b & a \end{bmatrix}, \quad (16)$$

where $a = a(Q_{1,2}, \dots, Q_{1,n}, P)$, $b = b(Q_{1,2}, \dots, Q_{1,n}, P) \in [0, 1]$ satisfy $nb + a - b = 1$. In particular, $R_\infty = \Pi$ if and only if $\text{Tr}(P) = 1$.

Proof. First, we shall prove by induction on $k \in \llbracket n \rrbracket$ that the first k rows and k columns of R_∞ is of the form

$$\begin{bmatrix} a & b & \dots & b & \dots \\ b & a & \ddots & b & \dots \\ \vdots & \ddots & \ddots & \vdots & \dots \\ b & \dots & b & a & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix},$$

that is, $R_\infty(x, x) = a$ for all $x \in \llbracket k \rrbracket$ and $R_\infty(x, y) = b$ for all $x \neq y, x, y \in \llbracket k \rrbracket$.

When $k = 1$, what we seek to prove obviously holds. When $k = 2$, since $R_\infty \in \mathcal{L}(\pi, Q_{1,2})$, we see that

$$\begin{aligned} R_\infty(1, 1) &= R_\infty(\psi_{1,2}(1), \psi_{1,2}(1)) = R_\infty(2, 2), \\ R_\infty(1, 2) &= R_\infty(\psi_{1,2}(1), \psi_{1,2}(2)) = R_\infty(2, 1). \end{aligned}$$

Assume that the induction hypothesis holds for some k . Since $R_\infty \in \bigcap_{j=2}^k \mathcal{L}(\pi, Q_{1,j})$, the first $k + 1$ rows and $k + 1$ columns of R_∞ can be written as

$$\begin{bmatrix} a & b & \dots & b & c & \dots \\ b & a & \ddots & b & c & \dots \\ \vdots & \ddots & \ddots & \vdots & \vdots & \dots \\ b & \dots & b & a & c & \dots \\ d & \dots & d & d & e & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix},$$

where $c, d, e \in [0, 1]$ are some constants. To see that $c = d$, we note $c = R_\infty(1, k + 1) = R_\infty(\psi_{1,k+1}(1), \psi_{1,k+1}(k + 1)) = R_\infty(k + 1, 1) = d$. Similarly, we have $a = e$ since $a = R_\infty(1, 1) = R_\infty(\psi_{1,k+1}(1), \psi_{1,k+1}(1)) = R_\infty(k + 1, k + 1) = e$. Finally, $b = c$ since $b = R_\infty(1, 2) = R_\infty(\psi_{1,k+1}(1), \psi_{1,k+1}(2)) = R_\infty(k + 1, 2) = d = c$. This completes the induction.

By Corollary 5.1, $\text{Tr}(P) = 1$ is a necessary condition of $R_\infty = \Pi$. In the opposite direction, if $\text{Tr}(P) = 1$, the trace-preserving property of projections in Proposition 4.2 gives $\text{Tr}(R_\infty) = 1$. We see that

$$\text{Tr}(R_\infty) = \text{Tr}((nb)\Pi + (a - b)I) = nb + (a - b)n = na = 1,$$

which gives $a = b = 1/n$, and hence $R_\infty = \Pi$. □

Using (16), we see that the right spectral gap of R_∞ is

$$\gamma(R_\infty) = nb.$$

In the following proposition, we give a lower bound of $1/2$ when P is closer to Π than to I in Frobenius norm:

Proposition 5.1. *In the setting of Theorem 5.1, if $\|P - \Pi\|_F \leq \|P - I\|_F$ or equivalently*

$$\mathrm{Tr}(P) \leq \frac{n+1}{2},$$

then

$$\gamma(R_\infty) \geq \frac{1}{2}.$$

Proof. By Proposition 4.2, the assumption $\|P - \Pi\|_F \leq \|P - I\|_F$ implies $\|R_\infty - \Pi\|_F \leq \|R_\infty - I\|_F$. Using (16), we compute that

$$\begin{aligned} \|R_\infty - \Pi\|_F &= |a - b| \|\Pi - I\|_F, \\ \|R_\infty - I\|_F &= |1 - (a - b)| \|\Pi - I\|_F. \end{aligned}$$

This leads to $|a - b| \leq |1 - (a - b)|$, and hence $a - b \leq 1/2$. Since $1 - nb = a - b$, this yields $nb \geq 1/2$.

To see the equivalence, we compute that

$$\begin{aligned} \|P - \Pi\|_F^2 &= \sum_{x,y} \left(P(x,y) - \frac{1}{n} \right)^2 \\ &= \sum_{x,y} P(x,y)^2 - \frac{2}{n} \sum_{x,y} P(x,y) + 1 \\ &= \sum_{x,y} P(x,y)^2 - 1, \\ \|P - I\|_F^2 &= \sum_{x,y} (P(x,y) - \delta_{x=y})^2 \\ &= \sum_{x,y} P(x,y)^2 - 2 \sum_{x,y} P(x,y) \delta_{x=y} + \sum_{x,y} \delta_{x=y} \\ &= \sum_{x,y} P(x,y)^2 - 2 \sum_x P(x,x) + n, \end{aligned}$$

and hence $\|P - \Pi\|_F \leq \|P - I\|_F$ is equivalent to

$$\sum_x P(x,x) \leq \frac{n+1}{2}.$$

□

In the remaining of this subsection, we let $c = c(P) := \mathrm{Tr}(P)$. Suppose that $c \in [0, 1)$, and by Theorem 5.1, we note that

$$R_\infty(Q_{1,2}, \dots, Q_{1,n}, P) \neq \Pi.$$

Consider instead the transition matrix P' given by

$$P' := \alpha I + (1 - \alpha)P, \quad \alpha := \frac{1 - c}{n - c} \in [0, 1],$$

then $P'^T = P' \in \mathcal{L}(\pi)$. Furthermore, $\text{Tr}(P') = 1$, and hence by Theorem 5.1 and Proposition 5.1 we have

$$R_\infty(Q_{1,2}, \dots, Q_{1,n}, P') = \Pi, \quad \gamma(R_\infty(Q_{1,2}, \dots, Q_{1,n}, P')) \geq \frac{1}{2}.$$

Thus, it is advantageous to consider first P' and then the sequence of alternating projections (R_l) induced by P' to improve mixing over the original P .

More generally, if P is such that $c \in [0, \frac{n+1}{2}] \setminus \{1\}$, then by Theorem 5.1 this is not an ideal situation since the limit of the projections is

$$R_\infty(Q_{1,2}, \dots, Q_{1,n}, P) \neq \Pi.$$

However, by Proposition 5.1

$$\gamma(R_\infty(Q_{1,2}, \dots, Q_{1,n}, P)) \geq \frac{1}{2}.$$

In other words, for $P \in \{P \in \mathcal{L}(\pi); \pi(x) = 1/n \text{ for all } x, \text{Tr}(P) \leq \frac{n+1}{2}\}$, the limit R_∞ induced from any member of this family mixes fast since it has a constant order relaxation time.

A special case arises when $c = 0$, or equivalently $P(x, x) = 0$ for all x . This leads to $a = 0, b = 1/(n - 1)$. Even if $R_\infty \neq \Pi$, R_∞ is an “optimal reversible stochastic matrix” that minimizes the worst-case asymptotic variance in the sense of (Frigessi et al., 1992, Remark 3).

6 Tuning strategies of Q

In this paper, given a $P \in \mathcal{L}(\pi)$, we propose projection samplers such as $\overline{P}(Q)$ or more generally the sequence of alternating projections $(R_l)_{l \in \mathbb{N}}$ as improved variants compared with the original P . In these cases, the isometric involution transition matrix $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$ can be understood as a parameter in these algorithms, and the improvement depends on the tuning of Q . For instance, the choice of $Q = I$ is always feasible, yet it leads to no improvement since $\overline{P}(I) = P$. On the other hand, we have seen in Section 5 that depending on P it might be possible to achieve $R_l = \Pi$ or $R_\infty = \Pi$ with suitable choices of Q s.

In this section, we explore some possible tuning strategies of Q .

6.1 Tuning Q via optimization and Markov chain assignment problems

The first strategy seeks to find an optimal Q that minimizes the discrepancy between $\bar{P}(Q)$ and Π or more generally between R_l and Π .

Precisely, we would like to find Q that minimizes the π -weighted KL divergence or the squared-Frobenius norm for a given $P \in \mathcal{S}(\pi)$:

$$Q_{*,KL} = Q_{*,KL}(P) := \arg \min_{Q \in \mathcal{I}(\pi) \cap \mathcal{L}} D_{KL}^\pi(\bar{P}(Q) \| \Pi),$$

$$Q_{*,F} = Q_{*,F}(P) := \arg \min_{Q \in \mathcal{I}(\pi) \cap \mathcal{L}} \|\bar{P}(Q) - \Pi\|_F^2.$$

The above optimization problems may not be solved in realistic time frame in practice, since π may involve normalization constant that is non-tractable. Fortunately, using the Pythagorean identities in Proposition 2.4 and 3.3, we see that

$$Q_{*,KL} = \arg \max_{Q \in \mathcal{I}(\pi) \cap \mathcal{L}} D_{KL}^\pi(P \| \bar{P}(Q)) = \arg \max_{\psi \in \Psi(\pi)} D_{KL}^\pi(P \| \bar{P}(Q_\psi)),$$

$$Q_{*,F} = \arg \max_{Q \in \mathcal{I}(\pi) \cap \mathcal{L}} \|P - \bar{P}(Q)\|_F^2 = \arg \max_{\psi \in \Psi(\pi)} \|P - \bar{P}(Q_\psi)\|_F^2.$$

The rightmost maximization problems can be understood as Markov chain assignment problems constrained to choosing permutations within the set $\Psi(\pi)$. While in general assignment problems can be solved in polynomial time in $|\mathcal{X}|$ Korte and Vygen (2018), this may still be computationally infeasible in practice since $|\mathcal{X}|$ might be exponentially large in many models of interest in the context of MCMC.

The above can be generalized to consider multidimensional Markov chain assignment problems. Specifically, we seek to solve, for $m, l \in \mathbb{N}$,

$$\begin{aligned} & \arg \min_{\psi_i \in \Psi(\pi), \forall i \in [0, m-1]} D_{KL}^\pi(R_l(Q_{\psi_0}, \dots, Q_{\psi_{m-1}}, P) \| \Pi) \\ &= \arg \max_{\psi_i \in \Psi(\pi), \forall i \in [0, m-1]} \sum_{j=0}^{l-1} D_{KL}^\pi(R_j(Q_{\psi_0}, \dots, Q_{\psi_{m-1}}, P) \| R_{j+1}(Q_{\psi_0}, \dots, Q_{\psi_{m-1}}, P)), \\ & \arg \min_{\psi_i \in \Psi(\pi), \forall i \in [0, m-1]} \|R_l(Q_{\psi_0}, \dots, Q_{\psi_{m-1}}, P) - \Pi\|_F^2 \\ &= \arg \max_{\psi_i \in \Psi(\pi), \forall i \in [0, m-1]} \sum_{j=0}^{l-1} \|R_j(Q_{\psi_0}, \dots, Q_{\psi_{m-1}}, P) - R_{j+1}(Q_{\psi_0}, \dots, Q_{\psi_{m-1}}, P)\|_F^2, \end{aligned}$$

where the equalities follow from the Pythagorean identities in Proposition 2.4 and 3.3. Note that in general multidimensional assignment problems are NP hard Nguyen et al. (2014) to solve, and there are heuristics to solve these in practice such as the cross-entropy method.

We remark that, this technique of converting the original problem of minimization of KL divergence to a maximization problem is in the spirit of evidence lower bound (ELBO) in variational inference, see for example Blei et al. (2017).

6.2 Tuning Q adaptively in a single run

Let $H : \mathcal{X} \rightarrow \mathbb{R}$ be a target Hamiltonian function, and π_β be its associated Gibbs distribution at inverse temperature $\beta \geq 0$, that is, for $x \in \mathcal{X}$,

$$\pi_\beta(x) := \frac{e^{-\beta H(x)}}{Z_\beta},$$

where $Z_\beta := \sum_{x \in \mathcal{X}} e^{-\beta H(x)}$ is the normalization constant. Thus, we see that $\pi_\beta(x) = \pi_\beta(y)$ if and only if $H(x) = H(y)$.

The second tuning strategy lies in adjusting Q adaptively on the fly as the algorithm progresses. Specifically, given a $P \in \mathcal{L}(\pi_\beta)$ such as the Metropolis-Hastings algorithm or the Gibbs sampler, we run a non-homogeneous and adaptive Markov chain with transition matrix at each time $l \in \mathbb{N}$ to be

$$\frac{1}{2}(P + Q_{\psi_l} P Q_{\psi_l}),$$

along with the initial condition $Q_{\psi_1} = I$. We record the trajectories of this adaptive Markov chain. At time $l \geq 2$, suppose the past trajectory is $\{x_0, x_1, \dots, x_{l-1}\}$. We search for an “equi-energy” pair that is not mapped in $Q_{\psi_{l-1}}$: if there exists i, j such that $H(x_i) = H(x_j)$, $\psi_{l-1}(x_i) = x_i$, $\psi_{l-1}(x_j) = x_j$, then we update the permutation to $\psi_l(x_i) = x_j$, $\psi_l(x_j) = x_i$, $\psi_l(x) = \psi_{l-1}(x)$ for all $x \in \mathcal{X} \setminus \{x_i, x_j\}$.

6.3 Tuning Q using an exploration chain in multiple runs

The third strategy uses an exploration Markov chain, such as the proposal chain in Metropolis-Hastings or the Metropolis-Hastings chain at high temperature, for $k \in \mathbb{N}$ times. Each time a permutation matrix Q_l is generated as outlined in Section 6.2. Then, we combine this sequence of matrices $(Q_l)_{l=1}^k$ using alternating projections as discussed in Section 4. This idea is inspired by the equi-energy sampler [Kou et al. \(2006\)](#).

7 Application to Metropolis-Hastings

The aim of this section is to concretely illustrate and quantify the benefit of using the projection sampler $\bar{P}(Q)$ over the original P , when the latter is taken to be the transition matrix of the classical Metropolis-Hastings (MH) algorithm. We also present a simple model in which π_β is a discrete bimodal distribution, where the relaxation time of the projection sampler, upon suitable choice of Q , is polynomial in β and size of the state space while that of the MH is exponential in these parameters. Thus, the relaxation (and hence mixing) time is improved from exponential to polynomial via this technique.

To this end, let us briefly recall the MH dynamics. Given a proposal Markov chain with transition matrix N that is ergodic and reversible, and a Gibbs distribution π_β associated with Hamiltonian H and inverse temperature β , the MH algorithm is a discrete-time Markov chain with transition matrix given by $P_\beta = P_\beta(N, H) = (P_\beta(x, y))_{x, y \in \mathcal{X}}$, where

$$P_\beta(x, y) := \begin{cases} N(x, y) \min \{1, e^{\beta(H(x) - H(y))}\} = N(x, y)e^{-\beta(H(y) - H(x))_+}, & \text{if } x \neq y; \\ 1 - \sum_{z: z \neq x} P_\beta(x, z), & \text{if } x = y. \end{cases}$$

For $\alpha \in [0, 1]$ and $\psi \in \Psi(\pi)$, we compute that, for $x \neq y$,

$$\begin{aligned} \overline{(P_\beta)_\alpha}(Q_\psi)(x, y) &= \alpha N(x, y)e^{-\beta(H(y) - H(x))_+} + (1 - \alpha)N(\psi(x), \psi(y))e^{-\beta(H(\psi(y)) - H(\psi(x)))_+} \\ &= (\alpha N(x, y) + (1 - \alpha)N(\psi(x), \psi(y)))e^{-\beta(H(y) - H(x))_+} \\ &= P_\beta(\alpha N + (1 - \alpha)Q_\psi N Q_\psi, H)(x, y), \end{aligned} \tag{17}$$

where the second equality follows from $H(x) = H(\psi(x))$. Therefore, the family $(\overline{(P_\beta)_\alpha}(Q_\psi))_{\alpha \in [0, 1]}$ can be interpreted as MH chains with modified proposals $(\alpha N + (1 - \alpha)Q_\psi N Q_\psi)_{\alpha \in [0, 1]}$ targeting the same H at the same inverse temperature β . This interpretation also illustrates it is perhaps advantageous to use $\overline{(P_\beta)_\alpha}(Q)$: the proposal $\alpha N + (1 - \alpha)Q N Q$ has at least as many connections as the original proposal N , that is, $\{(x, y); N(x, y) > 0\} \subseteq \{(x, y); (\alpha N + (1 - \alpha)Q N Q)(x, y) > 0\}$. In this sense, this technique to improve mixing is in the spirit of [Gerencsér and Hendrickx \(2019\)](#).

To quantify the speed of convergence towards π_β of the MH chain, we now recall an important parameter that is known as the hill-climbing constant, energy barrier or the critical height in the literature. In a broad sense, it measures the difficulty of navigating on the landscape of H . Precisely, we say that a path from x to y is any sequence of points starting from $x_0 = x, x_1, x_2, \dots, x_n = y$ such that $N(x_{i-1}, x_i) > 0$ for $i \in \llbracket n \rrbracket$. As N is irreducible, for any $x \neq y$ such path exists. We write $\Gamma^{x, y} = \Gamma^{x, y}(N)$ to be the set of paths from x to y , and elements of $\Gamma^{x, y}$ are denoted by $\gamma = (\gamma_i)_{i=0}^n$. The value of the Hamiltonian $H(x)$ can be interpreted as the elevation at x , and the highest elevation along a path $\gamma \in \Gamma^{x, y}$ is

$$\text{Elev}(\gamma) = \max\{H(\gamma_i); \gamma_i \in \gamma\},$$

and the lowest possible highest elevation along path(s) from x to y is

$$\mathbf{H}(x, y) := \min\{\text{Elev}(\gamma); \gamma \in \Gamma^{x, y}\}.$$

For $P_\beta(N, H)$, the associated critical height is defined to be

$$h(P_\beta) := \max_{x, y \in \mathcal{X}} \{\mathbf{H}(x, y) - H(x) - H(y)\} + \min_z H(z), \tag{18}$$

Using a classical result of ([Holley and Stroock, 1988](#), Lemma 2.3, 2.7), the right spectral gap of the MH chain can be bounded using $h(P_\beta)$: there exists constants $0 < c = c(N) \leq C = C(N) < \infty$ that do not depend on β such that

$$ce^{-\beta h(P_\beta)} \leq \gamma(P_\beta) \leq Ce^{-\beta h(P_\beta)}. \tag{19}$$

We now compare the critical heights of the family $(\overline{(P_\beta)_\alpha}(Q))_{\alpha \in [0,1]}$, and demonstrates the optimality of $\alpha = 1/2$: the sampler $(1/2)(P_\beta + QP_\beta Q)$ has the smallest critical height within this family, thus leading to improved convergence over the original P_β . In addition to critical height, $(1/2)(P_\beta + QP_\beta Q)$ also enjoys some advantageous properties over the original P in terms of entropic and spectral parameters as well as asymptotic variances if we recall Section 3. It justifies the decision to focus on analyzing $(1/2)(P_\beta + QP_\beta Q)$ in this context.

Proposition 7.1. *Let P_β be the transition matrix of the MH chain with ergodic proposal N and target distribution π_β , and $Q \in \mathcal{I}(\pi_\beta) \cap \mathcal{L}$. We have*

- (Similarity preserves critical height)

$$h(P_\beta) = h(QP_\beta Q).$$

- (Optimality of $\alpha = 1/2$) For $\alpha \in [0, 1]$,

$$h(\overline{(P_\beta)_\alpha}(Q)) \leq h(P_\beta).$$

In particular,

$$\min_{\alpha \in [0,1]} h(\overline{(P_\beta)_\alpha}(Q)) = h(\overline{(P_\beta)_{1/2}}(Q)).$$

Proof. We show the first item. Using Proposition 3.4, we have

$$\gamma(P_\beta) = \gamma(QP_\beta Q).$$

Now, if we consider (19) and since $QP_\beta Q = P_\beta(QNQ, H)$, we have

$$\begin{aligned} h(P_\beta) &= - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\gamma(P_\beta)) \\ &= - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\gamma(QP_\beta Q)) \\ &= h(QP_\beta Q). \end{aligned}$$

We proceed to prove the second item and it suffices to show for $\alpha \in (0, 1)$ in view of the first item. By Proposition 3.5, we see that

$$\gamma(\overline{(P_\beta)_\alpha}(Q)) \geq \gamma(P_\beta),$$

and using (19) and (17) again yield

$$\begin{aligned} h(P_\beta) &= - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\gamma(P_\beta)) \\ &\geq - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\gamma(\overline{(P_\beta)_\alpha}(Q))) \end{aligned}$$

$$= h(\overline{(P_\beta)_\alpha}(Q)).$$

To demonstrate the optimality of $\alpha = 1/2$, we note that

$$\overline{(P_\beta)_\alpha}(Q) = P_\beta(\alpha N + (1 - \alpha)Q N Q, H),$$

and applying the result above with P_β replaced by $\overline{(P_\beta)_\alpha}(Q)$ leads to

$$h(\overline{(P_\beta)_\alpha}(Q)) \geq h(\overline{\overline{(P_\beta)_\alpha}(Q)}_{1/2}(Q)) = h(\overline{(P_\beta)_{1/2}}(Q)).$$

□

The above result also illustrates a way to tune Q : we should seek to choose Q such that the critical height $h(\overline{(P_\beta)_{1/2}}(Q))$ is minimized. In the remaining of this section, we shall specialize into a discrete bimodal example on a line that has been investigated in the literature [Madras and Zheng \(2003\)](#).

Specifically, we consider $\mathcal{X} = \{-J, -J + 1, \dots, J - 1, J\}$ for $J \in \mathbb{N}$, $H(x) = -|x|$ for $x < J - 1$, $H(J - 1) = -J$ and $H(J) = -J - 1$, while the proposal chain N is taken to be a simple nearest-neighbor random walk on \mathcal{X} with holding probability of $1/2$ at the two boundaries $\pm J$. In this setting, there is a global mode of π_β at J and a local mode located at $-J$. It can readily be seen that

$$h(P_\beta) = J = H(0) - H(-J).$$

The bottleneck of mixing in this case is the hill at $x = 0$ that separates the two modes, in which the MH chain needs to climb over if it is initiated at $x < 0$ or $x > 0$, which is exponentially unlikely as $\beta \rightarrow \infty$.

Let $\psi(-J) = J - 1$, $\psi(J - 1) = -J$ and $\psi(x) = x$ for $x \in \mathcal{X} \setminus \{-J, J - 1\}$, and we take $Q = Q_\psi$. It can readily be seen that $Q^2 = I$ and $Q^* = Q$ since $H(-J) = H(J - 1) = -J$. It turns out this choice of Q is optimal since the critical height of $\overline{(P_\beta)_{1/2}}(Q)$ is zero. To see that, since $h(\overline{(P_\beta)_{1/2}}(Q))$ is attained in a path from a local minimum to a global minimum of H , the lowest elevation is zero since $Q N Q(-J, J) = N(J - 1, J) = 1/2 > 0$. This is graphically illustrated in [Figure 2](#).

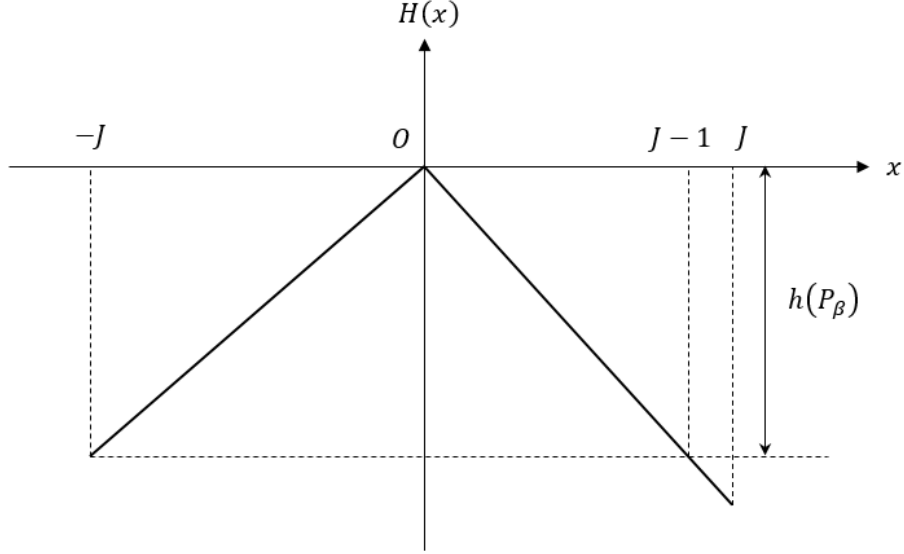


Figure 2: A landscape with a local minimum at $-J$ and a global minimum at J . The original critical height is $h(P_\beta) = J$, while $h(\overline{(P_\beta)}_{1/2}(Q)) = 0$. The reason is that there is a zero elevation path from $-J$ to $J-1$ to J owing to the choice of Q .

Using (19), the relaxation time of $\overline{(P_\beta)}_{1/2}(Q)$ is subexponential while that of P_β is exponential in β and J . Note that at each time there is at most two additional permutation steps in $(1/2)(P_\beta + QP_\beta Q)$ compared with the original P_β .

Proposition 7.2. *In the bimodal example, we have*

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(t_{\text{rel}}(\overline{(P_\beta)}_{1/2}(Q))) = 0,$$

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(t_{\text{rel}}(P_\beta)) = J.$$

In fact, a finer polynomial upper bound can be obtained for $t_{\text{rel}}(\overline{(P_\beta)}_{1/2}(Q))$. Precisely, in the notations of Ingrassia (1994), we have

$$b_\Gamma \leq \frac{2J(2J-1)}{2} = 2J^2 - J, \quad \gamma_\Gamma \leq 2(2J-1) + 4 = 4J + 2, \quad d^* = 4.$$

Applying (Ingrassia, 1994, Theorem 4.1) in view of these upper bounds leads to

Proposition 7.3. *In the bimodal example, we have*

$$t_{\text{rel}}(\overline{(P_\beta)}_{1/2}(Q)) \leq b_\Gamma \gamma_\Gamma d^* = \mathcal{O}(J^3).$$

8 Improving discrete-uniform samplers with general permutations and projections

In this section, we shall consider ergodic $P \in \mathcal{S}(\pi)$ where π is the discrete uniform distribution on \mathcal{X} . In earlier sections, we have restricted ourselves to $Q \in \mathcal{I}(\pi) \cap \mathcal{L}$, the set of isometric involution transition matrices, and shown that such Q s are induced by equi-probability permutations in Proposition 2.1. In this paper, we shall relax this assumption of Q to general permutation matrix in this section only.

In this setting, it is not necessary to use MCMC samplers to sample from the discrete uniform: if we have a Q_σ drawn uniformly at random from the set of permutation matrices, then we can consider $Q_\sigma e_1$, where e_1 is the vector with 1 in the first entry and 0 in all remaining entries. This resulting vector would have a 1 in a position sampled uniformly from $[[n]]$. The main message in this section is that the kernel $\overline{P}(Q)$ have improved mixing time over the original P .

Precisely, we define

$$\mathcal{Q} := \{Q_\psi; \psi \in \mathbf{P}\}$$

and let $Q \in \mathcal{Q}$. If $Q = Q_\psi$, we see that $Q^* = Q_{\psi^{-1}}$, the $\ell^2(\pi)$ -adjoint of Q . We also note that in general $Q^* \neq Q$. In addition, it is obvious to see that Q is unitary since $QQ^* = Q^*Q = I$. Generalizing (2) to $Q \in \mathcal{Q}$, we analogously define

$$\overline{P}(Q) := \frac{1}{2}(P + QP^*Q).$$

The advantage of working under the setting of discrete uniform π is that all of $P, QP, PQ, QPQ, \overline{P}(Q) \in \mathcal{S}(\pi)$, thus it is sensible to compare these transition matrices as candidate samplers of π .

We first demonstrate that a few results in earlier sections such as Section 2 and Section 3 can be generalized to a general permutation Q . Our first result states that, in terms of one-step KL divergence from Π or the KL-divergence Dobrushin coefficient, the samplers P, QP, PQ, QPQ cannot be distinguished. The proof is omitted as it is analogous to Proposition 8.1.

Proposition 8.1. *Let π be the discrete uniform distribution, $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{Q}$ be a permutation matrix. Let Π be the matrix where each row equals to π . We have*

- (One-step contraction measured by D_{KL}^π)

$$D_{KL}^\pi(P||\Pi) = D_{KL}^\pi(PQ||\Pi) = D_{KL}^\pi(QP||\Pi) = D_{KL}^\pi(QPQ||\Pi).$$

- (KL-divergence Dobrushin coefficient)

$$c_{KL}(P) = c_{KL}(PQ) = c_{KL}(QP) = c_{KL}(QPQ).$$

The second result gives a Pythagorean identity under D_{KL}^π , and its proof is similar to Proposition 3.3.

Proposition 8.2 (Pythagorean identity). *Let π be the discrete uniform distribution, $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{Q}$ be a permutation matrix. Let Π be the matrix where each row equals to π . We have*

$$D_{KL}^\pi(\bar{P}(Q) \parallel \Pi) \leq D_{KL}^\pi(P \parallel \bar{P}(Q)) + D_{KL}^\pi(\bar{P}(Q) \parallel \Pi) = D_{KL}^\pi(P \parallel \Pi),$$

and the equality holds if and only if $\bar{P}(Q) = P$.

Similarly, if P is further assumed to be π -reversible, then

$$c_{KL}(\bar{P}(Q)) \leq c_{KL}(P).$$

For $\alpha \in [0, 1]$, we see that

$$\overline{\alpha P + (1 - \alpha)QP^*Q}(Q) = \bar{P}(Q).$$

Together with Proposition 8.2, we observe that the choice of $\alpha = 1/2$ is optimal within the family $(\alpha P + (1 - \alpha)QP^*Q)_{\alpha \in [0,1]}$ as it minimizes the KL divergence D_{KL}^π :

Corollary 8.1 (Optimality of $\alpha = 1/2$). *Let π be the discrete uniform distribution, $P \in \mathcal{S}(\pi)$ and $Q \in \mathcal{Q}$ be a permutation matrix. We have*

$$\min_{\alpha \in [0,1]} D_{KL}^\pi(\alpha P + (1 - \alpha)QP^*Q \parallel \Pi) = D_{KL}^\pi(\bar{P}(Q) \parallel \Pi).$$

To apply the projection sampler $\bar{P}(Q)$ in practice, one may seek to tune Q using similar strategies discussed in Section 6. For instance, using the Pythagorean identity in Proposition 8.2, we see that

$$\arg \min_{Q \in \mathcal{Q}} D_{KL}^\pi(\bar{P}(Q) \parallel \Pi) = \arg \max_{\psi \in \mathbf{P}} D_{KL}^\pi(P \parallel \bar{P}(Q_\psi)),$$

where the rightmost optimization problem is an assignment problem.

8.1 The example of Diaconis-Holmes-Neal

In this subsection, we specialize into the following: let $\mathcal{X} = \llbracket n \rrbracket$, and consider P to be the nearest-neighbour simple random walk with holding probability of $1/2$ at the two endpoints 1 and n , that is, $P(1, 1) = P(n, n) = 1/2$, $P(x, x+1) = 1/2$ for $x \in \llbracket n-1 \rrbracket$ and $P(x, x-1) = 1/2$ for $x \in \llbracket 2, n \rrbracket$. Clearly P satisfies the assumption of this section: it is ergodic and admits the discrete uniform stationary distribution.

This P demonstrates a diffusive behaviour in the sense that the underlying Markov chain has a worst-case total variation mixing time of the order of n^2 . This motivates [Diaconis](#)

et al. (2000) to introduce a non-reversible lifting of P that aims at correcting the diffusive behaviour, who also prove that order n steps are necessary and sufficient for the lifted chain to mix in worst-case total variation distance.

Let us recall that for $\mu, \nu \in \mathcal{P}(\mathcal{X})$, the total variation distance between them is

$$\|\mu - \nu\|_{TV} := \frac{1}{2} \sum_{x \in \mathcal{X}} |\mu(x) - \nu(x)|,$$

and the worst-case total variation mixing time of the Markov chain associated with P is, for $\varepsilon > 0$,

$$t_{mix}(P, \varepsilon) := \inf \left\{ n \in \mathbb{N}; \max_{x \in \mathcal{X}} \|P^n(x, \cdot) - \pi\|_{TV} < \varepsilon \right\}.$$

The main result of this subsection is that, if the permutation matrix Q is drawn uniformly at random from \mathcal{Q} , then with high probability $t_{mix}(\bar{P}(Q), \varepsilon)$ is at most of the order $\ln n$:

Proposition 8.3. *Let $P \in \mathcal{S}(\pi)$ be the nearest-neighbour simple random walk on $\llbracket n \rrbracket$ described at the beginning of this subsection, and Q be a permutation matrix drawn uniformly at random from \mathcal{Q} . For all $\varepsilon \in (0, 1)$, there exists $C(\varepsilon)$ such that with high probability*

$$t_{mix}(\bar{P}(Q), \varepsilon) \leq \frac{\ln n}{\ln 2} + C(\varepsilon)\sqrt{\ln n}.$$

Proof. We apply (Dubail, 2024a, Theorem 1.1), where we note that P is π -reversible, and the entropy rate of P is $\ln 2$. \square

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References

- D. Aldous and J. A. Fill. Reversible Markov chains and random walks on graphs, 2002. Unfinished monograph, recompiled 2014, available at <http://www.stat.berkeley.edu/~aldous/RWG/book.html>.
- C. Andrieu and S. Livingstone. Peskun-Tierney ordering for Markovian Monte Carlo: beyond the reversible scenario. *Ann. Statist.*, 49(4):1958–1981, 2021.
- S. Apers, A. Sarlette, and F. Ticozzi. Characterizing limits and opportunities in speeding up Markov chain mixing. *Stochastic Process. Appl.*, 136:145–191, 2021.
- A. Ben-Hamou and Y. Peres. Cutoff for permuted Markov chains. *Ann. Inst. Henri Poincaré Probab. Stat.*, 59(1):230–243, 2023.
- L. J. Billera and P. Diaconis. A geometric interpretation of the Metropolis-Hastings algorithm. *Statistical Science*, pages 335–339, 2001.
- D. M. Blei, A. Kucukelbir, and J. D. McAuliffe. Variational inference: a review for statisticians. *J. Amer. Statist. Assoc.*, 112(518):859–877, 2017.
- P. Brémaud. *Markov chains*, volume 31 of *Texts in Applied Mathematics*. Springer-Verlag, New York, 1999. Gibbs fields, Monte Carlo simulation, and queues.
- P. Brémaud. *Discrete probability models and methods*, volume 78 of *Probability Theory and Stochastic Modelling*. Springer, Cham, 2017. Probability on graphs and trees, Markov chains and random fields, entropy and coding.
- S. Chatterjee and P. Diaconis. Speeding up Markov chains with deterministic jumps. *Probab. Theory Related Fields*, 178(3-4):1193–1214, 2020.
- T.-L. Chen, W.-K. Chen, C.-R. Hwang, and H.-M. Pai. On the optimal transition matrix for Markov chain Monte Carlo sampling. *SIAM J. Control Optim.*, 50(5):2743–2762, 2012.
- M. C. H. Choi and G. Wolfer. Systematic approaches to generate reversibilizations of Markov chains. *IEEE Trans. Inform. Theory*, 70(5):3145–3161, 2024.
- I. Csiszár. I -divergence geometry of probability distributions and minimization problems. *Ann. Probability*, 3:146–158, 1975.
- F. Deutsch. *Best approximation in inner product spaces*, volume 7 of *CMS Books in Mathematics/Ouvrages de Mathématiques de la SMC*. Springer-Verlag, New York, 2001.
- P. Diaconis and L. Miclo. On characterizations of Metropolis type algorithms in continuous time. *ALEA Lat. Am. J. Probab. Math. Stat.*, 6:199–238, 2009.
- P. Diaconis, S. Holmes, and R. M. Neal. Analysis of a nonreversible Markov chain sampler. *Ann. Appl. Probab.*, 10(3):726–752, 2000.

- P. Diaconis, K. Khare, and L. Saloff-Coste. Stochastic alternating projections. *Illinois J. Math.*, 54(3):963–979, 2010.
- B. Dubail. Cutoff for mixtures of permuted markov chains: reversible case, 2024a. URL <https://arxiv.org/abs/2401.03937>.
- B. Dubail. Cutoff for mixtures of permuted markov chains: general case, 2024b.
- A. Frigessi, C.-R. Hwang, and L. Younes. Optimal spectral structure of reversible stochastic matrices, Monte Carlo methods and the simulation of Markov random fields. *Ann. Appl. Probab.*, 2(3):610–628, 1992.
- A. Frigessi, P. di Stefano, C.-R. Hwang, and S. J. Sheu. Convergence rates of the Gibbs sampler, the Metropolis algorithm and other single-site updating dynamics. *J. Roy. Statist. Soc. Ser. B*, 55(1):205–219, 1993.
- B. Gerencsér and J. M. Hendrickx. Improved mixing rates of directed cycles by added connection. *J. Theoret. Probab.*, 32(2):684–701, 2019.
- R. Holley and D. Stroock. Simulated annealing via Sobolev inequalities. *Comm. Math. Phys.*, 115(4):553–569, 1988.
- R. A. Horn and C. R. Johnson. *Matrix analysis*. Cambridge University Press, Cambridge, second edition, 2013.
- S. Ingrassia. On the rate of convergence of the Metropolis algorithm and Gibbs sampler by geometric bounds. *Ann. Appl. Probab.*, 4(2):347–389, 1994.
- B. Korte and J. Vygen. *Combinatorial optimization*, volume 21 of *Algorithms and Combinatorics*. Springer, Berlin, sixth edition, 2018. Theory and algorithms.
- S. C. Kou, Q. Zhou, and W. H. Wong. Equi-energy sampler with applications in statistical inference and statistical mechanics. *Ann. Statist.*, 34(4):1581–1652, 2006. With discussions and a rejoinder by the authors.
- N. Madras and Z. Zheng. On the swapping algorithm. *Random Structures Algorithms*, 22(1):66–97, 2003.
- J. Melbourne. Strongly convex divergences. *Entropy*, 22(11):Paper No. 1327, 20, 2020.
- L. Miclo. *On the Markovian Similarity*, pages 375–403. Springer International Publishing, Cham, 2018.
- D. M. Nguyen, H. A. Le Thi, and T. Pham Dinh. Solving the multidimensional assignment problem by a cross-entropy method. *J. Comb. Optim.*, 27(4):808–823, 2014.
- Q. Qin. Analysis of two-component Gibbs samplers using the theory of two projections. *Ann. Appl. Probab.*, 34(5):4310–4341, 2024.

- L. Rey-Bellet and K. Spiliopoulos. Improving the convergence of reversible samplers. *J. Stat. Phys.*, 164(3):472–494, 2016.
- C. Sherlock. Reversible markov chains: variational representations and ordering, 2018.
- W. So. Commutativity and spectra of Hermitian matrices. In *Proceedings of the 3rd ILAS Conference (Pensacola, FL, 1993)*, volume 212/213, pages 121–129, 1994.
- Y. Wang and M. C. H. Choi. Information divergences of markov chains and their applications, 2023.
- G. Wolfer and S. Watanabe. Information geometry of reversible Markov chains. *Information Geometry*, 4(2):393–433, 2021.