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Peskun-Tierney ordering for Markov chain and process Monte Carlo: beyond the reversible scenario

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Abstract

Historically time-reversibility of the transitions or processes underpinning Markov chain Monte Carlo methods (MCMC) has played a key rôle in their development, while the self-adjointness of associated operators together with the use of classical functional analysis techniques on Hilbert spaces have led to powerful and practically successful tools to characterize and compare their performance. Similar results for algorithms relying on nonreversible Markov processes are scarce. We show that for a type of nonreversible Monte Carlo Markov chains and processes, of current or renewed interest in the Physics and Statistical literatures, it is possible to develop comparison results which closely mirror those available in the reversible scenario. We show that these results shed light on earlier literature, proving some conjectures and strengthening some earlier results.

1 Introduction

Markov chain Monte Carlo (MCMC) is concerned with the simulation of realisations of \( \pi \)–invariant and ergodic Markov chains, where \( \pi \) is a probability distribution of interest defined on some appropriate measurable space \((X, \mathcal{X})\). Such realisations can be used to produce samples of distributions arbitrarily close to \( \pi \), or approximate expectations with respect to \( \pi \). For a given probability distribution \( \pi \) the choice of a Markov chain is not unique, and understanding the nature of the approximation associated to particular choices is therefore of importance and has generated a substantial body of literature, both in statistical science and physics—among others and directly related to our work [45, 13, 35, 55, 26, 39, 40, 34, 29, 33, 37, 49, 51, 17, 52, 48, 4, 9, 53]. The present paper is a contribution to this literature and addresses a scenario currently barely covered by existing theory, despite recent interest motivated by applications.

Due to its wide applicability the Metropolis-Hastings update [38, 28] is the cornerstone of the design of general purpose MCMC algorithms. The corresponding Markov transition probability satisfies the so-called detailed balance property, ensuring that \( \pi \) is left invariant by this update, but also implies reversibility of the numerous algorithms of which it is a building block. An unintended benefit of reversibility is given at a theoretical level. Using the operator interpretation of Markov transition probabilities, the properties of reversible Markov chains can be studied with well established functional analysis techniques developed for self-adjoint operators. The celebrated result of Peskun and its extensions [45, 13, 55] are an example (see [39] for
a review), and allow for practical performance comparisons in numerous scenarios of interest (see Theorem 2.7 and its Corollary for a quick reference), providing in particular clear answers to questions concerned with the design of algorithms. While reversibility facilitates theoretical analysis and has historically enabled methodological developments, it is not necessarily a desirable property when performance is considered. Informally such processes have a tendency to “backtrack”, slowing down exploration of the support of the target distribution $\pi$.

Recently, there has been renewed interest in the design of $\pi$–invariant Markov chains which are not reversible. In several specific scenarios it has been shown that departing from reversibility can both improve the speed of convergence of a Markov chain [16], and reduce the asymptotic variance of resulting estimators [52] (although counterexamples also exist [50]). Certain nonreversible samplers have been known for some time [30, 27], but interest has been re-kindled more recently thanks to a suite of methods which are not instances of the Metropolis–Hastings class. All these Markov transition probabilities share a common structure, illustrated here with a very simple example. Assume that $X = \mathbb{Z}$, let $E := X \times \{-1, 1\}$, embed the distribution of interest $\pi$ into $\mu(x, v) := \frac{1}{2}\pi(x)\mathbb{I}\{v \in \{-1, 1\}\}$ and consider the Markov transition probability

$$P(x, v; y, w) := \alpha(x, v)\mathbb{I}\{y = x + v\}\mathbb{I}\{w = v\} + \mathbb{I}\{y = x\}\mathbb{I}\{w = -v\}[1 - \alpha(x, v)],$$

where $\alpha(x, v) := \min\{1, \pi(x + v)/\pi(x)\}$ and $\mathbb{I}S$ is the indicator function of set $S$. In words, starting at $(x, v)$, the first component of the Markov chain generated by $P$ will travel in the same direction $v$ in increments of size one until a rejection occurs and the direction is reversed. One can check that this does not satisfy detailed balance with respect to $\mu$ (or indeed $\pi$), but a similar looking property

$$\mu(x, v)P(x, v; y, w) = \mu(y, w)P(y, -w; x, -v),$$

for $(x, v), (y, w) \in E$. This is referred to as modified detailed balance in the literature [22] or skewed detailed balance [31], and leads to what is known as Yaglom reversibility [59]. It is instructive to write this identity in terms of the transition probability $Q(x, v; y, w) := \mathbb{I}\{y = x\}\mathbb{I}\{w = -v\}$, which now reads $\mu(x, v)P(x, v; y, w) = \pi(y, w)QPQ(y, w; x, v)$ where $QPQ$ is the composition of the three kernels. An interpretation of this identity is that the corresponding operator $QPQ$ is the adjoint of $P$, not $P$ as is the case in the self-adjoint scenario. This structure of the adjoint of $P$, together with the fact that $Q^2$ is the identity, play a central role in our analysis and covers a surprisingly large number of known scenarios and applications currently beyond the reach of earlier theory. Indeed our theory does not require the embedding $\mu$ of $\pi$ to be of the specific form above, and $Q$ is only required to be an isometric involution—see Subsection 2.1 for a precise definition in the present context. As we shall see this structure allows us to develop a theory for performance comparison for this class of MCMC algorithms which parallels that existing for reversible algorithms; see Subsection 2.2. Applications are given in Section 3, and include the proof of conjectures concerned with the lifted Metropolis–Hastings method of [56, 58] and improves and generalises the results of [52], provide a direct and rigorous proof of [40] in a more general set-up and a connection to the results of [37], which is generalised, permitting the characterization of algorithms (e.g. [30, 12]) currently not covered by existing theory.

We show that this structure is shared by nonreversible Markov process Monte Carlo (MPMC) methods, the continuous time pendant of MCMC, which have recently attracted some attention [46, 10, 11, 7, 6, 42]. Characterization of this property in the continuous time setup is precisely formulated in Subsection 4.1 and a concrete example discussed in Subsection 5.2. In Subsection 4.2 we propose new tools which enable performance comparison for this class of processes and an application is presented in Section 5.

Throughout this paper we will use the following standard notation. Let $(E, \mathcal{E})$ be a measurable space. For Markov kernels $T_1, T_2 : E \times \mathcal{E} \to [0, 1]$ we let $T_1T_2(z, A) := \int T_1(z, dz')T_2(z', A)$ for all $A \in \mathcal{E}$ and for any probability measure $\nu$ on $(E, \mathcal{E})$ and $f \in \mathbb{R}^E$ measurable, we let $\nu(f) := \int f d\nu$, sometimes simplified to
\( \nu f \) when no ambiguity is possible and whenever this quantity exists. We denote \( T \) the associated operators acting on functions to the right as \( Tf(z) := \int f(z')T(z,dz') \) for \( z \in E \), and on measures to the left as \( \nu T(A) := \int_E \int_A \nu(dz')T(z,dz') \) for every \( A \in \mathcal{E} \). Let \( \mu \) be a probability distribution defined on some measurable space \((E, \mathcal{E})\). Whenever the following exist, for \( f, g : E \to \mathbb{R} \), we define \( \langle f, g \rangle_\mu := \int fgd\mu \), \( \|f\|_\mu := \left( \int f^2d\mu \right)^{1/2} \) and the Hilbert spaces

\[
L^2(\mu) := \{ f \in \mathbb{R}^E : \|f\|_\mu < \infty \},
\]

and \( L^2_1(\mu) := L^2(\mu) \cap \{ f \in \mathbb{R}^E : \mu(f) = 0 \} \). We let \( \|T\|_\mu := \sup_{\|f\|_\mu = 1} \|Tf\|_\mu \) and denote \( T^* \) the adjoint of \( T \), whenever it is well defined. For a set \( S \) we let \( S^c \) be its complement in the ambient space.

## 2 Discrete time scenario – general results

### 2.1 The notion of \((\mu, Q)\)-self-adjointness

Here we formalize the notion of \((\mu, Q)\)-self-adjointness, and discuss its consequences in the discrete time setting.

**Definition 2.1.** We call a linear operator \( Q : L^2(\mu) \to L^2(\mu) \) an isometric involution if

(a) \( \langle f, g \rangle_\mu = \langle Qf, Qg \rangle_\mu \) for all \( f, g \in L^2(\mu) \),

(b) \( Q^2 = \text{Id} \), the identity operator.

**Remark 2.2.** We note the simple properties

- \( Q \) is \( \mu \)-self-adjoint since \( \langle f, Qg \rangle_\mu = \langle Qf, Qg \rangle_\mu = \langle Qf, g \rangle_\mu \) for \( f, g \in L^2(\mu) \),
- the operators \( \Pi_+ := (\text{Id} + Q)/2 \) and \( \Pi_- := (\text{Id} - Q)/2 \) are \( \mu \)-self-adjoint projectors and for any \( f \in L^2(\mu) \), \( f = \Pi_+ f + \Pi_- f \), \( Q \Pi_+ f = \Pi_+ f \) and \( Q \Pi_- f = -\Pi_- f \).
- for \( \Pi \) an orthogonal projector, \( Q = \pm(\text{Id} - 2\Pi) \) is an isometric involution.

Again we will use the same symbol for the associated Markov kernel \( Q : E \times \mathcal{E} \to [0,1] \) and that \( \mu Q = \mu \).

The following establishes that there exists an involution \( \xi : E \to E \) such that for all \( f \in \mathbb{R}^E \) and \( z \in E \), \( Qf(z) = f \circ \xi(z) \).

**Lemma 2.3.** Let \( T : E \times \mathcal{E} \to [0,1] \) be a Markov transition probability such that for any \( z \in E \), \( T^2(z, \{z\}) = 1 \), then there exists an involution \( \tau : E \to E \) such that for \( z, z' \in E \), \( T(z, dz') = \delta_{\tau(z)}(dz') \).

**Proof.** Let \( z \in E \) and \( A_z := \{ z' \in E : T(z', \{z\}) = 1 \} \). From \( T^2(z, \{z\}) = \int T(z, dz')T(z', \{z\}) = 1 \) we deduce by contradiction that \( T(z, A_z) = 1 \). Assume there exists \( z_1', z_2' \in A_z \) such that \( z_1' \neq z_2' \). Then for \( i \in \{1,2\} \), \( T^2(z_i', \{z_i\}) = \int T(z_i', dz'')T(z_i'', \{z_i\}) = T(z, \{z_i\}) = 1 \), which is not possible if \( z_1' \neq z_2' \). Therefore \( A_z \) is a singleton, whose element we denote \( \tau(z) \) and \( T(z, dz') = \delta_{\tau(z)}(dz') \). The involution property is immediate.

**Definition 2.4.** We say a Markov operator \( P : L^2(\mu) \to L^2(\mu) \) is \((\mu, Q)\)-self-adjoint if there is an isometric involution \( Q \) such that for all \( f, g \in L^2(\mu) \)

\[
\langle Pf, g \rangle_\mu = \langle f, PQg \rangle_\mu.
\]

We will say that the corresponding kernel \( P : E \times \mathcal{E} \to [0,1] \) is \((\mu, Q)\)-reversible. When \( Q = \text{Id} \) we will simply say that \( P \) is \( \mu \)-self adjoint or \( \mu \)-reversible. The following is a simple but important characterisation of \((\mu, Q)\)-self-adjoint operators.
Proposition 2.5. If the Markov operator $P$ is $(\mu, Q)$--self-adjoint (resp. $\mu$--self-adjoint) then $QP$ and $PQ$ are $\mu$--self-adjoint (resp. $(\mu, Q)$--self-adjoint). As a result a $(\mu, Q)$--self-adjoint Markov operator is always the composition of two $\mu$--self-adjoint Markov operators.

Proof. Let $f, g \in L^2(\mu)$. Assume that $P$ is $\mu$--self-adjoint, then $\langle QPf, g \rangle_\mu = \langle Pf, Qg \rangle_\mu = \langle f, PQg \rangle_\mu = \langle f, QPQg \rangle_\mu$. Similar arguments establish that $PQ$ is $(\mu, Q)$--self-adjoint. Now assume that $P$ is $(\mu, Q)$--self-adjoint then $\langle QPf, g \rangle_\mu = \langle Pf, Qg \rangle_\mu = \langle f, PQg \rangle_\mu$. Similar arguments establish that $PQ$ is $\mu$--self-adjoint. The last point is straightforward since $P = Q(QP) = (PQ)Q$. \hfill \qed

Definition 2.6. For $P$ a $(\mu, Q)$--self-adjoint operator we call $QP$ and $PQ$ its reversible parts.

2.2 Ordering of asymptotic variances

For an homogeneous Markov chain $\{Z_0, Z_1, \ldots\}$ of transition kernel $P$ leaving $\mu$ invariant, started at equilibrium and any $\mu$--measurable $f : E \to \mathbb{R}$, we define the asymptotic variance

$$\text{var}(f, P) := \lim_{n \to \infty} n\text{var}\left(n^{-1}\sum_{i=0}^{n-1} f(Z_i)\right),$$

whenever the limit exists. This limit always exists, but may be infinite, when $P$ is $\mu$--reversible and $f \in L^2(\mu)$. Beyond this scenario general criteria exist \cite{caracciolo1992asymptotic, peskun1976optimal, tierney1994k}, and often require a bespoke analysis. A general question of interest is, given two Markov transition probabilities $P_1$ and $P_2$ leaving $\mu$ invariant, can one find a simple criterion to establish that for some function $f$, $\text{var}(f, P_1) \geq \text{var}(f, P_2)$ or $\text{var}(f, P_1) \leq \text{var}(f, P_2)$, whenever these quantities are well defined. When $P_1$ and $P_2$ are $\mu$--reversible a criterion based on Dirichlet forms leads to a particularly simple solution. Beyond this scenario little is known in general.

For $P$ and $f \in L^2(\mu)$, define the Dirichlet form

$$\mathcal{E}(f, P) := \langle f, (\text{Id} - P)f \rangle_\mu = \frac{1}{2} \int (f(z') - f(z))^2 \mu(dz)P(z, dz').$$

Note that this is $\|f\|_\mu^2 - \langle f, Pf \rangle_\mu$ where the last term is the first order auto-covariance coefficient for $f \in L^2_0(\mu)$. Let $\text{Gap}_R(P) := \inf_{f \in L^2_0(\mu), \|f\|_\mu \neq 0} \mathcal{E}(f, P)/\|f\|_\mu^2$.

Theorem 2.7 (Caracciolo et al. \cite{caracciolo1992asymptotic}, Tierney \cite{tierney1994k}). Let $\mu$ be a probability distribution on some measurable space $(E, \mathcal{E})$, and let $P_1$ and $P_2$ be two $\mu$--reversible Markov transition probabilities. If for any $g \in L^2(\mu)$, $\mathcal{E}(g, P_1) \geq \mathcal{E}(g, P_2)$, then for any $f \in L^2(\mu)$

$$\text{var}(f, P_1) \leq \text{var}(f, P_2) \text{ and } \text{Gap}_R(P_1) \geq \text{Gap}_R(P_2).$$

Corollary 2.8 (Peskun \cite{peskun1976optimal}). Whenever for any $z \in E$ and $A \in \mathcal{E}$ such that $P_1(z, A \cap \{z\}^c) \geq P_2(z, A \cap \{z\}^c)$ then for any $f \in L^2(\mu)$,

$$\text{var}(f, P_1) \leq \text{var}(f, P_2) \text{ and } \text{Gap}_R(P_1) \geq \text{Gap}_R(P_2).$$

Our main result is that these conclusions extend in part to $(\mu, Q)$--reversible transitions. In order to ensure the existence of the quantities we consider, for any $\lambda \in [0, 1)$ we introduce the $\lambda$--asymptotic variance, defined for any $f \in L^2(\mu)$, with $\bar{f} := f - \mu(f)$, as

$$\text{var}_{\lambda}(f, P) := \|\bar{f}\|_\mu^2 + 2 \sum_{k \geq 1} \lambda^k \langle \bar{f}, P^k \bar{f} \rangle_\mu = 2\langle \bar{f}, [\text{Id} - \lambda P]^{-1} \bar{f} \rangle_\mu - \|\bar{f}\|_\mu^2.$$
Whether \( \lim_{\lambda \to 1} \var_{\lambda}(f, P) = \var(f, P) \) when the latter exists is problem specific and not addressed here, but we note that this is always true in the reversible scenario and that a general sufficient condition is that 
\[ \sum_{k \geq 1} \| \langle f, P^k f \rangle_{\mu} \| < \infty. \] Rather we focus on ordering \( \var_{\lambda}(P_1, f) \) and \( \var_{\lambda}(P_2, f) \) for \( \lambda \in [0, 1) \) and leave the convergence to the asymptotic variances as a separate problem.

**Theorem 2.9.** Let \( \mu \) be a probability distribution on some measurable space \( (E, \mathcal{E}) \), and let \( P_1 \) and \( P_2 \) be two \((\mu, Q)\)–reversible Markov transition probabilities. Assume that for any \( g \in L^2(\mu) \), \( \mathcal{E}(g, QP_1) \geq \mathcal{E}(g, QP_2) \), or for any \( g \in L^2(\mu) \), \( \mathcal{E}(g, P_1Q) \geq \mathcal{E}(g, P_2Q) \). Then for any \( \lambda \in [0, 1) \) and \( f \in L^2(\mu) \)

(a) satisfying \( Qf = f \) it holds that \( \var_{\lambda}(f, P_1) \leq \var_{\lambda}(f, P_2) \),

(b) satisfying \( Qf = -f \) it holds that \( \var_{\lambda}(f, P_1) \geq \var_{\lambda}(f, P_2) \).

**Corollary 2.10.** If \( P_1 \) and \( P_2 \) are such that for every \( z \in E \) and every \( A \in \mathcal{E} \) it holds that \( P_1Q(z, A \cap \{z\}^c) \geq P_2Q(z, A \cap \{z\}^c) \), or \( QP_1(z, A \cap \{z\}^c) \geq QP_2(z, A \cap \{z\}^c) \), then the conclusion of Theorem 2.9 holds.

**Proof of Theorem 2.9.** To compare \( P_1 \) and \( P_2 \) we follow the approach of [35], by introducing the mixture kernel \( P(\beta) = \beta P_1 + (1 - \beta)P_2 \) for \( \beta \in [0, 1] \) and establishing that the right derivative \( \partial_\beta \var_{\lambda}(f, P(\beta)) \) is of constant sign for \( \beta \in [0, 1) \). Using the representation \( \var_{\lambda}(f, P(\beta)) = 2\langle f, [\Id - \lambda P(\beta)]^{-1} f' \rangle_{\mu} - \| f \|_{\mu}^2 \) we have

\[
\partial_\beta \var_{\lambda}(f, P(\beta)) = 2\lambda \langle f, [\Id - \lambda P(\beta)]^{-1} (P_1 - P_2) [\Id - \lambda P(\beta)]^{-1} f' \rangle_{\mu},
\]

which is justified in detail in [3, Lemma 51]. Let \( P \) be \((\mu, Q)\)–self-adjoint, then for \( f, g \in L^2(\mu) \),

\[
\langle f, [\Id - \lambda P]^{-1} g \rangle_{\mu} = \sum_{k=0}^{\infty} \lambda^k \langle (QPQ)^k f, g \rangle_{\mu} = \sum_{k=0}^{\infty} \lambda^k \var_{\lambda}(f, P(\beta)) = \langle Q [\Id - \lambda P]^{-1} Qf, g \rangle_{\mu}.
\]

Noting that \( P(\beta) \) is \((\mu, Q)\)–self-adjoint, the above leads to

\[
\partial_\beta \var_{\lambda}(f, P(\beta)) = \lambda \var_{\lambda}(f, (P_1 - P_2) [\Id - \lambda P(\beta)]^{-1} f)_{\mu}.
\]

Set

\[
g := [\Id - \lambda P(\beta)]^{-1} f,
\]

then from the assumptions \( Qf = \pm f \) and on the Dirichlet forms, we deduce that

\[
\partial_\beta \var_{\lambda}(f, P(\beta)) = \pm \lambda \langle Qg, (P_1 - P_2) g \rangle_{\mu} = \pm \lambda \langle g, (\Id - QP_1) g \rangle_{\mu} \leq 0.
\]

Noting that \( \langle Qg, (P_1 - P_2) g \rangle_{\mu} = \langle Qg, (P_1 - P_2) Qg \rangle_{\mu} \) and that \( Q : L^2(\mu) \to L^2(\mu) \) is a bijection we conclude.

**Remark 2.11.** We note that in contrast with the reversible scenario the result never provides us with information about the speed of convergence to equilibrium. The practical guideline resulting from the theorem is that after “burn-in” an algorithm should be tuned to maximize or minimize \( \mathcal{E}(g, QP) \) or \( \mathcal{E}(g, PQ) \) for all \( g \in L^2(\mu) \).
Remark 2.12. From the proof it can be seen that ordering \( \text{var}_\lambda(f, P_1) \) and \( \text{var}_\lambda(f, P_2) \) for a specific \( f \in L^2(\mu) \) such that \( Qf = f \), only requires ordering Dirichlet forms for a particular subset of \( L^2(\mu) \), namely the \( \lambda \)-solutions of the Poisson equation (5). Although these quantities are generally intractable, in some scenarios their structure may be exploited to order the Dirichlet forms involved. Such ideas have been extensively used in the reversible scenario, for example in [3, 4] and we provide an example in the \((\mu, Q)\)-self-adjoint setup in Subsection 3.1. Another consequence of this is that strict inequalities can be obtained when the Dirichlet forms are strictly ordered for nonconstant functions and these \( \lambda \)-solutions are nonconstant.

Remark 2.13. More quantitative versions of this result, in the spirit of [13] can also be replicated using ideas of [33]. For \( \alpha \in (0, 1] \) consider the \((\mu, Q)\)-reversible transition \( P_1^\alpha := (1 - \alpha)I + \alpha P_1 \), notice that for \( f \in L^2(\mu), \langle \bar{f}, [\text{Id} - \lambda P_1^\alpha]^{-1} \bar{f} \rangle_\mu = \alpha^{-1} \langle \bar{f}, [\text{Id} - \lambda P_1]^{-1} \bar{f} \rangle_\mu \) and for \( g \in L^2(\mu) \)

\[
\langle g, [QP_2 - QP_1^\alpha]g \rangle_\mu = \alpha \langle g, (\text{Id} - QP_1^\alpha)g \rangle_\mu - \langle g, (\text{Id} - QP_2)g \rangle_\mu + (1 - \alpha)\langle g, (\text{Id} - Q)g \rangle_\mu.
\]

Therefore if for all \( g \in L^2(\mu), \langle g, (\text{Id} - QP_1^\alpha)g \rangle_\mu \geq \alpha^{-1} \langle g, (\text{Id} - QP_2)g \rangle_\mu \) then if in addition \( f = Qf \),

\[
\alpha^{-1} \langle \bar{f}, [\text{Id} - \lambda P_1]^{-1} \bar{f} \rangle_\mu \leq \langle \bar{f}, [\text{Id} - \lambda P_2]^{-1} \bar{f} \rangle_\mu,
\]

that is \( \text{var}_\lambda(f, P_1) \leq (1 - \alpha)\|\bar{f}\|_\mu^2 + \alpha \text{var}_\lambda(f, P_2) \).

3 Discrete time scenario: examples

The notion of \((\mu, Q)\)-reversibility, often described in terms of modified or skewed detailed balance, is known to hold for numerous processes of interest but its implications, beyond establishing that the corresponding Markov chain leaves \( \mu \) invariant, are to the best of our knowledge unknown. In this section we show that our framework contributes to filling this gap and revisit a wide range of simple, some foundational, questions. In some scenarios \((\mu, Q)\)-reversibility is not immediately apparent for a specific problem and we present basic strategies to remedy this. More complex examples are possible, such as extension of [3, 4] or [1], for example, but beyond the scope of this paper.

3.1 Links to 2-cycle based MCMC kernels

Recently [37], have shown that results for ordering of asymptotic variances of reversible time homogeneous Markov chains can be extended to certain inhomogeneous Markov chains arising naturally in the context of MCMC algorithms. Such chains are obtained by cycling between two reversible MCMC kernels, and it is a natural question to ask whether improving either of the kernels in terms of individual Dirichlet forms improves performance of the inhomogeneous chain resulting from their combination. Theorem 3.1 below provides us with a simple and practical characterization. We show that this result is in some sense dual to \((\mu, Q)\)-reversibility and provide a generalization which makes previously intractable analysis of some algorithms possible. For \( \pi \) a probability distribution on some space \((X, \mathcal{X})\), \( P_1 \) and \( P_2 \) two \( \pi \)-invariant Markov transitions and \( f \in L^2(\pi) \), we extend the definition of \( \lambda \)-asymptotic variance, for \( \lambda \in [0, 1) \) to the inhomogeneous scenario

\[
\text{var}_\lambda(f, \{P_1, P_2\}) := \sum_{k \geq 0} \lambda^{2k} \langle \bar{f}, (P_1 P_2)^k (\text{Id} + \lambda P_1) \bar{f} \rangle_\pi + \lambda^{2k} \langle \bar{f}, (P_2 P_1)^k (\text{Id} + \lambda P_2) \bar{f} \rangle_\pi - \| \bar{f} \|_\pi^2,
\]

where \( \bar{f} := f - \pi(f) \), which is well defined since for any \( g \in L^2(\pi) \) \( \|P_1 g\|_\pi \leq \|g\|_\pi \) and \( \|P_2 g\|_\pi \leq \|g\|_\pi \). Under additional assumptions (see for example [37, Proposition 9]) the following limits exist and satisfy

\[
\lim_{\lambda \uparrow 1} \text{var}_\lambda(f, \{P_1, P_2\}) = \lim_{n \to \infty} n \text{var} \left( n^{-1} \sum_{i=0}^{n-1} f(X_i) \right),
\]

6
where here \( \{X_0, X_1, \ldots \} \) is the time inhomogeneous Markov chain obtained by cycling through \( P_1 \) and \( P_2 \) and of initial distribution \( \pi \), that is for \( A \in \mathcal{X}^* \), \( \mathbb{P}(X_k \in A \mid X_0, \ldots, X_{k-1}) = P_{2-(k \mod 2)}(X_{k-1}, A) \) for \( k \geq 1 \) and \( X_0 \sim \pi \). The following is a reformulation of [37, Theorem 4 and Lemma 25] combined with a generalization of [37, Lemma 18].

**Theorem 3.1** (see [37, Theorem 4 and Lemma 25]). Let \( \pi \) be a probability distribution defined on \( (X, \mathcal{X}) \). For \( i, j \in \{1, 2\} \), let \( P_{i,j} : X \times \mathcal{X} \to [0, 1] \) be \( \pi \)-reversible Markov kernels such that for all \( g \in L^2(\pi) \) and \( i \in \{1, 2\} \) we have \( \mathcal{E}(g, P_{i,i}) \geq \mathcal{E}(g, P_{2,i}) \). Then for any \( f \in L^2(\pi) \) and \( \lambda \in [0,1) \)

\[
\var\lambda(f, \{P_{1,1}, P_{1,2}\}) \leq \var\lambda(f, \{P_{2,1}, P_{2,2}\}).
\]

Further, if \( f \in L^2(\pi) \) is such that \( P_{i,1}f = f \) (or \( P_{i,2}f = f \)) for \( i \in \{1,2\} \), then

\[
\var\lambda(f, \{P_{1,1}, P_{1,2}\}) \leq \var\lambda(f, \{P_{2,1}, P_{2,2}\}).
\]

**Corollary 3.2.** Let \( Q \) be an isometric involution and \( P_1 \) and \( P_2 \) be \( \pi \)-reversible. Note that for \( i \in \{1, 2\} \), \( P_i = Q(P_i) \) (resp. \( P_i = (P_i)Q \)) and that both \( P_{i,1} := Q \) (resp. \( P_{i,1} := P_i \)) and \( P_{i,2} := QP_i \) (resp. \( P_{i,2} := QP_i \)) are \( \pi \)-self-adjoint by Proposition 2.5. We can therefore apply Theorem 3.1 and the conclusion of Theorem 2.9 holds for \( f \in L^2(\pi) \) such that \( Qf = \pm f \).

Conversely one can show using a very simple argument that the first statement of Theorem 3.1 is a direct consequence of \((\mu, Q)\)-reversibility of a particular time homogeneous chain, where time is now part of the state, for a particular isometric involution. Apart from linking two seemingly unrelated ideas, an interest of the proof is that it highlights the difficulty with extending the results to \( m \)-cycles with \( m \geq 3 \).

**Proof of Theorem 3.1.** Here we let \( E = X \times V \) with \( V := \{1, 2\} \times \{-1, 1\} \), let \( v = (v_1, v_2) \in V \) and consider the target distribution \( \mu(\mathrm{d}(x,v)) = \pi(\mathrm{d}x)/4\mathbb{1}\{v \in V\} \). For \( i \in \{1, 2\} \) we define the Markov transition probabilities

\[ P_i(x, v; \mathrm{d}(y, w)) = P_{i,v_i}(x, \mathrm{d}y)\mathbb{1}\{v_1 = v_1 \oplus v_2, w_2 = v_2\}, \]

where \( 1 \oplus (+1) = 2 \) and \( 2 \oplus (+1) = 1 \), and \( Q(x, v; \mathrm{d}(y, w)) = \delta_x(\mathrm{d}y)\mathbb{1}\{v_1 = v_1 \oplus v_2, w_2 = -v_2\} \) whose corresponding operator is \( \mu \)-isometric and involutive. Notice that for \( f \in L^2(\mu) \) \( i \in \{1, 2\} \) and \( (x,v) \in E \),

\[ QP_i f(x,v) = P_i f(x, (v_1 \oplus v_2, -v_2)) = P_{i,v_1 \oplus v_2} f_{(v_1, -v_2)}(x), \]

with \( x \mapsto f_i(x) := f(x,v) \) and therefore

\[
\langle QP_i f, g \rangle_\mu = \frac{1}{4} \sum_{v \in V} \langle P_{i,v_1 \oplus v_2} f_{(v_1, -v_2)}, g_{(v_1, v_2)} \rangle_\pi = \frac{1}{4} \sum_{v \in V} \langle f_{(v_1, -v_2)}, P_{i,v_1 \oplus v_2} g_{(v_1, v_2)} \rangle_\pi = \frac{1}{4} \sum_{v \in V} \langle f_{(v_1, v_2)}, P_{i,v_1 \oplus v_2} g_{(v_1, v_2)} \rangle_\pi = \langle f, QP_i g \rangle_\mu, \tag{6} \]

where we have used that for \( v \in V \), \( P_{i,v_1 \oplus v_2} \) is \( \pi \)-self-adjoint and the property that \( v_1 \oplus (-v_2) = v_1 \oplus v_2 \). From Proposition 2.5 \( P_i \) is \((\mu, Q)\)-self-adjoint and we now follow the proof of Theorem 2.9 and its notation. For \( \beta \in [0,1) \), from (4) and (6) we deduce that for any \( f \in L^2(\pi) \), with \( (x,v) \mapsto \hat{f}(x,v) := f(x) \) (which satisfies \( Q\hat{f} = \hat{f} \)),

\[
\delta_\beta \var\lambda(\hat{f}, P(\beta)) = \frac{1}{4} \sum_{v \in V} \langle (P_{i,v_1 \oplus v_2} - P_{i,v_1 \oplus v_2}) g_{(v_1, -v_2)}(\beta), g_{(v_1, v_2)}(\beta) \rangle_\pi, \]

7
where
\[ g(\beta)(x,v) = \left[ \text{Id} - \lambda P(\beta) \right]^{-1} \bar{f}(x,v) = \sum_{k \geq 0} \lambda^{2k} (P_{v_1} P_{v_2},\bar{f}(x_1)) + \lambda^{2k+1} (P_{v_1} P_{v_2},\bar{f}(x)). \]

By noting that \( g(v_1, v_2)(\beta) = g(v_1, v_2) \) since \( v_1 \oplus (-v_2) = v_1 \oplus v_2 \) we deduce \( c(\beta \varLambda(\bar{f}, P(\beta)) \geq 0 \) and \( \varLambda(f, P_{1}) \leq \varLambda(f, P_{2}) \). The first claim follows from the fact that \( \varLambda(f, P_{1}) = \varLambda(f, \{P_{1}, P_{2}\}) \) for \( i \in \{1, 2\} \). The second statement is immediate once we establish that for \( f \in L^2(\pi) \) such that \( P_{1} f = f \) for \( i \in \{1, 2\} \), then
\[ \varLambda(f, \{P_{1}, P_{2}\}) = \frac{2 + \lambda + \lambda^{-1}}{2} \varLambda(f, P_{1} P_{2}) + \frac{\lambda - \lambda^{-1}}{2} \|\bar{f}\|^2. \]

Notice that
\[
\sum_{k \geq 0} \lambda^{2k} \langle \bar{f}, (P_{1} P_{2})^{k}\rangle x = \|\bar{f}\|^2 + (1 + \lambda^{-1}) \sum_{k \geq 0} \lambda^{2k} \langle \bar{f}, (P_{1} P_{2})^{k}\rangle x,
\]
and from the definition of \( \varLambda(f, \{P_{1}, P_{2}\}) \) and the fact that for \( i \in \{1, 2\} \) and \( k \geq 1 \)
\[ \langle \bar{f}, (P_{1} P_{2})^{k}\rangle x = \langle \bar{f}, (P_{1} P_{2})^{k}\rangle x, \]
we conclude. When \( P_{i} f = f \) for \( i \in \{1, 2\} \) the result follows from the case above and the symmetry \( \varLambda(f, \{P_{1}, P_{2}\}) = \varLambda(f, \{P_{2}, P_{1}\}) \).

**Remark 3.3.** Note that the instrumental Markov chains introduced in the proof are never ergodic, but can be marginally. It is possible to revisit this proof for \( m \)-cycles and \( m \geq 3 \), but the property \( v_1 \oplus (-v_2) = v_1 \oplus v_2 \) fails in this scenario, in general, and it is not possible to conclude.

Theorem 3.4 below extends Theorem 3.1 to 2-cycles of \( (\mu, Q) \)-reversible Markov kernels–applications of this result are given in Subsection 3.2.

**Theorem 3.4.** Let \( \pi \) be a probability distribution defined on some probability space \( (X, \mathcal{F}) \). For \( i,j \in \{1, 2\} \), let \( P_{i,j} : X \times \mathcal{F} \rightarrow [0, 1] \) be \( (\mu, Q) \)-reversible Markov kernels for some isometric involution \( Q \), and such that for all \( \pi \in \{1, 2\} \) we have \( E(g, Q P_{1,j}) \geq E(g, Q P_{2,i}) \) for all \( g \in L^2(\pi) \), or \( E(g, P_{1,i}) \geq E(g, P_{2,i}) \) for all \( g \in L^2(\pi) \). Then for any \( f \in L^2(\pi) \) such that \( Q f = f \) and \( \lambda \in [0, 1] \)
\[ \varLambda(f, \{P_{1}, P_{2}\}) \leq \varLambda(f, \{P_{2}, P_{1}\}). \]

Further, if \( f \in L^2(\pi) \) is such that \( P_{1,j} f = f \) (or \( P_{2,j} f = f \) for \( i \in \{1, 2\} \)), then
\[ \varLambda(f, P_{1,j} P_{2}) \leq \varLambda(f, P_{2,j} P_{2}). \]

**Proof.** Notice that for \( f = Q f \in L^2(\pi) \) we have \( \varLambda(f, \{P_{1}, P_{2}\}) = \varLambda(f, \{P_{1}, Q P_{2}\}) \) since
\[
\sum_{k \geq 0} \lambda^{2k} \langle \bar{f}, (P_{1} Q P_{2})^{k}\rangle x = \sum_{k \geq 0} \lambda^{2k} \langle \bar{f}, (P_{1} Q P_{2})^{k}\rangle x,
\]
and for \( k \geq 0 \), \( (Q P_{1} Q P_{2})^{k} = (P_{1} Q P_{2})^{k} \), \( Q \) is an isometry, \( Q^2 = \text{Id} \) and \( Q \bar{f} = \bar{f} \). From Proposition 2.5
\[ P_{1} Q \text{ and } Q P_{2} \text{ are } \mu \text{-self-adjoint and we conclude with Theorem 3.1.} \]
Similarly one establishes that for \( f = Q f \in L^2(\pi) \) we have \( \varLambda(f, \{P_{1}, P_{2}\}) = \varLambda(f, \{Q P_{1}, P_{2} Q\}) \) and conclude in a similar way. \( \square \)
### 3.2 Construction of Markov kernels from time-reversible flows

A generic way to construct \((\mu, Q)\)-reversible Markov transition probability consists of the following slight generalization of [30, 22]. For a probability distribution \(m\) on \((E, \mathcal{E})\) and measurable mapping \(\psi : E \to E\) we let for any \(A \in \mathcal{E}, m^\psi(A) := m(\psi^{-1}(A))\). The presentation parallels that of [55, Section 2, second example] in order to avoid specificities concerned with densities and, for example, the presence of Jacobians.

**Proposition 3.5.** Let \(\mu\) be a probability distribution on \((E, \mathcal{E})\),

\[(a) \ \psi : E \to E\) is a bijection such that \(\psi^{-1} = \xi \circ \psi \circ \xi\) for \(\xi : E \to E\) corresponding to an isometric involution \(Q\),

\[(b) \ \phi : \mathbb{R}_+ \to [0, 1]\) such that \(r(\phi(r^{-1}) = \phi(r)\) for \(r > 0\) and \(\phi(0) = 0\),

\[(c) \ \text{define for } z \in E,

\[r(z) := \begin{cases} \frac{d\mu_{z \circ \psi}}{d\mu(z)} & \text{if } d\mu_{z \circ \psi}/d\mu(z) > 0 \text{ and } d\mu/d\mu(z) > 0, \\ 0 & \text{otherwise.} \end{cases}\]

where \(\nu := \mu + \mu_{z \circ \psi}\)

then

\[P(z, dz') := \phi \circ r(z)\delta_{z}(dz') + \delta_{\xi(z)}(dz')[1 - \phi \circ r(z)],\]

is \((\mu, Q)\)-reversible.

**Proof.** This can be checked directly, but we instead check that \(PQ\) is \(\mu\)-self-adjoint and conclude with Proposition 2.5. For any measurable and bounded \(f \in \mathbb{R}^E\),

\[PQf(z) = \phi \circ r(z) (Qf) \circ \psi(z) + [1 - \phi \circ r(z)](Qf) \circ \xi(z) = \phi \circ r(z) f \circ \xi \circ \psi(z) + [1 - \phi \circ r(z)] f(z).\]

The property on \(\psi\) implies that \(\xi \circ \psi \circ \xi \circ \psi = \text{Id}\), that is \(\xi \circ \psi\) is an involution and hence \(PQ\) is \(\mu\)-reversible from [55, Section 2, second example]. From Proposition 2.5 \(P\) is \((\mu, Q)\)-self-adjoint.

**Example 3.6.** Assume \(E = \mathbb{X} \times \mathbb{V}\) and for \((x, v) \in E\) and \(f \in \mathbb{R}^E\) let \(Qf(x, v) := f(x, -v)\). Then for any \(t \in \mathbb{R}\), \(\psi_t(x, v) = (x + tv, v)\) satisfies \(\psi_t^{-1} = \xi \circ \psi_t \circ \xi\) and was considered in [27] to define the Guided Random Walk Metropolis. More general examples satisfying this condition include \(\psi_t(x, v) = \psi_{\frac{t}{2}} \circ \psi_{\frac{t}{2}} (x, v)\) where \(\psi_t^A(x, v) := (x + t\nabla_x H(x, v), v)\) and \(\psi_t^B(x, v) := (x, v - t\nabla_x H(x, v))\) for a separable Hamiltonian \(H : E \to \mathbb{R}\). This is the Störmer–Verlet scheme considered in [30] to define the Hybrid Monte Carlo algorithm in the situation where \(H := -\log d\mu/d\mu_{\text{Lab}}\) is well defined and separable. More generally dynamical systems with the time reversal symmetry (e.g. [32] and also [21, Lemma 3.14]) provide ways of constructing such mappings (see also [47, 43, 54, 12, 42] and [22]).

**Example 3.7.** Choices of \(\phi(r)\) in Proposition 3.5 include \(\phi(r) = \min\{1, r\}\), which leads to the standard Metropolis-Hastings acceptance probability, or \(\phi(r) = r/(1 + r)\) which corresponds to Barker’s dynamic. It is well known that for any \(\phi\) satisfying Proposition 3.5-(b) one has \(\phi(r) \leq \min\{1, r\}\) and that for Barker’s choice \(\min\{1, r\} \leq \phi(r)\).
In order to be useful in practice a Markov transition of the type given in (7) must be combined with another transition in order to lead to an ergodic Markov chain [27, 30]. We focus here on 2–cycles of $(\mu, Q)$–reversible Markov transitions.

**Theorem 3.8.** Let $\mu$ be a probability distribution on $(E, \mathcal{E})$ and let $\psi$ satisfy Proposition 3.5-(a) for some isometric involution $Q$. Further for $i \in \{1, 2\}$, let $P_{i,2}$ be as in (7) for a mapping $\psi_i = \psi$ and some mapping $\phi_i$ satisfying Proposition 3.5-(b) and let $P_{1,1} = P_{2,2}$ be a $(\mu, Q)$–reversible Markov transition. Assume that $\phi_1 \geq \phi_2$, then for any $f \in L^2(\mu)$ such that $Qf = f$ and $\lambda \in [0,1)$ we have

$$\text{var}_\lambda(f, \{P_{1,1}, P_{2,2}\}) \leq \text{var}_\lambda(f, \{P_{2,1}, P_{2,2}\}).$$

In particular $\phi(r) = \min\{1, r\}$ achieves the smallest $\lambda$–asymptotic variance.

**Proof.** The expression in (3) leads to

$$\mathcal{E}(g, P_{i,2}Q) = \frac{1}{2} \int \phi_i \circ r(z)(g \circ \xi(z) - g(z))^2 \mu(dz),$$

for $i \in \{1, 2\}$ and we conclude with Theorem 3.4. \hfill $\Box$

**Example 3.9 (Example 3.6 (cd)).** Assume here for presentational simplicity that $X = V = \mathbb{R}$ that $\mu$ has a density with respect to the Lebesgue measure and $\mu(x, v) = \pi(x)\varpi(v)$ where $\varpi$ is a $\mathcal{N}(0, \sigma^2)$ for some $\sigma^2 > 0$. In this setup a popular choice [18] for $P_{1,1} = P_{2,2}$ is a momentum refreshment of the type, for some $\omega \in (0, \pi/2]$,

$$R_\omega((x, v); d(y, w)) = \int \delta_{(x,v \cos \omega + w \sin \omega)}(d(y, w))\varpi(d\omega').$$

Lemma 3.10 below establishes that the corresponding operator is $(\mu, Q)$–self-adjoint. We can therefore apply Theorem 3.8 and deduce, for example, that the choice $\phi(r) = \min\{1, r\}$ for all $\omega \in (0, \pi/2]$ is optimum. Further since $R_\omega(x,v; \{x\} < V) = 1$ we note that the second statement of Theorem 3.1 holds, a result partially known for $\omega = \pi/2$ since in this case for $i \in \{1, 2\}$ $P_{i,1}P_{i,2}$ is $\mu$–reversible and Theorem 2.7 can be applied.

**Lemma 3.10.** For any $\omega \in (0, \pi/2]$, $R_\omega$ is $(\mu, Q)$–self-adjoint for $Q$ such that $Qf(x, v) = f(x, -v)$ for $f \in \mathbb{R}^E$.

**Proof.** Let $f, g \in L^2(\mu)$. Note that for $x \in X$,

$$\int f(x,v)QR_\omega Qg(x,v)\varpi(dv) = \int f(x,v)R_\omega Qg(x,-v)\varpi(dv) = \int f(x,v)Qg(x,-v\cos \omega + w\sin \omega)\varpi(dv)\varpi(dw)$$

$$= \int f(x,v)g(x,v\cos \omega - w\sin \omega)\varpi(dv)\varpi(dw)$$

$$= \int f(x,v')\varpi(dv')\varpi(dw)\varpi'(d\omega'),$$

where on the last line we have used the change of variable $(v', \omega') = (v \cos \omega - w \sin \omega, v \sin \omega + w \cos \omega)$ and the fact that $\varpi \otimes \varpi$ is invariant by rotation. We therefore deduce that $\langle f, QR_\omega Qg \rangle_\mu = \langle R_\omega f, g \rangle_\mu$ and conclude. \hfill $\Box$

Another application of the results above is the extra chance HMC method presented in [12], equivalent to the ideas of [54], which can be seen as an extension to Horowitz’s scheme [30]. Using the notation of Proposition 3.5 the main idea is to define a variation of (7) where transitions to $\xi \circ \psi(x,v), \xi \circ \psi \circ \psi(x,v), \ldots$ are attempted in sequence until success.
Example 3.11. Here $X = \mathbb{R}$ for simplicity and $\mu(dx, v) = \pi(dv)\varpi(dv)$ where $\varpi(dv)$ is a $\mathcal{N}(0, \sigma^2)$. With $Qf(x, v) = f(x, -v)$ for $f \in \mathbb{R}^E$ and $\psi$ as in Proposition 3.5-(a) we let $\psi^0 = \text{Id}$ and $\psi^k = \psi \circ \psi^{k-1}$ for $k \in \mathbb{N}\setminus\{0\}$. Define for $K \in \mathbb{N}\setminus\{0\}$,

$$
P_K((x, v); d(y, w)) := \sum_{k=1}^{K} \beta_k(x, v)\delta_{\psi^k(x, v)}(d(y, w)) + \rho_K(x, v)\delta_{\xi(x, v)}(d(y, w)),
$$

where, with $\alpha_0(x, v) = 0$ and for $k = 1, \ldots, K$ $\alpha_k(x, v) = \max\{\alpha_{k-1}(x, v), \min\{1, r_k(x, v)\}\}$, with

$$
r_k(x, v) := \begin{cases} 
\frac{d\mu^{\xi \circ \psi^k}(dx, dv)}{d\mu(dx)dv} & \text{if } d\mu^{\xi \circ \psi^k}/d\nu_k(z) > 0 \text{ and } d\mu/d\nu_k(z) > 0, \\
0 & \text{otherwise},
\end{cases}
$$

and $\nu_k := \mu + \mu^{\xi \circ \psi^k}$, $\beta_k(x, v) = \alpha_k(x, v) - \alpha_{k-1}(x, v)$ and $\rho_K(x, v) := 1 - \sum_{k=1}^{K} \beta_k(x, v)$. It is shown in [12, Appendix A] that this update is $(\mu, Q)$-reversible, while it is pointed out that for $\omega \in (0, \pi/2]$, $R_\omega P_K$ is not. We can apply Theorem 3.4 to deduce that for any $f \in L^2(\mu)$ such that $Qf = f$ and any $\omega \in (0, \pi/2]$, the mapping $K \mapsto \var{\lambda(f, \{R_\omega, P_K\})}$ is non increasing, since from Lemma 3.12 below, $K \mapsto \mathcal{E}(g, P_K)$ is nondecreasing. In fact, since $R_\omega(x, v; \{x\} \times V) = 1$, for $f \in L^2(\pi)$ and $\bar{f}(x, v) := f(x)$ for $(x, v) \in E$, we also deduce that $K \mapsto \var{\lambda(\bar{f}, R_\omega P_K)}$ is nonincreasing.

Lemma 3.12. For any $g \in L^2(\mu)$, $K \mapsto \mathcal{E}(g, P_K)$ is non-decreasing.

Proof. For $g \in L^2(\mu)$, we have from (3.1)

$$
\mathcal{E}(g, P_K) = \frac{1}{2} \int \mu(dx, v) P_K\{ (x, v); d(y, w)\} [g(x, v) - g(y, w)]^2 = \frac{1}{2} \sum_{k=1}^{K} \int \mu(dx, v) \beta_k(x, v) [g(x, v) - g \circ \xi \circ \psi^k(x, v)]^2.
$$

The result follows. 

Remark 3.13. As pointed out by [12] the rational behind the approach is that for $(x, v) \in E$, $k \mapsto H \circ \xi \circ \psi^k(x, v)$ typically fluctuates around $H(x, v)$. As a result if there exist $(x_0, v_0) \in E$ and $k_0 \in \mathbb{N}_\alpha$ such that $\min_{1 \leq k \leq k_0} H \circ \xi \circ \psi^k(x_0, v_0) > \max \{H(x_0, v_0), H \circ \xi \circ \psi^{k_0+1}(x_0, v_0)\}$ and, for example, $(x, v) \mapsto H \circ \xi \circ \psi^{k_0+1}(x, v)$ is continuous in a neighbourhood of $(x_0, v_0)$ then $\mu\{H_{k_0+1}(X, V) > 0\} > 0$ and $\mathcal{E}(g, P_{k_0+1}) - \mathcal{E}(g, P_k) > 0$ for $L^2(\mu) \ni g \neq g \circ \xi \circ \psi^{k_0+1}$ on the aforementioned neighbourhood, suggesting that the strict performance improvement observed numerically in [12] for specific functions holds more generally. A more precise investigation of this point is far beyond the scope of the present work.

It is natural to try to assess the impact of $\omega \in (0, \pi/2]$ involved in the definition of $R_\omega$ on the performance of the type of algorithms presented in this section. In particular, a long-standing question is whether partial momentum refreshment is preferable to full refreshment, meaning replacing $R_\omega$ by $R_{\pi/2}$. Application of Theorem 3.4 requires establishing that $\langle y, Q(R_{\pi/2} - R_\omega)g \rangle$ does not change sign for all $g \in L^2(\mu)$. This, however, is not the case. For example, setting $g_1(x, v) := v$ then the quantity is positive but for $g_2(x, v) := v^2$ it is negative and we cannot conclude.

11
3.3 Lifted MCMC algorithms

Assume we are interested in sampling from $\pi$ defined on $(X, \mathcal{X})$ and are given two sub-stochastic kernels $T_1$ and $T_{-1}$ such that for $x, y \in X$ the following “skewed” detailed balance holds,

$$\pi(dx)T_1(x, dy) = \pi(dy)T_{-1}(y, dx). \quad (8)$$

A generic example, related to the Metropolis-Hastings algorithm is as follows.

**Example 3.14.** Let $\{q_1(x, \cdot), x \in X\}$ and $\{q_{-1}(x, \cdot), x \in X\}$ be two families of probability distributions on $(X, \mathcal{X})$, then the kernel defined for $v \in \{-1, 1\}$ and $x, y \in X$ as

$$T_v(x, dy) = \min \{1, r_v(x, y)\} q_v(x, dy) \text{ with } r_v(x, y) := \left\{ \begin{array}{ll} \frac{\gamma_v(dy)/q_v(y, x)}{\gamma_v(dx)/q_v(x, y)} & \text{if } \gamma_v(dy)/q_v(y, x) \times \gamma_v(dx)/q_v(x, y) > 0, \\
0 & \text{otherwise,} \end{array} \right.$$ 

where $\gamma_v(d(x, y)) := \pi(dx)q_v(x, dy)$ and $\nu(d(x, y)) := \gamma_v(d(x, y)) + \gamma_{-v}(d(y, x))$.

A standard way of constructing a $\pi$–reversible Markov transition probability based on the above sub-kernels consists of the following

$$P(x, dy) = \frac{1}{2} T_1(x, dy) + \frac{1}{2} T_{-1}(x, dy) + \delta_x(dy) \left( 1 - \frac{1}{2} T_1(x, X) - \frac{1}{2} T_{-1}(x, X) \right). \quad (9)$$

The standard Metropolis-Hastings algorithm corresponds to the scenario where $T_1 = T_{-1}$. The aim of the lifting is to stratify the choice between $T_1$ and $T_{-1}$ by embedding the sampling problem into that of sampling from $\mu(dx)\mathcal{X}(v) = \frac{1}{2} \pi(dx)\mathcal{X}\{v \in \{-1, 1\}\}$ and using a Markov kernel defined on the corresponding extended space $E = X \times \{-1, 1\}$ which promotes contiguous uses of $T_1$ or $T_{-1}$ along the iterations. As shown in [56, 58] one possible solution, which imposes $P_{\text{lifted}}((x, v); (A \backslash \{x\}) \times \{v\}) = 0$ for any $A \in \mathcal{X}$, is

$$P_{\text{lifted}}((x, v); d(y, w)) = \mathcal{I}(w = v) \left[ T_v(x, dy) + \delta_x(dy)(1 - T_v(x, X) - \rho_{v,-v}(x)) \right] + \mathcal{I}(w = -v) \delta_x(dy) \rho_{v,-v}(x),$$

where $\rho_{1,-1}(x)$ and $\rho_{-1,1}(x)$ are free parameters, the “switching rates”, required to satisfy for all $(x, v) \in E$ $0 \leq \rho_{v,-v}(x) \leq \rho_{v,-v}(x) \leq 1 - T_v(x, X)$ and

$$\rho_{v,-v}(x) - \rho_{v,v}(x) = T_{-v}(x, X) - T_v(x, X). \quad (10)$$

It is not difficult to check that under (8) and (10) $P_{\text{lifted}}$ is $(\mu, Q)$–self-adjoint, for $Q$ such that $Qf(x, v) = f(x, -v)$ for $f \in L^2(\mu)$. There are numerous known solutions to the condition above [31], including

$$\hat{\rho}_{v,-v}(x) := \max \{0, T_{-v}(x, X) - T_v(x, X)\}.$$ 

It is remarked as intuitive in [58] that among the possible solutions to (10), this choice should promote fastest exploration. We prove below that this is indeed true, in the sense that this choice minimizes asymptotic variances, as a consequence of Theorem 2.9. We let $P_{\text{lifted, } \gamma}$ denote the transition probability which uses $\rho_{v,-v}$.

**Theorem 3.15.** For any switching rate $\rho_{v,-v}$ satisfying $0 \leq \rho_{v,-v}(x) \leq 1 - T_v(x, X)$ for all $(x, v) \in E$ and (10), any $f \in L^2(\mu)$ such that $Qf = f$ and $\lambda \in [0, 1)$, we have

$$\text{var}^\lambda(f, P_{\text{lifted, } \gamma}) = \text{var}^\lambda(f, P_{\text{lifted, } \gamma}) = \text{var}^\lambda(f, P_{\text{lifted, } 1-T_v}).$$
Proof. Let $\rho_{1,v,v}$ and $\rho_{2,v,v}$ be switching rates such that $0 \leq \rho_{1,v,v}(x,v) \leq \rho_{2,v,v}(x,v) \leq 1 - T_v(x,X)$ for all $(x,v) \in E$, then from the identity in (3)

$$
\mathcal{E}(g, P_{\text{lifted,}\rho_1} Q) - \mathcal{E}(g, P_{\text{lifted,}\rho_2} Q) = \frac{1}{2} \int \mu(d(x,v)) \left( \rho_{2,v,v}(x) - \rho_{1,v,v}(x) \right) \left[ g(x,v) - g(x,v) \right] \geq 0,
$$

and the application of Theorem 2.9 leads to $\text{var}_\lambda(f, P_{\text{lifted,}\rho_1}) \leq \text{var}_\lambda(f, P_{\text{lifted,}\rho_2})$ for any $f \in L^2(\mu)$ such that $Qf = f$. We now establish that $\rho_{v,v}$ satisfying $0 \leq \rho_{v,v}(x) \leq 1 - T_v(x,X)$ and (10) implies $\tilde{\rho}_{v,v}(x,v) \leq 1 - T_v(x,X)$ for all $(x,v) \in E$, notice that $1 - T_v(x,X)$ satisfies (10) and apply the result above twice to conclude. We proceed by contradiction to establish the first inequality. Assume there exists a switching rate $\rho_{v,v}$ such that for some $(x,v) \in E$ such that $\tilde{\rho}_{v,v}(x) > 0$ we have $\rho_{v,v}(x) < \rho_{v,v}(x)$. Then from (10),

$$
\tilde{\rho}_{v,v}(x) - \tilde{\rho}_{v,v}(x) = \rho_{v,v}(x) - \rho_{v,v}(x),
$$
or equivalently

$$
\tilde{\rho}_{v,v}(x) - \rho_{v,v}(x) = \tilde{\rho}_{v,v}(x) - \rho_{v,v}(x) > 0,
$$
which is impossible since $\tilde{\rho}_{v,v}(x) > 0$ implies $\tilde{\rho}_{v,v}(x) = 0$ and we must have $\rho_{v,v}(x) \geq 0$. Therefore we must necessarily have $\rho_{v,v}(x) \geq \tilde{\rho}_{v,v}(x)$ for all $(x,v) \in E$.

Remark 3.16. Readers familiar with the delayed rejection Metropolis-Hastings update may notice the similarity here since

$$
P_{\text{lifted}}((v,w); d(w,y)) = \mathbb{I}\{w = v\} \frac{T_v(x,X)}{T_v(x,X)}
$$

$$
+ \left[ 1 - T_v(x,X) \right] \left[ \mathbb{I}\{w = v\} \delta_x(dy) \left( 1 - \frac{\rho_{v,v}(x)}{1 - T_v(x,X)} \right) + \mathbb{I}\{w = -v\} \delta_x(dy) \frac{\rho_{v,v}(x)}{1 - T_v(x,X)} \right],
$$

where we require the property

$$
\left[ 1 - T_v(x,X) \right] \left( 1 - \frac{\rho_{v,v}(x)}{1 - T_v(x,X)} \right) = \left[ 1 - T_v(x,X) \right] \left( 1 - \frac{\rho_{v,v}(x)}{1 - T_v(x,X)} \right),
$$
and notice that

$$
1 - \frac{\tilde{\rho}_{v,v}(x)}{1 - T_v(x,X)} = \min \left\{ 1, \frac{1 - T_v(x,X)}{1 - T_v(x,X)} \right\}.
$$

The theorem above establishes that this latter form of acceptance probability for the second stage of the update is again optimum in this setup. The update however differs from the standard delayed rejection update in that here the accept/rejection probability is integrated, restricting implementability of the approach. We also note that our results can be used to established superiority of the standard delayed rejection strategy in the context of $(\mu, Q)$--reversible updates and that integration of the rejection probability in the scenario above is beneficial.

One can compare the performance of algorithms relying on $P_{\text{lifted}}$ and $P$. With a slight abuse of notation for any $\lambda \in [0,1)$ and $f \in L^2(\mu)$ we let $\text{var}_\lambda(f, P_{\text{lifted}}) = \text{var}_\lambda(f, P_{\text{lifted}})$ where for $(x,v) \in E$ we let $\tilde{f}(x,v) := f(x)$.

**Theorem 3.17.** For any $\lambda \in [0,1)$ and $f \in L^2(\mu)$, any switching rate $\rho_{v,v}$ satisfying $\tilde{\rho}_{v,v}(x,v) \leq \rho_{v,v}(x,v) \leq 1 - T_v(x,X)$ for all $(x,v) \in E$, $\text{var}_\lambda(f, P_{\text{lifted},\rho}) \leq \text{var}_\lambda(f, P)$, with $P$ given in (9).
Proof. Fix \( \lambda \in [0, 1] \). First consider the additive symmetrization of \( P^{\text{lifted}} \), \( S(P^{\text{lifted}}) := [P^{\text{lifted}} + (P^{\text{lifted}})^*]/2 \), which is \( \mu \)-self-adjoint. From a classical result, see for example [1, Lemma 2], we have for \( g \in L^2(\mu) \),
\[
\operatorname{var}_\lambda (g, P^{\text{lifted}}) \leq \operatorname{var}_\lambda (g, S(P^{\text{lifted}})).
\]
For \( h \in \mathbb{R}^E \) measurable and bounded,
\[
P^{\text{lifted}} Q_h(x, v) = \int T_v(x, dy) h(y, -v) + (1 - T_v(x, X) - \rho_{v, -v}(x)) h(x, -v) + \rho_{v, -v}(x) h(x, v),
\]
and therefore
\[
Q^{\text{lifted}} P_h(x, v) = \int T_{-v}(x, dy) h(y, v) + (1 - T_{-v}(x, X) - \rho_{-v, v}(x)) h(x, v) + \rho_{-v, v}(x) h(x, -v).
\]
Consequently,
\[
S(P^{\text{lifted}}) h(x, v) = \int \frac{1}{2} [T_v(x, dy) + T_{-v}(x, dy)] h(y, v) + \left( 1 - \frac{T_v(x, X) + T_{-v}(x, X)}{2} \right) h(x, v) + \frac{\rho_{v, -v}(x) + \rho_{-v, v}(x)}{2} (h(x, -v) - h(x, v)).
\]
Therefore, for \( f \in L^2(\pi) \) and \( (x, v) \in E, S(P^{\text{lifted}}) \tilde{f}(x, v) = P f(x) \) and by a straightforward induction one can establish \( S(P^{\text{lifted}})^k \tilde{f}(x, v) = P^k f(x) \) for \( k \geq 1 \). As a consequence for \( f \in L^2(\pi) \) and \( \lambda \in [0, 1] \) we have \( \operatorname{var}_\lambda (f, P) = \operatorname{var}_\lambda (\tilde{f}, S(P^{\text{lifted}})) \) and we conclude. \( \lhd \)

Example 3.18. In the scenario where \( X = \mathbb{R} \) or \( X = \mathbb{Z} \) and \( \pi \) has a density with respect to the Lebesgue or counting measure, [27] introduced the guided walk Metropolis, whose transition probability is
\[
P^{\text{GRW}}((v, x); d(w, y)) = T^{\text{guided}}_v(x, dy) 1_{\{w = v\}} + \delta_x(dy) 1_{\{w = -v\}} \left[ 1 - T^{\text{guided}}_v(x, X) \right]
\]
where,
\[
T^{\text{guided}}_v(x, dy) := \int_X \min \left\{ 1, \frac{\pi(x + |z|v)}{\pi(x)} \right\} q(dz) \delta_{x+|z|v}(dy),
\]
for some symmetric distribution \( q(\cdot) \) on \( V = \mathbb{R} \) or \( V = \{-1, 1\} \). It is straightforward to check that \( T^{\text{guided}}_v \) satisfies (8), and hence we can construct a lifted version of Gustafson’s algorithm. We also notice that \( P \) corresponds in this case to the random walk Metropolis algorithm with proposal distribution \( q(\cdot) \)–we denote this algorithm \( P^{\text{RW}} \). Our two earlier results establish that for any switching rate \( \rho_{v, -v} \), \( f \in L^2(\pi) \) and \( \lambda \in [0, 1] \),
\[
\operatorname{var}_\lambda (f, P^{\text{GRW}, \rho}) \leq \operatorname{var}_\lambda (f, P^{\text{RW}}) \leq \operatorname{var}_\lambda (f, P_{\text{GRW}}).
\]

3.4 Neal’s scheme to avoid backtracking

In [40] the author describes a generic way of modifying a reversible Markov chain defined on a finite state space \( X \) to reduce “backtracking” (a special case is also discussed in [16]). More specifically, assume we are interested in sampling from some probability distribution \( \pi \) defined on \( X \) and that we do so by using a \( \pi \)-reversible (first order) Markov transition \( T_2 \) defined on \( X \). Informally the idea in [40] is to modify the first order Markov chain of transition \( T_2 \) into a second order Markov chain \( T_1 \) to ensure that given a realization
X_0, X_1, \ldots, X_{k-1}, X_k \text{ for some } k \geq 1 \text{ the new chain samples } X_{k+1} \text{ conditional upon } X_k \text{ and } X_{k-1} \text{ and prevents the occurrence of the event } X_{k+1} = X_{k-1}. \text{ A probabilistic argument is developed in [40] for } X \text{ finite to establish that the resulting chain produces estimators with an asymptotic variance that cannot exceed that of estimators from the original chain. We show here that this holds more generally for countable spaces and is a direct consequence of } (\mu, Q) \text{—self-adjointness for a particular } Q, \text{ the bivariate first order representation of a second order univariate Markov chain, as used in [40] and the application of Theorem 2.9. For simplicity of exposition we assume } 0 < T_2(x_1, x_2) < 1 \text{ for } x_1, x_2 \in X. \text{ First define the extended probability distribution on } X \times X

\mu(x_1, x_2) := \pi(x_1)T_2(x_1, x_2) = \pi(x_2)T_2(x_2, x_1),

\text{for } (x_1, x_2) \in X \times X. \text{ Setting } Qf(x_1, x_2) := f(x_2, x_1), \text{ we notice that } T_2 \text{ implies that } Q \text{ is an } \mu \text{—isometric involution. Let } M_2((x_1, x_2); (y_1, y_2)) := \mathbb{P}(y_1 = x_1) T_2(x_1, y_2) \text{ for } (x_1, x_2) \in X \times X \text{ and notice that } M_2 \text{ is } \mu \text{—reversible. The Markov chain of transition } P_2 = QM_2 \text{ is therefore } (\mu, Q) \text{—reversible from Proposition 2.5. Following an idea of Liu [35], it is suggested in [40] to use instead the transition } P_1 = QM_1, \text{ where the } \mu \text{—reversible component } M_2 \text{ is replaced with the following } (\mu \text{—reversible) Metropolis-Hastings update,}

M_1((x_1, x_2); (y_1, y_2)) := \mathbb{P}(y_1 = x_1) \left[ U((x_1, x_2); (y_1, y_2)) + \mathbb{P}(y_2 = x_2) \left( 1 - U((x_1, x_2); X \times X) \right) \right],

\text{where}

U((x_1, x_2); (y_1, y_2)) := \frac{T_2(x_1, y_2) \mathbb{P}(y_2 \neq x_2)}{1 - T_2(x_1, x_2)} \min \left( 1, \frac{1 - T_2(x_1, x_2)}{1 - T_2(y_1, y_2)} \right).

\text{The } (\mu, Q) \text{—reversible kernel } P_1 \text{ is designed so that backtracking, the probability of returning to } x_1 \text{ when sampling } y_2 \text{ conditional upon } x_2 \text{ of the chain is reduced, compared to } P_2. \text{ Let } \{Z_k, k \geq 0\} \text{ denote a realization of the homogeneous Markov chain of transition } P_i \text{ (for } i \in \{1, 2\}) \text{ and arbitrary initial condition, one can check that its first component is a realisation } \{X_k, k \geq 0\} \text{ of the Markov chain of transition } T_i, \text{ and in fact } Z_k = (X_k, X_{k+1}) \text{ for } k \geq 0. \text{ With an abuse of notation, for any } \lambda \in [0, 1) \text{ and } f \in L^2(\pi) \text{ we let } \var_{\lambda}(f, T_i) := \var_{\lambda}(f, P_i) \text{ where for any } x_1, x_2 \in X, f(x_1, x_2) := f(x_1).

\textbf{Theorem 3.19. For any } g \in L^2(\mu) \text{ such that } Qg = g, \text{ and } \lambda \in [0, 1) \text{ we have } \var_{\lambda}(g, P_1) \leq \var_{\lambda}(g, P_2) \text{ and as a consequence, for any } f \in L^2(\pi) \text{ we have}\n
\var_{\lambda}(f, T_1) \leq \var_{\lambda}(f, T_2).

\textbf{Proof. Since for } (x_1, x_2) \neq (y_1, y_2),

\begin{align*}
M_1((x_1, x_2); (y_1, y_2)) &= \mathbb{P}(y_1 = x_1) T_2(x_1, y_2) \mathbb{P}(y_2 \neq x_2) \min \left( \frac{1}{1 - T_2(x_1, x_2)}, \frac{1}{1 - T_2(y_1, y_2)} \right) \\
&\geq \mathbb{P}(y_1 = x_1) T_2(x_1, y_2),
\end{align*}

\text{we deduce } QP_1((x_1, x_2); (y_1, y_2)) \geq QP_2((x_1, x_2); (y_1, y_2)) \text{ for } (x_1, x_2) \neq (y_1, y_2) \text{ and consequently from the identity in (3) } \mathcal{E}(g, QP_i) \geq \mathcal{E}(g, QP_2) \text{ for any } g \in L^2(\mu). \text{ The first statement follows from Theorem 2.9 (or Theorem 3.1). The second statement will follow by letting } g(x_1, x_2) = f(x_1) + f(x_2) \text{ for an arbitrary } f \in L^2(\pi) \text{ and once we have established that for } \lambda \neq 0 \text{ and } i \in \{1, 2\}

\var_{\lambda}(g, P_i) = -(1 - \lambda^2) \lambda^{-1} \var_{\lambda}(f) + (1 + \lambda) \lambda^{-1} \var_{\lambda}(f, T_i).
Without loss of generality assume that $\pi(f) = 0$. For both homogeneous Markov chains of transitions $P_1$ and $P_2$ with initial condition $Z_0 = (X_0, X_1) \sim \mu$ we have $\mathbb{E}[g^2(Z_0)] = 2\mathbb{E}[f^2(X_0)] + 2\mathbb{E}[f(X_0)f(X_1)]$ and for $k \geq 1$, with $Z_k = (X_k, X_{k+1})$, we have
\[
\mathbb{E}[g(Z_0)g(Z_k)] = \mathbb{E}[(f(X_0) + f(X_1))(f(X_k) + f(X_{k+1}))]
= \mathbb{E}[f(X_0)f(X_{k-1})] + 2\mathbb{E}[f(X_0)f(X_k)] + \mathbb{E}[f(X_0)f(X_{k+1})],
\]
therefore implying
\[
\sum_{k \geq 1} \lambda^k \mathbb{E}[g(Z_0)g(Z_k)] = \lambda \sum_{k \geq 1} \lambda^k \mathbb{E}[f(X_0)f(X_k)] + 2 \sum_{k \geq 1} \lambda^k \mathbb{E}[f(X_0)f(X_k)] + \sum_{k \geq 2} \lambda^{k-1} \mathbb{E}[f(X_0)f(X_k)]
= \lambda \mathbb{E}[f^2(X_0)] + (\lambda^2 + 2\lambda) \mathbb{E}[f(X_0)f(X_1)] + (\lambda^2 + 2\lambda + 1) \sum_{k \geq 2} \lambda^{k-1} \mathbb{E}[f(X_0)f(X_k)].
\]
This yields for $i \in \{1, 2\}$ and $\lambda \neq 0$,
\[
\text{var}_\lambda(g, P_i) = 2(1 + \lambda) \mathbb{E}[f^2(X_0)] + 2(\lambda^2 + 2\lambda + 1) \mathbb{E}[f(X_0)f(X_1)] + (1 + \lambda)^2 \sum_{k \geq 2} \lambda^{k-1} \mathbb{E}[f(X_0)f(X_k)]
= -(1 - \lambda^2)\lambda^{-1} \mathbb{E}[f^2(X_0)] + (1 + \lambda^2)\lambda^{-1} \left( \mathbb{E}[f^2(X_0)] + 2 \sum_{k \geq 1} \lambda^k \mathbb{E}[f(X_0)f(X_k)] \right).
\]
Finally note that for $k \geq 0 \mathbb{E}[\hat{f}(Z_0)\hat{f}(Z_k)] = \mathbb{E}[f(X_0)f(X_k)]$ and therefore $\text{var}_\lambda(\hat{f}, P_1) = \mathbb{E}[f^2(X_0)] + 2 \sum_{k \geq 1} \lambda^k \mathbb{E}[f(X_0)f(X_k)]$. We can therefore conclude.

4 Continuous time scenario – general results

The continuous time scenario follows in part ideas similar to those developed in the discrete time scenario, but requires the introduction of the generator of the semigroup associated with the continuous time process, leading to additional technical complications. In Subsection 4.1 we develop a crucial result of practical interest, Theorem 4.4, which allows one to deduce that a (in general intractable) semigroup is $(\mu, Q)$-self-adjoint when its generator is $(\mu, Q)$-symmetric on a type of dense subset of its domain. In Subsection 4.2 we establish the continuous time counterpart of Theorem 2.9, that is that showing that order of tractable quantities involving the generators of two $(\mu, Q)$-reversible processes implies an order on their asymptotic variances (Theorem 4.6). We remark that while establishing order rigorously may appear complex and technical, checking the criterion suggesting order involves in general elementary calculations. To the best of our knowledge no general result is available in the continuous time reversible setup, that is when $Q = \text{Id}$ in our setup, but note the works [34, 49], focused on particular scenarios.

4.1 Set-up and characterization of $(\mu, Q)$-self-adjointness

Let $(Z_t, t \geq 0)$ be a Markov process taking values in the space $D(\mathbb{R}_+, E)$ of cadlag functions endowed with the Skorokhod topology and corresponding probability space $(\Omega, \mathcal{F}, \mathbb{P})$. We denote $\{P_t, t \geq 0\}$ the associated semi-group, assumed to have an invariant distribution $\mu$ defined on $(E, \mathcal{E})$ and let $(D^2(L, \mu), L)$ be the generator associated with $\{P_t, t \geq 0\}$ i.e. $L$ and $D^2(L, \mu) \subset L^2(\mu)$ are such that, with $\text{Id}$ the identity operator,
\[
D^2(L, \mu) := \left\{ f \in L^2(\mu) : \lim_{t \downarrow 0} \left| t^{-1} (P_t - \text{Id}) f - Lf \right|_\mu = 0 \right\}.
\]
From above \( \{P_t, t \geq 0\} \) is a strongly continuous contraction, \( \mathcal{D}^2(L, \mu) \) is dense in \( L^2(\mu) \) and \( L \) is closed [20, Corollary 1.6]. For any \( t \in \mathbb{R}_+ \) we let \( P^*_t \) denote the \( L^2(\mu) \)–adjoint of \( P_t \), and it is classical that \( \{P^*_t, t \geq 0\} \) is a strongly continuous contraction of invariant distribution \( \mu \) and generator \( (\mathcal{D}^2(L^*, \mu), L^*) \), the adjoint of \( L \) [14], that is it holds that for \( f \in \mathcal{D}^2(L, \mu) \) and \( g \in \mathcal{D}^2(L^*, \mu) \), 

\[
\langle Lf, g \rangle_{\mu} = \langle f, L^*g \rangle_{\mu}.
\]

In order to avoid repetition we group our basic assumptions on the triplet \( (\mu, Q, \{P_t, t \geq 0\}) \) used throughout this section.

(A1) \( (a) \) \( \mu \) is a probability distribution defined on \( (E, \mathcal{E}) \),

\( (b) \) \( \{P_t, t \geq 0\} \) is a strongly continuous Markov semi-group of invariant distribution \( \mu \),

\( (c) \) \( Q \) is a \( \mu \)–isometric involution.

**Definition 4.1.** We will say that the semi-group \( \{P_t, t \geq 0\} \) is \( (\mu, Q) \)–self-adjoint, if for all \( f, g \in L^2(\mu) \) and \( t \geq 0 \)

\[
\langle P_tf, g \rangle_{\mu} = \langle f, QP_tQg \rangle_{\mu}.
\]

We aim to characterise the adjoint of the generator of a \( (\mu, Q) \)–self-adjoint semigroup \( \{P_t, t \geq 0\} \) and provide a practical simple condition to establish this property for a given semigroup. We preface our first results with a technical lemma. For two operators \( (\mathcal{D}^2(A, \mu), A) \) and \( (\mathcal{D}^2(B, \mu), B) \), \( \mathcal{D}^2(AB, \mu) := \{ f \in \mathcal{D}^2(B, \mu) : Bf \in \mathcal{D}^2(A, \mu) \} \).

**Lemma 4.2.** Let \( (\mu, Q, \{P_t, t \geq 0\}) \) satisfying (A1) and let \( \{T_t := QP_tQ, t \geq 0\} \). Then

(\( a \) \( (\mu, Q, \{T_t, t \geq 0\}) \) satisfies (A1),

(\( b \) \( \) the generator of \( \{T_t, t \geq 0\} \) is \( (\mathcal{D}^2(QLQ, \mu), QLQ) \).

**Proof.** From the properties of \( Q \) and \( \{P_t, t \geq 0\} \), it is immediate that \( \{T_t, t \geq 0\} \) is a semigroup leaving \( \mu \) invariant. Further for \( f \in L^2(\mu) \) \( \|QP_tQf - f\|_\mu = \|P_tQf - Qf\|_\mu \) from which the continuity follows. Denote \( (\mathcal{D}^2(\hat{L}, \mu), \hat{L}) \) the generator of \( \{T_t, t \geq 0\} \). For \( f \in \mathcal{D}^2(QLQ, \mu) \) we have \( Qf \in \mathcal{D}^2(L, \mu) \) and therefore by (A1),

\[
\lim_{t \downarrow 0} \|t^{-1}(QP_tQ - \text{Id})f - QLQf\|_\mu = \lim_{t \downarrow 0} \|t^{-1}(P_t - \text{Id})Qf - LQf\|_\mu = 0,
\]

implying \( \mathcal{D}^2(QLQ, \mu) \subset \mathcal{D}^2(\hat{L}, \mu) \) and \( \hat{L}f = QLQf \) for \( f \in \mathcal{D}^2(QLQ, \mu) \). Similarly for any \( f \in \mathcal{D}^2(\hat{L}, \mu) \)

\[
0 = \lim_{t \downarrow 0} \|t^{-1}(QP_tQ - \text{Id})f - \hat{L}f\|_\mu = \lim_{t \downarrow 0} \|t^{-1}(P_t - \text{Id})Qf - QLQf\|_\mu,
\]

implying \( Qf \in \mathcal{D}^2(L, \mu) \) and hence \( f \in \mathcal{D}^2(QLQ, \mu) \). We conclude.

As a corollary one can characterise the generator of a \( (\mu, Q) \)–self-adjoint semigroup.

**Proposition 4.3.** Let \( (\mu, Q, \{P_t, t \geq 0\}) \) satisfying (A1) be \( (\mu, Q) \)–self-adjoint. Then the generator of \( \{P^*_t, t \geq 0\} \) is \( (\mathcal{D}^2(QLQ, \mu), L^* = QLQ) \).

**Proof.** We use Lemma 4.2 and the fact that here \( P^*_t = QP_tQ \) for \( t \geq 0 \).
Theorem 4.4. Let $(\mu, \{P_t, t \geq 0\}, Q)$ satisfying (A1). Assume that $\mathcal{A}$ is a core for $(L, \mathcal{D}^2(L, \mu))$ such that

(a) $f \in \mathcal{A}$ implies $Qf \in \mathcal{A}$,

(b) for all $f, g \in \mathcal{A}$ we have $\langle Lf, g \rangle_\mu = \langle f, QLg \rangle_\mu$,

then $\{P_t, t \geq 0\}$ is $(\mu, Q)$–self-adjoint.

Proof. Since $\mathcal{A}$ is a core for $(\mathcal{D}^2(L, \mu), L)$, $Q \mathcal{A} = \mathcal{A}$ and $Q$ is continuous, we have $\langle Lf, g \rangle_\mu = \langle f, QLg \rangle_\mu$ for $f \in \mathcal{D}^2(L, \mu)$ and $g \in \mathcal{D}^2(QLQ, \mu)$. Indeed, since $\mathcal{A}$ is a core for $L$, for any $f \in \mathcal{D}^2(L, \mu)$ there exists $\{f_n \in \mathcal{A}, n \in \mathbb{N}\}$ such that $\lim_{n \to \infty} \|f_n - f\|_\mu + \|Lf_n - Lf\|_\mu = 0$. Similarly for $g \in \mathcal{D}^2(QLQ, \mu)$, then $Qg \in \mathcal{D}^2(L, \mu)$ and from the definition of a core one can find $\{\gamma_n \in \mathcal{A}, n \in \mathbb{N}\}$ such that $\lim_{n \to \infty} \|\gamma_n - Qg\|_\mu + \|L\gamma_n - LQg\|_\mu = 0$ implying $\lim_{n \to \infty} \|g_n - g\|_\mu + \|LQg_n - LQg\|_\mu = 0$ with $\{g_n := Q\gamma_n \in \mathcal{A}, n \in \mathbb{N}\}$. Further $\mathcal{D}^2(QLQ, \mu) \subset \mathcal{D}^2(L^*, \mu)$ as for any $g \in \mathcal{D}^2(QLQ, \mu)$ we have that $\mathcal{D}^2(L, \mu) \ni f \mapsto \langle Lf, g \rangle_\mu = \langle f, QLQg \rangle_\mu$

which is bounded and can be extended to $L^2(\mu)$ by density of $\mathcal{D}^2(L, \mu)$, and we conclude by definition of the adjoint [44, Paragraph 5.1.2]. From Lemma 4.2 and the Hille-Yosida theorem, we have that for all $\lambda > 0$ \text{Ran}(\lambda \text{Id} - QLQ) = L^2(\mu)$. Fix $\lambda > 0$, then for any $g \in \mathcal{D}^2(L^*, \mu)$ there exists $h \in \mathcal{D}^2(QLQ, \mu)$ such that $(\lambda \text{Id} - QLQ)h = (\lambda \text{Id} - L^*)g$ and hence for any $f \in \mathcal{D}^2(L, \mu)$

$$\langle (\lambda \text{Id} - L)f, g \rangle_\mu = \langle f, (\lambda \text{Id} - L^*)g \rangle_\mu = \langle f, (\lambda \text{Id} - QLQ)h \rangle_\mu = \langle (\lambda \text{Id} - L)f, h \rangle_\mu.$$ Again from the Hille-Yosida theorem we can take $\lambda > 0$ as above and have $\text{Ran}(\lambda \text{Id} - L) = L^2(\mu)$, and the equality above translates into $\langle k, g \rangle_\mu = \langle k, h \rangle_\mu$ for any $k \in L^2(\mu)$ and hence $g = h \in \mathcal{D}^2(QLQ, \mu)$, $\mathcal{D}^2(L^*, \mu) = \mathcal{D}^2(QLQ, \mu)$ and $L^* = QLQ$. From the Duhamel formula we deduce that $P_t^\mu = QP_tQ$ for $t \geq 0$.

4.2 Ordering of asymptotic variances

For $f \in L^2(\mu)$ we are interested, when this quantity exists, in the limit of

$$\var(f, L) := \lim_{t \to \infty} \var \left( t^{-1/2} \int_0^t f(Z_s) ds \right),$$

where $Z_0 \sim \mu$. In some circumstances (for instance when a Foster-Lyapunov function can be identified [25, Theorem 4.3]) the limit above exists and has the following expression

$$\var(f, L) = 2\langle f, RF \rangle_\mu,$$

where $RF := \int_0^{+\infty} P_t f dt$. For $\lambda > 0$ and $f \in L^2(\mu)$ we introduce $\var(\lambda f, L) := 2\langle \lambda f, R_* f \rangle_\mu$, where $R_\lambda$ is the bounded operator defined as

$$R_\lambda f := \int_0^{+\infty} \exp(-\lambda t) P_t f dt,$$

referred to as the resolvent from now on. It is classical that for any $f \in L^2(\mu)$, $(\lambda \text{Id} - L)R_\lambda f = f$ and for $f \in \mathcal{D}(L, \mu)$, $R_\lambda(\lambda \text{Id} - L)f = f$. As in the discrete time setup, we leave the issue of checking whether $\lim_{\lambda \to 0+} \var(\lambda f, L) = \var(f, L)$ as separate. We note the following straightforward result.

**Lemma 4.5.** If $(\mu, Q, \{P_t, t \geq 0\})$ satisfies (A1) and is $(\mu, Q)$–self-adjoint, then for any $\lambda > 0$ the bounded operator $R_\lambda$ is also $(\mu, Q)$–self-adjoint.
For two semi-groups \( \{P_t, t \geq 0\} \) leaving \( \mu \) invariant and of generators \( L_1 \) and \( L_2 \) with domains \( D^2(L_1, \mu) \) and \( D^2(L_2, \mu) \), we are interested in ordering \( \text{var}_\lambda(f, L_1) \) and \( \text{var}_\lambda(f, L_2) \) for \( \lambda > 0 \). As in the discrete time set-up the comparison relies on the Dirichlet forms, defined as follows for a generator \( L \) and \( f \in D^2(L, \mu) \),

\[
\mathcal{E}(f, L) := \langle f, -Lf \rangle_\mu.
\]

Our proof requires the introduction of interpolating processes, defined at the level of their generators.

(A2) \( \{\mu, Q, \{P_t, t \geq 0\}\} \) and \( \{\mu, Q, \{P_t, t \geq 0\}\} \) satisfy (A1) and are \( (\mu, Q) \)–self-adjoint. Their respective generators \( \{L_1, D^2(L_1, \mu)\} \) and \( \{L_2, D^2(L_2, \mu)\} \) are assumed

(a) to have a common core \( A \) dense in \( L^2(\mu) \) such that \( QA \subset A \),

(b) to be such that for any \( \beta \in [1, 2] \) the operator \( ((2 - \beta)L_1 + (\beta - 1)L_2, D^2(L_1, \mu) \cap D^2(L_2, \mu)) \)

(i) has an extension defining a unique continuous contraction semigroup \( \{P_t(\beta), t \geq 0\} \) on \( L^2(\mu) \)

of invariant distribution \( \mu \) and of (closed) generator \( (L(\beta), D^2(L(\beta), \mu)) \),

(ii) and for any \( f \in A \) we have \( P_t(\beta)f \in A \) for any \( t \geq 0 \).

From [20, Proposition 3.3] the last assumption and density of \( A \) in \( L^2(\mu) \) imply that \( A \) is a core for \( L(\beta), \beta \in [1, 2] \). Establishing that for \( \beta \in [1, 2] \) the contraction semigroup \( \{P_t(\beta), t \geq 0\} \) exists may require one to resort to the Hille-Yosida theory and/or perturbation theory results [57, 20], but turns out to be straightforward in some scenarios such as those treated in Section 5. For \( \lambda > 0 \) and \( \beta \in [1, 2] \) we let \( R_\lambda(\beta) \) be the corresponding resolvent operators. Differentiability of \( \beta \rightarrow R_\lambda(\beta)f \) and the expression for the corresponding derivative are key to our result, as is the case in the discrete time scenario. The right derivatives of operators below are to be understood as limits in the Banach space \( L^2(\mu) \) equipped with the norm \( \| \cdot \|_\mu \). We only state the results for \( f \in L_2(\mu) \) such that \( Qf = f \) and note that the case \( Qf = -f \) is straightforward.

\textbf{Theorem 4.6.} Assume (A2) and that for any \( \lambda > 0, \beta \in [1, 2] \) and \( f \in A \),

(a) \( R_\lambda(\beta)f \in D^2(L_1, \mu) \cap D^2(L_2, \mu) \) and there exists \( \{g_n(\beta) \in A, n \in \mathbb{N}\} \) such that \( \lim_{n \to \infty} (L_1 - L_2)g_n(\beta) = (L_1 - L_2)R_\lambda(\beta)f \),

(b) \( [1, 2] \ni \beta \rightarrow R_\lambda(\beta)f \) is right differentiable with

\[
\partial_\beta R_\lambda(\beta)f = R_\lambda(\beta)(L_2 - L_1)R_\lambda(\beta)f,
\]

and \( \beta \rightarrow \langle f, \partial_\beta R_\lambda(\beta)f \rangle_\mu \) is continuous,

(c) either \( \mathcal{E}(g, QL_1 - QL_2) \geq 0 \) for any \( g \in A \) or \( \mathcal{E}(g, L_1Q - L_2Q) \geq 0 \) for any \( g \in A \),

then

(a) for any \( f \in A \) satisfying \( Qf = f \) and \( \beta \in [1, 2] \),

\[
\partial_\beta \langle f, R_\lambda(\beta)f \rangle_\mu = \mathcal{E}(QR_\lambda(\beta)f, L_1Q - L_2Q) = \mathcal{E}(R_\lambda(\beta)f, QL_1 - QL_2) \geq 0,
\]

(b) for any \( f \in L_2(\mu) \) such that \( Qf = f \),

\[
\text{var}_\lambda(f, L_1) = 2\langle f, R_\lambda(1)f \rangle_\mu \leq \text{var}_\lambda(f, L_2) = 2\langle f, R_\lambda(2)f \rangle_\mu.
\]
Proof. For $\beta \in [1, 2)$, $\delta \in (0, 2 - \beta]$ and $f \in \mathcal{A}$ such that $Qf = f$ we have $\delta^{-1}[\langle f, R_\lambda(\beta + \delta)f \rangle_\mu - \langle f, R_\lambda(\beta)f \rangle_\mu] = \langle f, \delta^{-1}[R_\lambda(\beta + \delta) - R_\lambda(\beta)]f \rangle_\mu$ and from the assumption we deduce

$$
\partial_\beta \langle f, R_\lambda(\beta)f \rangle_\mu = \langle f, \partial_\beta R_\lambda(\beta)f \rangle_\mu = \langle f, R_\lambda(\beta)(L_2 - L_1)R_\lambda(\beta)f \rangle_\mu
$$

$$= \langle R_\lambda^*(\beta)f, (L_2 - L_1)R_\lambda(\beta)f \rangle_\mu = \langle Q R_\lambda(\beta)Qf, (L_2 - L_1)R_\lambda(\beta)f \rangle_\mu = \langle R_\lambda(\beta)f, -Q(L_2 - L_1)R_\lambda(\beta)f \rangle_\mu,
$$

where we have used that $Qf = f$ and the fact that $Q$ is $\mu-$self-adjoint. Using in addition that $Q^2 = \text{Id}$, it is not difficult to establish the alternate expression $\partial_\beta \langle f, R_\lambda(\beta)f \rangle_\mu = \langle QR_\lambda(\beta)f, -(L_1 - L_2)QQR_\lambda(\beta)f \rangle_\mu$. The first claim follows from $\mathcal{E}(R_\lambda(\beta)f, QL_1 - QL_2) = \lim_{n \to \infty} \mathcal{E}(g_n, QL_1 - QL_2) \geq 0$. The second claim follows from

$$
\langle f, R_\lambda(2)f \rangle_\mu - \langle f, R_\lambda(1)f \rangle_\mu = \int_1^2 \mathcal{E}(R_\lambda(\beta)f, QL_1 - QL_2)d\beta \geq 0,
$$

continuity of $R_\lambda(1), R_\lambda(2)$ on $L^2(\mu)$ and the density of $\mathcal{A}$ in $L^2(\mu)$. \hfill \Box

The following allows us to check the conditions of the theorem above.

**Lemma 4.7.** Assume (A2) and that for any $\lambda > 0$, $\beta \in [1, 2)$ and $f \in \mathcal{A}$,

(a) $t \mapsto (L_2 - L_1)P_t(\beta)f$ and $t \mapsto (L_2 - L_1)QP_t(\beta)f$ are continuous,

(b) there exists $\delta(\beta) > 0$ such that

$$
\left\{ \int_0^\infty \exp(-\lambda t)\|L_2 - L_1\|_\mu dt \right\} \vee \left\{ \sup_{|\beta' - \beta| \leq \delta(\beta)} \int_0^\infty \exp(-\lambda t)\|L_2 - L_1\|_\mu dt \right\} < \infty.
$$

Then for any $\beta \in [1, 2)$ and $\lambda > 0$, for any $f \in \mathcal{A}$,

(a) $R_\lambda(\beta)f \in D^2(L_1, \mu) \cap D^2(L_2, \mu)$ and there exists $\{g_n(\beta) \in \mathcal{A}, n \in \mathbb{N}\}$ such that $\lim_{n \to \infty} (L_1 - L_2)g_n(\beta) = (L_1 - L_2)R_\lambda(\beta)f$,

(b) $[1, 2) \ni \beta \mapsto R_\lambda(\beta)f$ is right differentiable with

$$
\partial_\beta R_\lambda(\beta)f = R_\lambda(\beta)(L_2 - L_1)R_\lambda(\beta)f,
$$

and $\beta \mapsto \langle f, \partial_\beta R_\lambda(\beta)f \rangle_\mu$ is continuous.

**Proof.** Let $f \in \mathcal{A}, \beta, \beta' \in [1, 2)$ and $\lambda > 0$. Then for $t \geq 0$ $P_t(\beta)f \in \mathcal{A} \subset D(L(\beta'), \mu)$, by definition $L(\beta') = L(\beta) + (\beta' - \beta)[L_2 - L_1]$ on $\mathcal{A} \subset D^2(L_1, \mu) \cap D^2(L_2, \mu)$ and $L(\beta)P_t(\beta)f = P_t(\beta)L(\beta)f$ from [20, Proposition 1.5]. Therefore from the assumptions $t \mapsto \exp(-\lambda t)L(\beta')P_t(\beta)f$ is continuous and summable and from [20, Lemma 1.4] we have

$$
\int_0^\infty \exp(-\lambda t)L(\beta')P_t(\beta)f dt = L(\beta') \int_0^\infty \exp(-\lambda t)P_t(\beta)f dt,
$$

20
since \( L(\beta') \) is closed, implying that \( R_\lambda(\beta)f \in \mathcal{D}(L(\beta'), \mu) \). Using the identity above for \( \beta_1' \neq \beta_2' \) and taking the difference we deduce that \( R_\lambda(\beta)f \in \mathcal{D}^2(L_1, \mu) \cap \mathcal{D}^2(L_2, \mu) \) and that we can take \( \{g_n(\beta) \in \mathcal{A}, n \in \mathbb{N} \} \) such that for \( n \in \mathbb{N} \)

\[
g_n(\beta) := \frac{1}{n} \sum_{k=1}^{n^2} \exp(-\lambda k/n) P_{k/n}(\beta)f,
\]

in the first claim. Now let \( \beta \in [1, 2) \) and \( \delta \in \mathbb{R} \) such that \( \beta + \delta \in [1, 2] \). From the above we deduce that for \( f \in \mathcal{A} \),

\[
[R_\lambda(\beta + \delta) - R_\lambda(\beta)]f = R_\lambda(\beta + \delta)\left[\text{Id} - (\lambda \text{Id} - L(\beta + \delta))R_\lambda(\beta)\right]f
\]

\[
= R_\lambda(\beta + \delta) \left[ (\lambda \text{Id} - L(\beta)) - (\lambda \text{Id} - L(\beta + \delta)) \right] R_\lambda(\beta)f
\]

\[
= R_\lambda(\beta + \delta) \left[ L(\beta + \delta) - L(\beta) \right] R_\lambda(\beta)f
\]

\[
= \delta R_\lambda(\beta + \delta) \left[ L_2 - L_1 \right] R_\lambda(\beta)f.
\]

Using that \( \|R_\lambda(\beta)\|_\mu \leq \lambda^{-1} \) for \( \beta \in [1, 2] \) we conclude that for any \( f \in \mathcal{A} \) the mapping \( \beta \mapsto R_\lambda(\beta)f \) is continuous. Let \( f \in \mathcal{A} \) and \( \epsilon > 0 \), then from the density of \( \mathcal{A} \) in \( L^2(\mu) \), there exists \( g \in \mathcal{A} \) such that \( \|L_2 - L_1\|_\mu R_\lambda(\beta)f - g\|_\mu \leq \lambda \epsilon/4 \), and using the bound

\[
\|\left[R_\lambda(\beta + \delta) - R_\lambda(\beta)\right][L_2 - L_1] R_\lambda(\beta)f\|_\mu \leq\|\left[R_\lambda(\beta + \delta) - R_\lambda(\beta)\right][L_2 - L_1] R_\lambda(\beta)\|_\mu \|g\|_\mu,
\]

the fact that \( \|R_\lambda(\beta)\|_\mu \leq \lambda^{-1} \) for \( \beta \in [1, 2] \) and the continuity of \( \beta \mapsto R_\lambda(\beta)g \) we conclude that for \( \delta \) sufficiently small, \( \|\left[R_\lambda(\beta + \delta) - R_\lambda(\beta)\right][L_2 - L_1] R_\lambda(\beta)f\|_\mu \leq \epsilon \). Therefore together with (12) we have established that for any \( \beta \in [1, 2] \) and \( f \in \mathcal{A} \)

\[
\lim_{\delta \downarrow 0} \delta^{-1}\left[R_\lambda(\beta + \delta) - R_\lambda(\beta)\right] f - R_\lambda(\beta) \left[L_2 - L_1\right] R_\lambda(\beta)f\|_\mu = 0.
\]

Further for \( f \in \mathcal{A} \) such that \( Qf = f \) and any \( \beta, \beta' \in [1, 2] \)

\[
\langle R_\lambda(\beta')f, Q(L_2 - L_1) R_\lambda(\beta')f \rangle_\mu - \langle R_\lambda(\beta)f, Q(L_2 - L_1) R_\lambda(\beta)f \rangle_\mu
\]

\[
= \langle [R_\lambda(\beta') - R(\beta)]f, Q(L_2 - L_1) R_\lambda(\beta')f \rangle_\mu - \langle [L_2 - L_1] Q R_\lambda(\beta')f, [R_\lambda(\beta) - R(\beta')]f \rangle_\mu
\]

and we conclude with the Cauchy-Schwarz inequality, another use of [20, Lemma 1.4] and the continuity of \( \beta \mapsto R_\lambda(\beta)f \).

\[\square\]

5 Continuous time scenario – example

In this section we show how the results of the previous section can be applied to a particular class of processes designed to perform Monte Carlo simulation, which has recently received some attention (Subsection 5.1). In Subsection 5.2 we establish that most processes considered in the literature are indeed \( (\mu, Q) \)-self-adjoint—this includes in particular the Zig-Zag (ZZ) process. In Subsection 5.3 we show that with some smoothness conditions on the intensities involved in the definition of the ZZ process, then all the conditions required to apply our general results, namely Theorem 4.6 and Lemma 4.7, are satisfied. In Subsection 5.1 we apply our general theory and present some applications. In addition we show how one can consider more general versions of ZZ relying on nonsmooth intensities using smooth approximation strategies which have the advantage of preserving the correct invariant distribution.
5.1 PDMP-Monte Carlo

We assume here that \( E = X \times V \) and that the distribution \( \mu \) of interest has density (also denoted \( \mu \))

\[
\mu(x,v) \propto \exp \left( -U(x) \right) \varpi(v)
\]

with respect to some \( \sigma \)-finite measure denoted \( d(x,v) \), where \( U : X = \mathbb{R}^d \to \mathbb{R} \) is an energy function and \( \varpi : V \subset \mathbb{R}^d \to \mathbb{R}_+ \) are such that \( \mu \) induces a probability distribution. Piecewise deterministic Markov processes (PDMPs) [15] are continuous time processes with various applications in engineering and science, but it has recently been shown [21, 46, 10, 11, 7, 6] that such processes can be used in order to sample from large classes of distributions defined as above. The particular cases derived for this purpose are known to be non-reversible, but we establish here that they are in fact \((\mu,Q)\)-reversible for a specific isometric involution \( Q \). This allows us to apply the theory developed in the previous section and to compare their performance in terms of some of their design parameters.

For \( k \in \mathbb{Z}_+ \), for \( i \in \llbracket 1, k \rrbracket \) define intensities \( \lambda_i : E \to \mathbb{R}_+ \), \( \lambda := \sum_{i=1}^k \lambda_i \), for \( (x,v) \in E \) and \( t \geq 0 \)

\[
\Lambda_i(t,x,v) := \int_0^t \lambda_i(x + uv,v)du,
\]

\( \Lambda(t,x,v) := \sum_{i=1}^k \Lambda_i(t,x,v) \) and kernels \( R_i : E \times \mathcal{E} \to [0,1] \) such that for any \( (x,v) \in E \), \( R_i((x,v),\{x\} \times V) = 1 \). For any \( x \in X \) and \( i \in \llbracket 1, k \rrbracket \) we let \( R_{x,i} : V \times \mathcal{Y} \to [0,1] \) be such that \( R_{x,i}(v,A) := R_i((x,v),\{x\} \times A) \) for \( (v,A) \in V \times \mathcal{Y} \). For \( \varsigma_1, \ldots, \varsigma_k \in \mathbb{R}_+ \) we let \( \mathcal{P}(\varsigma_1, \ldots, \varsigma_k) \) denote the probability distribution of the random variable \( M \) such that \( \mathbb{P}(M = m) \propto \varsigma_m \). The PDMPs of interest here can be described algorithmically as in Algorithm 1.

Algorithm 1: A piecewise deterministic Markov process to sample from \( \mu \).

- Initialization \( z(0) = (x(0),v(0)) \), \( T_0 = 0 \) and \( l = 1 \).
- Repeat
  1. Draw \( T_i \) such that \( \mathbb{P}(T_i \geq \tau \mid T_{i-1}) = \exp \left( -\Lambda(\tau - T_{i-1},X_{T_{i-1}},V_{T_{i-1}}) \right) \),
  2. \( (X_t,V_t) = (X_{T_{i-1}} + (t - T_{i-1})V_{T_{i-1}},V_{T_{i-1}}) \) for \( t \in [T_{i-1},T_i) \),
  3. \( X_{T_i} = \lim_{t \uparrow T_i} X_t \) and with \( M \sim \mathcal{P}(\lambda_1(Z_{T_i}), \ldots, \lambda_d(Z_{T_i})) \) set \( V_{T_i} \sim R_{X_{T_i},M}(V_{T_{i-1}}) \),
  4. \( l \leftarrow l + 1 \),

Davis [15] (see also [19] for an alternative construction) shows that this defines a process, of corresponding semigroup \( \{P_t, t \in \mathbb{R}_+ \} \), as soon as the following standard two conditions on the intensity are satisfied [15, p. 62]:

(A3) For \( i \in \llbracket 1, k \rrbracket \),

1. \( \lambda_i \) is measurable and \( t \mapsto \lambda_i(x + tv,v) \) is integrable for all \( (x,v) \in E \),
2. for any \( t > 0 \) and \( (x,v) \in E \), \( \mathbb{E}_{x,v}(N(t)) < \infty \), where \( N(t) := \sum_{i=1}^\infty \mathbb{I}[T_i \leq t] \),
Define for any \((x, v) \in E\) and \(f \in \mathbb{R}^E\), whenever the limit exists,

\[
Df(x, v) := \lim_{h \to 0} \frac{f(x + hv, v) - f(x, v)}{h},
\]

then the extended generator of the process above, which solves the Martingale problem, is of the form

\[
Lf := Df + \sum_{i=1}^{k} \lambda_i \cdot \left[ R_i f - f \right],
\]

for \(f \in \mathcal{D}(L)\), a domain fully characterized by Davis [15, Theorem 26.14, p. 69 and Remark 26.16]. Let \( \mathbf{M}(E) \subset \mathbb{R}^E \) be the set of measurable functions and \( \mathbf{B}(E) \subset \mathbf{M}(E) \) be the set of bounded measurable functions. It can be shown that \( \{P_t, t \geq 0\} \) is a contraction semigroup on \( \mathbf{B}(E) \) equipped with the \( \| \cdot \|_{\infty} \) norm. Further with

\[
\mathbf{B}_0(E) := \left\{ f \in \mathbf{B}(E) : \lim_{t \to 0} \|P_t f - f\|_{\infty} = 0 \right\},
\]

one can show that \( \{P_t, t \geq 0\} \) is a strongly continuous contraction semigroup on \( \mathbf{B}_0(E) \) [15, p. 28-29] of strong generator \((\mathcal{D}_x(L_\infty), L_\infty)\), with \( \mathcal{D}_x(L_\infty) \subset \mathcal{D}(L) \) and for any \( f \in \mathcal{D}_x(L_\infty), L_\infty f = Lf \).

When \( V = \mathbb{R}^d \) (or such that \( E \) is a Riemannian sub-manifold) we define \( \mathbf{C}(E) := \mathbf{C}^0(E) := \{f \in \mathbb{R}^E : f \text{ is continuous}\} \) and

\[
\mathbf{C}^i(E) := \{f \in \mathbb{R}^E : f \text{ is } i \text{ times continuously differentiable}\},
\]

for \( i \in \mathbb{N}_+ \), \( \mathbf{C}^i(X) := \{f \in \mathbb{R}^X : f \text{ is } i \text{ times continuously differentiable}\}, \)

use the simplified notation \( \mathbf{C}(E) := \mathbf{C}^0(E) \), and let \( \mathbf{C}_c(E), \mathbf{C}_c^1(E) \) be the corresponding restrictions to functions \( x \mapsto f(x, v) \) of compact support for any \( v \in V \). We let \( \mathbf{C}_0(E) \) be the set of \( f \in \mathbf{C}(E) \) such that for any \( \epsilon > 0 \) there exists \( M \in \mathbb{R}_+ \) such that \( |f(x, v)| \leq \epsilon \) for \( (x, v) \in B^{\epsilon}(0, M) \times V \) where \( B(0, M) = \{x \in X : \|x\| \leq M\} \) and \( \| \cdot \| \) is the Euclidian norm.

### 5.2 \((\mu, Q)\)-symmetry of some PDMP-Monte Carlo processes

From now on \( Qf(x, v) = f(x, -v) \) for \( f \in \mathbb{R}^E \) and \((x, v) \in E\). In the following we establish simple conditions implying that \( L \) is \((\mu, Q)\)-symmetric on \( \mathbf{C}_c^1(E) \), which cover most known scenarios. Hereafter we will need the following assumption on the potential \( U \).

**(A4)** The potential \( U: X \to \mathbb{R} \) is \( \mathbf{C}^2(X) \) and

\[
\int [1 + \|U(x)\|] \exp \left( -U(x) \right) dx < \infty.
\]

The following was shown in [21, Proposition 3.2] for example.

**Lemma 5.1.** Assume (A4). Then for \( f, g \in \mathbf{C}_c^1(E) \)

\[
\langle Df, g \rangle_\mu = \langle f, -Dg + DU \cdot g \rangle_\mu,
\]

and \(-Df = QDf\).
Proof. Let \( v \in \mathbf{V} \) and for \( h \in \mathbb{R}^E \) define \( x \mapsto h_v(x) := h(x,v) \) then, for \( f,g \in C^1_v(E) \), an integration by part gives

\[
\langle Df_v, g_v \rangle_x = \langle f_v, -Dg_v + DU \cdot g_v \rangle_x,
\]

and we conclude by Fubini’s theorem and integration with respect to \( \varpi \). The second statement follows from the fact that for \( g \in C^1_v(E) \) \( Dg(x,v) = \langle \nabla g(x,v), v \rangle_\mu \) and therefore for \( g = Qf \), \( DF(x,v) = \langle \nabla f(x,-v), v \rangle_\mu \).

The following establishes that a simple property on the family of operators \( \{R_i, i \in [1,k]\} \) ensures \((\mu, Q)-\)symmetry of \( L \), and hence invariance of \( \mu \) if \( C^1_v(E) \) is a core.

**Theorem 5.2.** Let \( \mu \) be a probability distribution defined on \((E,E')\) and consider the semigroup \( \{P_t, t \geq 0\} \) with extended generator \( L \) given in (14). Assume (A4), \( \lambda - Q\lambda = DU \) and that for any \( i \in [1,k] \) the operator \((\lambda_i \cdot R_i)\) is \((\mu, Q)-\)symmetric on \( C^1_v(E) \). Then \( L \) is \((\mu, Q)-\)symmetric on \( C^1_v(E) \).

**Proof.** Let \( f,g \in C^1_v(E) \). By assumption, for \( i \in [1,k] \)

\[
\langle (\lambda_i \cdot R_i)f, g \rangle_\mu = \langle f, Q\lambda_i \cdot QR_iQg \rangle_\mu,
\]

and using \( \lambda - Q\lambda = DU \)

\[
\langle \lambda \cdot f, g \rangle_\mu = \langle f, \lambda \cdot g \rangle_\mu = \langle f, (Q\lambda + DU) \cdot g \rangle_\mu.
\]

Together with Lemma 5.1, the above leads to

\[
\langle LF, g \rangle_\mu = \langle f, QDG \rangle_\mu + \langle f, DG \rangle_\mu + \sum_{i=1}^d \langle f, Q\lambda_i \cdot QR_iQg \rangle_\mu - \langle f, Q\lambda_i \cdot Q^2g \rangle_\mu - \langle f, DU \cdot g \rangle_\mu,
\]

that is \( \langle LF, g \rangle_\mu = \langle f, QLG \rangle_\mu \) and we conclude.

**Remark 5.3.** With an abuse of notation, for \( f \in \mathbb{R}^Y \) let \( Qf := Q\hat{f} \) where for \((x,v) \in E \) \( \hat{f}(x,v) = f(v) \). For \( f \in \mathbb{R}^E \) and for \( x \in X \) denote \( f_x(\cdot) := f(x,\cdot): \mathbf{V} \to \mathbb{R} \). Let \( i \in [1,k] \). If for any \( x \in X \), \( \lambda_{x,i} \cdot R_{x,i} \) is \((\varpi(\cdot),Q)-\)symmetric on \( \mathbf{B}_c(V) \) then for \( f,g \in C^1_v(E) \)

\[
\langle (\lambda_i \cdot R_i)f, g \rangle_\mu = \int \langle (\lambda_{i,x} \cdot R_{i,x})f_x, g_x \rangle_x \pi(dx) = \int \langle f_x, Q(\lambda_{i,x} \cdot R_{i,x})Qg_x \rangle_x \pi(dx) = \langle f, Q\lambda_i \cdot QR_iQg \rangle_\mu,
\]

that is \( (\lambda_i \cdot R_i) \) is \((\mu, Q)-\)symmetric on \( C^1_v(E) \).

The most popular PDMP-MC processes satisfy the properties of Theorem 5.2 and are covered by the following examples. For notational simplicity we may drop the index \( i \) below.

**Example 5.4.** Let \( x \mapsto n(x) \) be a unit vector field and assume that for any \((x,v) \in E \) we have \( v - 2\langle n(x), v \rangle n(x) \in \mathbf{V} \). Consider the operator such that for any \( f \in \mathbb{R}^E \) and \((x,v) \in E \) \( Rf(x,v) := f(x, v - 2\langle n(x), v \rangle n(x)) \) and assume that the property \( R\lambda = Q\lambda \) holds. Note that \( R^2 = \text{Id} \) and that for any \( f \in \mathbb{R}^E \) and \((x,v) \in E \), \( RQf(x,v) = f(x, -v + 2\langle n(x), v \rangle n(x)) \) and hence \( QRQf = Rf \). Therefore for any \( f,g \in C^1_v(E) \),

\[
\langle (\lambda \cdot R)f, g \rangle_\mu = \langle Rf, \lambda \cdot g \rangle_\mu = \langle f, R\lambda \cdot Rg \rangle_\mu = \langle f, Q\lambda \cdot QRQg \rangle_\mu.
\]
Now let \( \{ n_i : X \to \mathbb{R}^d, i \in [1, k] \} \) be unitary vector fields and \( \{ a_i : X \to \mathbb{R}, i \in [1, k] \} \) such that \( \nabla U = \sum_{i=1}^{k} a_i n_i \). Assume that for \( i \in [1, k] \) the intensities are of the form \( \lambda_i(x, v) = \varphi(a_i(x) \langle n_i(x), v \rangle) \) for \( \varphi : \mathbb{R} \to \mathbb{R}^+ \) such that \( \varphi(s) - \varphi(-s) = s \) and \( R, f(x, v) := f(x, v - 2\langle n_i(x), v \rangle n_i(x)) \) for \( f \in \mathbb{R}^E \) and \( (x, v) \in E \). Possible choices of \( \varphi \) are discussed later on and include \( \varphi(s) = \max\{0, s\} \). Then for \( i \in [1, k] \), \( R_i \lambda_i = Q \lambda_i \), \( (\lambda_i \cdot R_i) \) is \((\mu, Q)-\)symmetric on \( C^1_c(E) \) and \( \lambda - Q \lambda = DU \). Therefore Theorem 5.2 holds. This covers the Zig-Zag and Bouncy Particle Sampler processes, for example [2].

**Example 5.5.** The choice \( R_f(x, v) = \int f(x, w) \varpi(dw) \) for \((x, v) \in E \) and \( f \in L^2(\mu) \), the “refreshment” operator, is such that for any \( f, g \in L^2(\mu) \), \( \langle Rf, g \rangle_\mu = \langle f, Rg \rangle_\mu \), \( Rf = Rf \) and \( QRF = RF \) since for any \( x \in X \), \( v \mapsto RF(x, v) \) is constant. If for any \( x \in X \) the mapping \( v \mapsto \hat{\lambda}(x, v) \) is constant (implying \( \hat{\lambda} = Q \hat{\lambda} = 0 \)) we deduce that for any \( f, g \in C^1_c(E) \)

\[
\langle (\hat{\lambda} \cdot R) f, g \rangle_\mu = \langle Rf, \hat{\lambda} \cdot g \rangle_\mu = \langle f, \hat{\lambda} \cdot Rg \rangle_\mu = \langle f, Q \hat{\lambda} \cdot QRFg \rangle_\mu,
\]

that is \((\hat{\lambda} \cdot R) \) is \((\mu, Q)-\)symmetric on \( C^1_c(E) \). In fact, from the proof of Lemma 3.10 we note that \( R \) can be taken to be Horowitz’s refreshment operator.

**Example 5.6.** The choice \( R_x f_x(v) = \int f_x(w) \lambda(x, w) \varpi(dw) \) with \( R_x 1(v) = 1 \) when possible, for any \((x, v) \in E \) and \( f \in C^1_c(E) \) has been suggested in [23]. It is such that for \( f, g \in C^1_c(E) \) and \( x \in X \),

\[
\int f_x(v) g_x(w) \lambda(x, v) \lambda(x, w) \varpi(dw) \varpi(dv) = \int Q f_x(v) g_x(w) \lambda(x, v) \lambda(x, w) \varpi(dw) \varpi(dv),
\]

and we conclude that \( (\lambda_x \cdot R_x) \) is \((\varpi, Q)-\)self-adjoint.

**Remark 5.7.** We note that Theorem 5.2 holds more generally when the operator \( D \) is replaced with the generator \( D_F \) of a dynamic with time-reversal symmetry [32] for which \( \langle D_F f, g \rangle_\mu = \langle f, Q D_F Qg + D_F U \cdot g \rangle_\mu \), which is the case for the Liouville operator for an arbitrary potential \( H(x, v) \), and the condition on the total intensity rate adjusted accordingly. We do not pursue this here for brevity.

### 5.3 Zig-Zag: generator and semigroup properties

Zig-Zag (ZZ) is a particular continuous time Markov process designed to sample from \( \mu \) and described in Alg. 1. The name was coined in [7] and further extended in [6], and can be interpreted as being a particular case of the process studied in [21]. In this scenario \( k = d + 1 \), \( V := \{-1, 1\}^d \), \( \varpi \) is the uniform distribution and, with \( \{ e_i \in \mathbb{R}^d, i \in [1, d] \} \) the canonical basis of \( \mathbb{R}^d \), for \( i \in [1, d] \) and \( (x, v) \in E \) we let \( R_x f(x, v) := f(x, v - 2v_i e_i) \) where \( v_i := \langle v, e_i \rangle \). Note that this corresponds to \( n_i(x) = e_i \) in Example 5.4. For \( i = d + 1 \) we let \( \lambda_{d+1}(x, v) = \hat{\lambda} \) for \( \hat{\lambda} \in \mathbb{R}^+ \) and \( R_{d+1} \) is as in Example 5.5. We require the following assumptions on the intensities.

**A5** For any \( i \in [1, d] \) and \((x, v) \in E \) we have

(a) \( \lambda_i \in C^1(E) \) and \( \lambda_i > 0 \),

(b) \( \lambda_i(x, v) - Q \lambda_i(x, v) = \partial_i U(x)v_i \),

(c) \( R_i \lambda_i(x, v) = Q \lambda_i(x, v) \).

The following establishes the existence of such intensities.
Proposition 5.8. Assume (A4). Let $\phi : \mathbb{R} \rightarrow [0,1]$ be such that $r\phi(r^{-1}) = \phi(r)$ for $r \geq 0$ and define for any $(x,v) \in E$ and $i \in [1,d]$, 
\[ \lambda_i^\phi(x,v) := - \log \left( \phi \left( \exp(\partial_i U(x)v_i) \right) \right) \geq 0. \]
If further $\phi < 1$ and $\phi \in C^1(\mathbb{R})$ then $\{\lambda_i, i \in [1,d]\}$ satisfies (A5).

Proof. The first property is direct. For the second property, from the assumption on $\phi$, we have
\[ \lambda_i^\phi(x,v) - \lambda_i^\phi(x,-v) = \lambda_i^\phi(x,v) - \partial_i U(x)(-v_i) + \log \left( \phi \left( \exp(\partial_i U(x)v_i) \right) \right) \]
\[ = \lambda_i^\phi(x,v) + \partial_i U(x)v_i - \lambda_i^\phi(x,v). \]
The last property was established in Example 5.4 (here $n_i = e_i$ for $i \in [1,d]$).

Corollary 5.9. The choice $\phi(r) = r/(1+r)$ satisfies the assumptions of Proposition 5.8, but this is not the case for the canonical choice $\phi(r) = \min\{1,r\}$.

We now establish properties required of $\{P_t, t \geq 0\}$ and its generator in order to check (A2) and apply Theorem 4.6 and Lemma 4.7.

Proposition 5.10. Let $L$ be the extended generator of the ZZ process and assume (A4)-(A5). Then $L$ is $(\mu,Q)$--symmetric on $C^1_c(E)$.

Proof. This follows the discussion of Example 5.4 and application of Theorem 5.2.

For $A, B \subseteq M(E)$ and $t > 0$ we let $P_t A \subseteq B$ mean that for any $f \in A$ such that $P_t f$ exists, then $P_t f \in B$.

A semigroup $\{P_t, t \geq 0\}$ is said to be Feller if $C_0(E) \subseteq B_0(E)$ and $\{P_t, t \geq 0\}$ is a strongly continuous contraction semigroup on $C_0(E)$ equipped with $\| \cdot \|_x$, that is for any $s, t > 0$, $P_{s+t} = P_s P_t$, $\|P_t f\|_x \leq \|f\|_x$, $P_t C_0(E) \subseteq C_0(E)$ and for any $f \in C_0(E)$, $\lim_{t \to 0} \|P_t f - f\|_x = 0$.

Theorem 5.11. Consider a ZZ process of intensities $\{\lambda_i, i \in [1,d+1]\}$ satisfying (A5). Then

(a) $\{P_t, t \geq 0\}$ is Feller,
(b) for any $t > 0$, $P_t C^1_c(E) \subseteq C^1_c(E)$,
(c) $C^1_c(E)$ is a core for the strong generator of the Feller semigroup $\{P_t, t \geq 0\}$,
(d) $\mu$ is invariant for $\{P_t, t \geq 0\}$,
(e) $\{P_t, t \geq 0\}$ can be extended to a strongly continuous semigroup on $L^2(\mu)$ equipped with $\| \cdot \|_\mu$,
(f) $C^1_c(E)$ is a core for the strong generator of the extended semigroup on $L^2(\mu)$.

Proof. The proof is an adaptation of [19, Proposition 15 and Lemma 17] to the present ZZ scenario for which $V$ consists of a finite set of bounded velocities. Note that due to the discrete nature of $V$ gradients of the form $\nabla_{x,v} f(x,v)$ (for suitable functions) appearing in the statements of [19] should be replaced throughout with derivatives with respect to the position only, that is $\nabla_x f(x,v)$. Establishing [19, Lemma 17 and Corollary 19] requires checking that the ZZ process is non-explosive and that its characteristics satisfy in particular conditions [19, (A2) and (A3)] which we refer to as (A2) and (A3) in the present manuscript in order to avoid confusion. For convenience we provide simplified formulations, adapted to the specific ZZ process considered here, of (A2) and (A3) and statements of [19, Proposition 15 and Lemma 17] in Appendix A where we also check that these hold.
Once the conditions for [19, Lemma 17 and Corollary 19] to hold are satisfied the reasoning is as follows. [19, Proposition 15 (b)] allows us to conclude that $C^1_c(E) \subset D(\mu)$ and [19, Lemma 17] implies that for $i \in \{0,1\}$ and $t \geq 0$, $P_t C^i(E) \subset C^i(E)$. Let $f \in C_0(E)$, $\epsilon > 0$ and $M > 0$ be such that $|f(x,v)| \leq \epsilon$ for $(x,v) \in B^c(0,M) \times V$. Then for $(x,v) \in B^c(0,M + d^{1/2}t) \times V$, $\sup \{P_t(x,v,:)\} \subset B^c(0,M) \times V$ and therefore $|P_t f(x,v)| \leq \epsilon$ and with [19, Lemma 17] for $i = 0$, we deduce $P_t f \in C_0(E)$. Therefore for any $t \geq 0$ $P_t C_0(E) \subset C_0(E)$ and from [19, Proposition 15 (a)] $C_0(E) \subset B_0(E)$ from which we conclude that $\{P_t, t \geq 0\}$ is a strongly continuous contraction semigroup on $C_0(E)$ equipped with $\| \cdot \|_\infty$, that is $\{P_t, t \geq 0\}$ is Feller. Let $f \in C^1_c(E)$, then using the reasoning above with $\epsilon = 0$ and [19, Lemma 17] for $i = 1$ we deduce that for any $t \geq 0$ $P_t f \in C^1_c(E)$, that is for any $t \geq 0$ $P_t C^1_c(E) \subset C^1_c(E)$. This stability property, together with the Feller property and density of $C^1_c(E)$ in $C_0(E)$ allows us to conclude that $C^1_c(E)$ is a core for the strong generator $L_\infty$ of $\{P_t, t \geq 0\}$ as a semigroup defined on $C_0(E)$ equipped with $\| \cdot \|_\infty$. [20, Proposition 3.3] from which we deduce that $C^1_c(E)$ is a core for $(L\mu, D^2(L\mu, \mu))$. □

### 5.4 Zig-Zag - main results and some examples

The main result of this section is the ordering of Theorem 5.12, which we illustrate with two examples.

**Theorem 5.12.** Assume (A4) and consider two ZZ processes of intensities $\{\lambda_{1,i}, i \in [1,d+1]\}$ and $\{\lambda_{2,i}, i \in [1,d+1]\}$ satisfying (A5) such that for $i \in [1,d+1]$, $\|\lambda_{1,i} - \lambda_{2,i}\|_\mu < \infty$. Then if for all $g \in C^1_c(E)$,

$$\langle g, -(L_1 - L_2)Qg \rangle_\mu = \sum_{i=1}^{d+1} \langle g, (\lambda_{1,i} - \lambda_{2,i}) \cdot [\Id - R_iQ]g \rangle_\mu - \langle g, (\lambda_1 - \lambda_2) \cdot [\Id - Q]g \rangle_\mu \geq 0,$$  

(15)

then $\var_\lambda(L_1, f) \leq \var_\lambda(L_2, f)$ for $\lambda > 0$ and $f \in L^2(\mu)$ such that $Qf = f$.

**Remark 5.13.** The assumption on the intensity is satisfied as soon as for some $c, C > 0$, for any $i \in [1,d+1]$ and $(x,v) \in E$, $\lambda_{1,i}(x,v) \leq c + C\|\nabla U(x)\|$ and $\int \|\nabla U\|^2 d\pi < \infty$. As we shall see this can be checked for various examples.

**Proof.** We check that the assumptions in (A2) are satisfied. First we note that for any $\beta \in [1,2]$ one can define a ZZ process with intensities $((2-\beta)\lambda_{1,i} + (\beta - 1)\lambda_{2,i}$ for $i \in [1,d+1]$ and extended generator $(2-\beta) L_1 + (\beta - 1)L_2$. Further note that for $i \in [1, d+1]$, $(2-\beta)\lambda_{1,i} + (\beta - 1)\lambda_{2,i}$ satisfies (A5). From Theorem 5.11 for $\beta \in [1,2]$ we have that $C^1_c(E) \subset D^2(L\mu(\beta), \mu)$ is a core for $L_\mu(\beta)$, the generator of $\{P_t(\beta), t \geq 0\}$ on $L^2(\mu)$, dense in $L^2(\mu)$ and such that for any $t \geq 0$, $P_t(\beta)C^1_c(E) \subset C^1_c(E)$. From the definition of $C^1_c(E)$, $QC^1_c(E) \subset C^1_c(E)$ and from Proposition 5.10 $L_\mu(\beta)$ is $\mu, Q$–symmetric on $C^1_c(E)$ for any $\beta \in [1,2]$. One can therefore apply Theorem 4.4 and deduce that for any $\beta \in [1,2]$, $\{P_t(\beta), t \geq 0\}$ is $\mu, Q$–self-adjoint. We now turn to checking the assumptions of Lemma 4.7. First note that we have for $g \in C^1_c(E)$

$$-(L_1 - L_2)g = \sum_{i=1}^{d+1} (\lambda_{1,i} - \lambda_{2,i}) \cdot [\Id - R_i]g,$$
where for $i \in [1, d + 1]$
\[
\| (\lambda_{1,i} - \lambda_{2,i} \cdot [\text{Id} - R_i]g) \|_{\mu} \leq \| \lambda_{1,i} - \lambda_{2,i} \|_{\mu} \| [\text{Id} - R_i]g \|_{\infty} \\
\leq 2 \| \lambda_{1,i} - \lambda_{2,i} \|_{\mu} \| g \|_{\infty},
\]
with $\| \lambda_{1,i} - \lambda_{2,i} \|_{\mu} < \infty$ by assumption. Now for $\beta \in [1, 2], f \in C^1_\text{c}(E)$ and $t \in \mathbb{R}^+$, we choose $g_t = P_t(\beta)f \in C^1_\text{c}(E)$ or $g_t = QP_t(\beta)f \in C^1_\text{c}(E)$ (from Theorem 5.11), note that in both scenarios $\| g \|_{\infty} \leq \| f \|_{\infty}$ and deduce the continuity and summability conditions of Lemma 4.7. We conclude with Theorem 4.6.

**Example 5.14.** When $d = 1$, $R_1 = Q$ and therefore $R_1Q = \text{Id}$. If we further assume that $\lambda_{1,2} = \lambda_{2,2} = \lambda$ then for all $g \in C^1_\text{c}(E)$
\[
\langle g, -(L_1 - L_2)Qg \rangle_{\mu} = -\langle g, (\lambda_{1,1} - \lambda_{2,2}) \cdot [\text{Id} - Q]g \rangle_{\mu} \geq 0,
\]
whenever $\lambda_{2,1} \geq \lambda_{1,1}$, a result similar to that of [5].

The situation where the total event rate is constant, that is $\lambda_1 = \lambda_2$ in the expression above, but distributed differently between updates of the velocity leads to the following.

**Example 5.15.** Let $d = 2$ and for $g \in C^1_\text{c}(E)$ let
\[
Lg = Dg + \sum_{i=1}^{2} \lambda_i \cdot [R_i - \text{Id}]g
\]
and consider the ZZ processes of generators, for $C^1(X) \ni \tilde{\gamma}: X \rightarrow \mathbb{R}^+$,
\[
L_1g = Lg + \tilde{\gamma}/2 \cdot \sum_{i=1}^{2} [R_i - \text{Id}]g
\]
\[
L_2g = Lg + \tilde{\gamma} \cdot [I - \text{Id}]g.
\]
Then for $g \in C^1_\text{c}(E)$,
\[
\langle g, -(L_1 - L_2)Qg \rangle_{\mu} = \langle g, \tilde{\gamma}/2 \cdot \sum_{i=1}^{2} [\text{Id} - R_iQ]g \rangle_{\mu} - \langle g, \tilde{\gamma} \cdot [\text{Id} - I]\rangle_{\mu} \geq 0,
\]
where the equality follows from $R_1Q = R_2, R_2Q = R_1, \text{Lemma B.1 and } [41, \text{p. 52}]. \text{ We therefore conclude that in this setup partial refreshment of the velocity is superior to full refreshment in terms of asymptotic variance.}

We note that checking (15) involves the difference of two non-negative terms (from Lemma B.1) and may be challenging to establish for this class of processes. For example we have not been able to extend the result of Example 5.14 to the situation where $d \geq 2$, yet. We have not explored comparisons involving other updates $R_i$, which would require establishing Theorem 5.11 for this setup, and rather focus on the following issue. Intensities of interest may not satisfy (A5) and we may not be able to apply Theorem 5.11. This is the case for the so-called canonical choice $\lambda(x, v) = (\partial U(x)v)_+$, which may however be of interest as suggested by the following. In the following discussion we assume $d = 1$ for presentational simplicity, but the approach is valid for $d \geq 1$. 

28
Proposition 5.16. Let \( \lambda : E \to \mathbb{R}_+ \) be an intensity satisfying \( \lambda(x, v) - Q\lambda(x, v) = \partial U(x)v, \) then \( \lambda(x, v) \geq (\partial U(x)v)_+ \).

**Proof.** For \( x \in X \) consider the sets \( V_+(x) = \{ v \in V : \pm \partial U(x)v \geq 0 \} \). From the assumption, for \( (x, v) \in E \)
\[ \lambda(x, v) - Q\lambda(x, v) = (\partial U(x)v)_+ - (\partial U(x)v)_+, \]
and we deduce that for \( v \in V_+(x) \)
\[ \lambda(x, \pm v) = \lambda(x, \mp v) + (\pm \partial U(x)v)_+ \geq (\pm \partial U(x)v)_+, \]
and conclude since \( V = \{-1, 1\} \).

A natural question is whether we can establish that the choice \( \lambda^0(x, v) := (\partial U(x)v)_+ \) is optimum in terms of asymptotic variance. Our argument relies on the existence of regularizing intensities satisfying the following properties.

(A6) The family of intensities \( \{\lambda^\epsilon, \epsilon \geq 0\} \) satisfies for any \( (x, v) \in E \) and \( \epsilon > 0 \),
- (a) \( \lambda^\epsilon \in C^1(E) \) and \( \lambda^\epsilon > 0 \),
- (b) \( \epsilon \mapsto \lambda^\epsilon(x, v) \) is non-increasing,
- (c) \( \lambda^\epsilon(x, v) - Q\lambda^\epsilon(x, v) = \partial U(x)v \),
- (d) \( \lim_{\epsilon \downarrow 0} \sup_{(x, v) \in E} |\lambda^\epsilon(x, v) - \lambda^0(x, v)| = 0 \).

Intensities satisfying these properties exist:

Proposition 5.17. Assume (A4) and for any \( \epsilon > 0 \) define the intensities such that for \( (x, v) \in E \),
\[ \lambda^\epsilon(x, v) := -\log \left( \phi_\epsilon \left( \exp(\partial U(x)v) \right) \right), \]
where for \( r > 0 \)
\[ \phi_\epsilon(r) := r[1 - \Phi(\epsilon/2 + \log(r)/\epsilon)] + [1 - \Phi(\epsilon/2 - \log(r)/\epsilon)] > 0, \]
with \( \Phi(\cdot) \) the cumulative distribution function of the \( \mathcal{N}(0, 1) \). Then \( \{\lambda^\epsilon, \epsilon > 0\} \) satisfies (A6).

**Proof.** As shown in Proposition D.1 \( \phi_\epsilon(r) \) is the acceptance probability of the penalty method [14], a particular instance of the Metropolis-Hastings algorithm, and therefore satisfies the assumptions of Proposition 5.8. Condition (A6)-(d) is a consequence of the corollary of Proposition D.1.

Theorem 5.18. Let \( d = 1 \), assume (A4) and \( \int \|\nabla U\|^2 \phi_\epsilon < \infty \), and consider two ZZ processes of common invariant distribution and of intensities \( \lambda_1 \) and \( \lambda_2 \) where \( \lambda_1(x, v) := (\partial U(x) \cdot v)_+ \) and \( \lambda_2(x, v) := \lambda_1(x, v) + \gamma(x, v) \) with \( 0 \leq \gamma \leq c + C \|\nabla U\| \) for \( c, C > 0 \), \( \gamma \in C^1(E) \) and such that \( \gamma - Q\gamma = 0 \). Then for any \( f \in L^2(\mu) \) such that \( Qf = f \) and \( \lambda \in [0, 1] \)
\[ \text{var}_\lambda(f, L_1) \leq \text{var}_\lambda(f, L_2). \]

**Proof.** We consider regularized intensities \( \lambda_2^\epsilon(x, v) := \lambda_1^\epsilon(x, v) + \gamma(x, v) \) satisfying (A6) (we have shown that we can construct such intensities in Proposition 5.17). From Example 5.14 and Theorem 5.12, for any \( f \in L^2(\mu) \) such that \( Qf = f \) and \( \epsilon > 0 \) we have
\[ \text{var}_\lambda(f, L_1^\epsilon) \leq \text{var}_\lambda(f, L_2^\epsilon). \]

We can now conclude with Theorem C.2 and Lemma C.1.
One can consider more general forms for $\lambda_2$ in the theorem above. For example the result will hold when $\gamma$ can be uniformly approximated by a sequence $\{\gamma^\epsilon \in C^1(E), \epsilon > 0\}$ such that $\gamma^\epsilon \geq 0$ for $\epsilon_0 > \epsilon > 0$ for some $\epsilon_0 > 0$. Another possibility is to consider generalizations of the ideas of Proposition 5.17: for example with $\hat{\phi}(r) = r/(1 + r)$ instead of $\phi(r) = \min\{1, r\}$ as a starting point in Proposition D.1 one can analogously define a family of acceptance ratios which is automatically such that $\hat{\phi}_\epsilon(r) \leq \phi_\epsilon(r)$ for $\epsilon > 0$ and $r \geq 0$, define the corresponding intensities, and then proceed as above to compare the processes with intensities derived from $\hat{\phi}(\cdot)$ and $\phi(\cdot)$.

6 Conclusion

We have extended the set of practical tools available to characterize existing Markov chain or process Monte Carlo algorithms to the scenario where the building blocks involved are not reversible. We have shown how they can be used to characterize algorithms previously beyond the reach of earlier theory, confirming in some cases their good properties in full generality. A natural question, not addressed here, is that of the comparison of speed of convergence to equilibrium for the class of processes considered here, for which a partial result exists in the time-reversible setup (see Theorem 2.7). Consider for example the scenario where $\pi$ has finite support $[1,d]$ and the transition in (1) is combined into a $2$--cycle (cf. Subsection 3.1) with the $(\mu, Q)$--reversible transition $P'_\alpha = (1 - \alpha)\text{Id} + \alpha Q$ for $\alpha \in [0,1]$, as suggested in [16] (see also references therein). The analysis of [16] (see also [24]), in the situation where $\pi$ is the uniform distribution, shows that near optimal convergence speed to equilibrium is achieved for $\alpha(d) = c/d > 0$, whereas application of Theorem 3.4 shows that $\alpha$ closer to zero is a better choice when asymptotic variance is of interest, since $E(g, QP'_\alpha) = (1 - \alpha)/2 \{g(x,v) - g(x,-v)\}^2 \mu(dx,v)$. To the best of our knowledge no systematic spectral theory exists in the setup considered in this manuscript, despite the numerous analogies with the $\mu$--self-adjoint scenario and its practical interest. We note the very recent work [8] (focused on a restricted scenario) and [2] (which provides lower bounds on the spectral gap) which both suggest difficulties and the need for the development of new tools.

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A Key results of \([19]\)

For the reader’s convenience we reformulate the results of \([19]\) for the specific scenario where the flow used is linear, that is we consider the PDMP of extended generator

\[
Lf = Df + \lambda[R - \text{Id}]f,
\]

where here

\[
Rf = \lambda^{-1} \sum_{i=1}^{d} \lambda_i R_i f.
\]

Following the terminology of \([19]\), we refer to \((\lambda, R)\) as characteristics of the process. The deterministic flow for this process is \(\varphi_t(x, v) = (x + tv, v)\) and the associated regularity condition required in \([19]\) translates to: for any \(v \in \mathcal{V}\), \((x, t) \mapsto x + tv\) is continuously differentiable (which is trivially satisfied). For brevity we omit this property from the statements of \([19]\), leading to:

\(\langle A2 \rangle\) Let \(\{P_t, t \geq 0\}\) be a non-explosive PDMP semigroup with characteristics \((\lambda, R)\). Assume that for any \(T \in \mathbb{R}_+\) there exists \(M \in \mathbb{R}_+\) such that for all \((x, v) \in E\) and \(t \in [0, T]\), \(\text{supp}(P_t(x, v; \cdot)) \subset B(x, M) \times \mathcal{V}\).

\(\langle A3 \rangle\) The characteristics \((\lambda, R)\) satisfy

(a) for all compact sets \(K \subset E\) and \(T \in \mathbb{R}_+\) there exists a compact set \(\bar{K} \subset E\) such that for all \(n \in \mathbb{N}_+\) and \(\{t_i \in \mathbb{R}_+\), \(i \in [1, n]\}\) such that \(\sum_{i=1}^{n} t_i \leq T\), there exists a sequence of compact sets \(\{K_i \subset E, i \in [0, n]\}\) such that \(\bigcup_{i=0}^{n} K_i \subset \bar{K}\) with \(K_0 := K\) and

(i) \(K_i, i \in [1, n]\) dependent on \(\{t_i \in \mathbb{R}_+, j \in [1, i]\}\),

(ii) for \(i \in [0, n - 1]\), \(s_i \in [0, t_{i+1}]\) and \(s_{n+1} \in [0, T - \sum_{i=1}^{n} t_j]\)

\[
\bigcup_{(x,v) \in K_i} \text{supp}\{R(x + t_{i+1}v, v; \cdot)\} \subset K_{i+1},
\]

and for any \((x, v) \in K_i\), then \((x + s_{i+1}v, v) \in \bar{K}\).

(b) \(\lambda \in \mathcal{C}^1(E), (\lambda R)\mathcal{C}^1(E) \subset \mathcal{C}^1(E)\) and there exists a locally bounded function \(\Psi: E \to \mathbb{R}_+\)

such that for all \((x, v) \in K, K\) compact, and \(f \in \mathcal{C}^1(E)\)

\[
\|\nabla_x (\lambda Rf)(x, v)\| \leq \sup_{(x,v) \in K} \|\Psi(x, v)\|_{\infty} \sup \|f(y, w) + \|\nabla_x f(y, w)\| : (y, w) \in \text{supp} \{R(x, v; \cdot)\} \|.
\]

As pointed out in \([19]\), the first property (which the authors refer to as compact compatibility) implies that the process is non-explosive. The two results of \([19]\) we use are:

**Proposition** \([\text{[19, Proposition 15]}]\). Let \(\{P_t, t \geq 0\}\) be a PDMP semigroup of characteristics \((\lambda, R)\) satisfying \(\langle A2 \rangle\). Then

(a) \(\mathcal{C}_0(E) \subset \mathcal{B}_0(E)\),

(b) if \(\lambda \in \mathcal{C}(E)\) and \((\lambda R)\mathcal{C}_c(E) \subset \mathcal{C}_c(E)\) then \(\mathcal{C}_c^1(E) \subset \mathcal{D}_\alpha(L_\infty)\).

**Lemma** \([\text{[19, Lemma 17]}]\). Let \(\{P_t, t \geq 0\}\) be a non-explosive PDMP semigroup of characteristics \((\lambda, R)\) satisfying \(\langle A3 \rangle\). Then for \(i \in \{0, 1\}, t \geq 0\) \(P_t \mathcal{C}^i(E) \subset \mathcal{C}^i(E)\).
We now establish that these results hold for the ZZ process considered here.

Checking \( \langle A2 \rangle \) is identical to the argument \([19, \text{Proposition 23}]\) concerned with the scenario where the velocity is bounded, since for any \( t \in \mathbb{R}_+ \) and \((x, v) \in E, P_t(x, v; B(x, \sqrt{dt}) \times V) = 1\). We turn to checking the conditions of \([19, \text{Proposition 15}]\). From \( \langle A5 \rangle \) \( \lambda \in C^1(E) \) and \( \lambda > 0 \) and for any \( f \in C_c(E) \) then \( Rf(x,v) \in C_c(E) \) since for \( i \in [1,d] \), \( R_i f \in C_c(E) \). We conclude.

Establishing that \( \langle A3 \rangle \)-\( (a) \) is identical to the result in the proof of \([19, \text{Proposition 23}]\) concerned with the linear flow and bounded velocities. We repeat their argument adapted to the present scenario: for all \( M \in \mathbb{R}_+ \) let \( B(0,M) \subset X \) then for all \((x, v) \in B(0,M) \times V, R(x,v;B(0,M) \times V) = 1\). Therefore, for any \( K \subset B(0,M_k) \times V \) (with \( M_k \) such that the projection of \( K \) on \( X \) is contained in \( B(0, M_K) \)) and \( T \in \mathbb{R}_+ \) \( \langle A3 \rangle \)-\( (a) \) is satisfied with \( K = B(0, M_K + \sqrt{d}T) \times V \) and \( K_i := B(0, M_K + \sqrt{d} \sum_{j=0}^3 t_j) \times V \). As a result the process is non-explosive. Finally we check that \( \langle A3 \rangle \)-\( (b) \) holds. For \( f \in C^1(E) \)

\[
\|\nabla_x(\lambda Rf)(x,v)\| \leq \sum_{i=1}^{d+1} |R_i f(x,v)| \|\nabla x \lambda_i(x,v)\| + \lambda_i(x,v) \|\nabla x (R_i f)(x,v)\| \\
\leq \left( \lambda(x,v) \vee \sum_{i=1}^{d+1} \|\nabla x \lambda_i(x,v)\| \right) \sup \{|f(y,w)| + \|\nabla x f(y,w)\|, (y,w) \in \text{supp} \{R(x,v; \cdot)\}|.
\]

From \( \langle A5 \rangle \) \((x,v) \mapsto \lambda(x,v) \vee \sum_{i=1}^{d+1} \|\nabla x \lambda_i(x,v)\| \) is locally bounded. We conclude that \([19, \text{Lemma 17}]\) holds.

## B Expression for Dirichlet forms

Computation of \( \mathcal{E}(f, LQ) \) requires computation of terms of the form \( \langle f, \lambda \cdot [\text{Id} - R]Qf \rangle \). The identity

\[
\langle f, \lambda \cdot [\text{Id} - R]Qf \rangle = \langle f, \lambda \cdot [\text{Id} - R]Qf \rangle - \langle f, \lambda \cdot [\text{Id} - Q]f \rangle
\]

motivates the following result.

**Lemma B.1.** Assume that the operator \( R \) is such that for any \( x \in X \), \( \lambda_x \cdot R_x \) is \((\mathcal{F}, Q)\)-symmetric on \( \mathcal{D}(R_x) \). Then for any \( f \in L^2(\mu) \) such that for any \( x \in X \), \( f_x \in \mathcal{D}(R_x) \) and the integral exists, we have

\[
\langle f, \lambda \cdot [\text{Id} - R]Qf \rangle = \frac{1}{2} \int \left( (f(x,v) - f(x,w))^2 \lambda(x,v) \mu(dx,v) R_x Q(v,dw) \right).
\]

**Corollary B.2.** Note that \( R_x = \text{Id} \) is \((\mathcal{F}, Q)\)-symmetric and therefore

\[
\langle f, \lambda \cdot [\text{Id} - Q]f \rangle = \frac{1}{2} \int (f(x,v) - Qf(x,v))^2 \lambda(x,v) \mu(dx,v).
\]

**Proof.** By assumption \( \langle \lambda \cdot RQf, g \rangle = \langle Qf, Q(\lambda \cdot R)Qg \rangle = \langle f, \lambda \cdot RQg \rangle \), that is \( \lambda \cdot RQ \) is symmetric. Now we use polarization

\[
\langle f, \lambda \cdot [\text{Id} - R]Qf \rangle = \frac{1}{2} \int \left( 2f^2(x,v) + (f(x,v) - f(x,w))^2 - f^2(x,v) - f^2(x,w) \right) \lambda(x,v) \mu(dx,v) R_x Q(v,dw)
\]

\[
= \frac{1}{2} \left( \int (f(x,v) - f(x,w))^2 \lambda(x,v) \mu(dx,v) R_x Q(v,dw) - \int f^2(x,v) [\lambda(x,v) - \lambda(x,v)] \mu(dx,v) \right),
\]

where, with \((x,v) \mapsto 1(x,v) = 1\) we have used \( \langle 1, \lambda \cdot RQf^2 \rangle = \langle \lambda, f^2 \rangle \) since \( \lambda \cdot RQ \) is symmetric. \( \square \)
C Continuity of $\varepsilon \mapsto \var\lambda(f, L_\varepsilon)$ for

Lemma C.1. For any $\varepsilon \geq 0$ let $\{P^\varepsilon_t, t \geq 0\}$ be a semigroup on $L^2(\mu)$ leaving $\mu$ invariant, or generator $(L_\varepsilon, D^2(L_\varepsilon, \mu))$ and assume that for any $t \geq 0$ and $f \in L^2(\mu)$

$$\lim_{\varepsilon \downarrow 0} \|P^\varepsilon_t f - P^0_t f\|_\mu = 0.$$  

Then for any $f \in L^2(\mu)$ and $\lambda > 0$,

$$\lim_{\varepsilon \downarrow 0} \var\lambda(f, L_\varepsilon) = \var\lambda(f, L_0).$$

Proof. For $\lambda > 0$ and $f \in L^2(\mu)$ we have

$$|\var\lambda(f, L_\varepsilon) - \var\lambda(f, L_0)| \leq \int \int \exp(-\lambda t)|f(x, v)||P^\varepsilon_t f(x, v) - P^0_t f(x, v)|\mu(d(x, v))dt,$$

$$\leq \|f\|_\mu \int \exp(-\lambda t)||P^\varepsilon_t f - P^0_t f\|_\mu dt,$$

from the Cauchy-Schwarz inequality. Since for $t \geq 0$ $\|P^\varepsilon_t f - P^0_t f\|_\mu \leq 2\|f\|_\mu$ we can apply the dominated convergence theorem and conclude.

Theorem C.2. Let $d = 1$. For any $\varepsilon > 0$, let $\{P^\varepsilon_t, t \geq 0\}$ be a ZZ process of intensity $A$ as in Proposition 5.17. Then, with $\{P_t, t \geq 0\}$ the semigroup of the ZZ process using canonical intensities,

(a) for any $f \in B(E)$, $(x, v) \in E$ any $t \geq 0$ and $\varepsilon > 0$ such that $1 - \left[\exp(\varepsilon) - 1\right]^{1/2} > 0$,

$$|P_t f(x, v) - P^\varepsilon_t f(x, v)| \leq -2 \log \left\{1 - \left[\exp(\varepsilon) - 1\right]^{1/2}\right\} t\|f\|_\infty,$$

(b) $\{P_t, t \geq 0\}$ is Feller and $C^1_\varepsilon(E)$ is a core for the corresponding strong generator,

(c) $\mu$ is invariant for $\{P_t, t \geq 0\}$,

(d) $\{P_t, t \geq 0\}$ can be extended to a strongly continuous semigroup on $L^2(\mu)$ equipped with $\|\cdot\|_\mu$.

(e) For any $f \in L^2(\mu)$ and $t > 0$ we have

$$\lim_{\varepsilon \downarrow 0} \|P_t f - P^\varepsilon_t f\|_\mu = 0.$$  

Proof. For any $\varepsilon > 0$ (A6) implies (A5) from which we deduce that the conclusions of Theorem 5.11 hold for $\{P^\varepsilon_t, t \in \mathbb{R}_+\}$. Further from Proposition D.1 and its corollary, for any $\varepsilon > 0$ such that $1 - \left[\exp(\varepsilon) - 1\right]^{1/2} > 0$ we have $R^\varepsilon_1 = R_1$ and $\|\lambda - \lambda^\varepsilon\|_\infty \leq -\log \left\{1 - \left[\exp(\varepsilon) - 1\right]^{1/2}\right\}$. Consequently we can apply [19, Proposition 11, Theorem 21, Corollary 22] and deduce the first three claims. The fourth claim is direct and obtained by density of $C_0(E)$ in $L^2(\mu)$. For the fifth claim note that for any $t \geq 0$, $\varepsilon > 0$, $f \in L^2(\mu)$ and $\hat{f} \in C_0(E)$ we have

$$\|P_t f - P^\varepsilon_t f\|_\mu \leq \|P_t f - P_1 \hat{f}\|_\mu + \|P_1 \hat{f} - P^\varepsilon_t \hat{f}\|_\mu + \|P^\varepsilon_t f - P_t \hat{f}\|_\mu \leq 2\|f - \hat{f}\|_\mu - 2 \log \left\{1 - \left[\exp(\varepsilon) - 1\right]^{1/2}\right\} t\|\hat{f}\|_\infty,$$

where we have used the contraction property of $P_t$ and $P^\varepsilon_t$, the first claim and the corollary of Proposition D.1. Now for any $\varepsilon > 0$, by density of $C_0(E)$ in $L^2(\mu)$ we can find $\hat{f} \in C_0(E)$ such that $2\|f - \hat{f}\|_\mu \leq \varepsilon/2$ and $\varepsilon_0 > 0$ such that for any $0 \leq \varepsilon \leq \varepsilon_0$, $-2 \log \left\{1 - \left[\exp(\varepsilon) - 1\right]^{1/2}\right\} t\|\hat{f}\|_\infty \leq \varepsilon/2$. We conclude.
D Regularized intensities

Proposition D.1. With the notation of Proposition 5.17 we have the alternative expression for \( r \geq 0 \) and \( \epsilon \geq 0 \),

\[
\phi_\epsilon(r) = \int \min \{1, r \exp(-\epsilon/2 + \epsilon^{1/2}z)\} \mathcal{N}(z; 0, 1) dz ,
\]

\( \phi_\epsilon(r) < 1 \) for \( \epsilon > 0 \) and

\[
0 \leq \phi_0(r) - \phi_\epsilon(r) \leq \phi_0(r) \left\lfloor \exp(\epsilon) - 1 \right\rfloor^{1/2} .
\]

Proof. First claim. This is direct for \( r = 0 \). For \( \epsilon, r > 0 \), with \( A_r := \{ z \in \mathbb{R} : \log r - \epsilon/2 + \epsilon^{1/2}z \geq 0 \} \)

\[
\phi_\epsilon(r) := 1 - \Phi(\epsilon^{1/2}/2 - \epsilon^{-1/2} \log r) + r \int_{A_r} \exp \left(-\epsilon/2 + \epsilon^{1/2}z\right) \mathcal{N}(z; 0, 1) dz .
\]

Noting that \( \epsilon^{1/2}z - z^2/2 = -(z - \epsilon^{1/2})^2/2 + \epsilon/2 \), and together with \( Z \sim \mathcal{N}(0, 1) \), we have

\[
(2\pi)^{-1/2} \int_{A_r} \exp \left(-\epsilon/2 + \epsilon^{1/2}z - \frac{1}{2} z^2\right) dz = \mathbb{P} \left(Z + \epsilon^{1/2} < \epsilon^{1/2}/2 - \epsilon^{-1/2} \log r\right)
\]

\[
= \mathbb{P} \left(Z < -\epsilon^{1/2}/2 - \epsilon^{-1/2} \log r\right)
\]

\[
= 1 - \Phi(\epsilon^{1/2}/2 + \epsilon^{-1/2} \log r) ,
\]

and we conclude. Second claim. The leftmost inequality follows from Jensen’s inequality (twice). Since for \( a, b > 0 \), \( \min \{1, ab\} \geq \min \{1, a\} \min \{1, b\} \) and using the expressions for the mean and variance of the log-normal distribution,

\[
\phi_0(r) - \phi_\epsilon(r) = \int \left[ \min \{1, r\} - \min \{1, r \exp \left(-\epsilon/2 + \epsilon^{1/2}z\right)\} \right] \mathcal{N}(z; 0, 1) dz
\]

\[
\leq \min \{1, r\} \int \left[ 1 - \min \{1, \exp \left(-\epsilon/2 + \epsilon^{1/2}z\right)\} \right] \mathcal{N}(z; 0, 1) dz
\]

\[
= \phi_0(r) \int \max \{0, 1 - \exp \left(-\epsilon/2 + \epsilon^{1/2}z\right)\} \mathcal{N}(z; 0, 1) dz
\]

\[
\leq \phi_0(r) \int \left|1 - \exp \left(-\epsilon/2 + \epsilon^{1/2}z\right)\right| \mathcal{N}(z; 0, 1) dz
\]

\[
\leq \phi_0(r) \left\lfloor \exp(\epsilon) - 1 \right\rfloor^{1/2} .
\]

Corollary D.2. As a result we have for \( r > 0 \)

\[
0 \leq 1 - \frac{\phi_\epsilon(r)}{\phi_0(r)} \leq \left\lfloor \exp(\epsilon) - 1 \right\rfloor^{1/2} 
\]

and consequently for \( \epsilon > 0 \) such that \( 1 - \left\lceil \exp(\epsilon) - 1 \right\rceil^{1/2} > 0 \) and \( \lambda^\epsilon \) as in Proposition 5.17, for any \( (x, v) \in E \),

\[
0 \leq \lambda^\epsilon(x, v) - \lambda^0(x, v) = \log \\left\{ \frac{\phi_0(\exp(\hat{U}(x)v))}{\phi_\epsilon(\exp(\hat{U}(x)v))} \right\}
\]

\[
\leq -\log \left\{ 1 - \left\lfloor \exp(\epsilon) - 1 \right\rfloor^{1/2} \right\} .
\]
References


