On the Hill relation and the mean reaction time for metastable processes

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Abstract

We illustrate how the Hill relation and the notion of quasi-stationary distribution can be used to analyse the error introduced by many algorithms that have been proposed in the literature, in particular in molecular dynamics, to compute mean reaction times between metastable states for Markov processes. The theoretical findings are illustrated on various examples demonstrating the sharpness of the error analysis as well as the applicability of our study to elliptic diffusions.

Index Terms: Source-sink process, Hill relation, Transition path process, Reactive trajectory, Quasi-stationary distribution.

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Contents

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1 Introduction

This work is motivated by the computation of reaction times in thermostated molecular dynamics. In this context, the evolution of a molecular system is typically modelled by the Langevin dynamics

$$\begin{cases} dq_t = M^{-1}p_t dt, \\ dp_t = -\nabla V(q_t)dt - \gamma M^{-1}p_t dt + \sqrt{2\gamma\beta^{-1}}dW_t, \end{cases} \tag{1.1}$$

where $q_t \in \mathbb{R}^d$ and $p_t \in \mathbb{R}^d$ denote the positions and momenta of the nuclei, or the overdamped Langevin dynamics, which is in position space only:

$$dq_t = -\nabla V(q_t)dt + \sqrt{2\beta^{-1}}dW_t. \tag{1.2}$$

In these equations, $\beta = (k_{\mathrm{B}}T)^{-1}$ is the inverse temperature, M is the mass matrix, $V : \mathbb{R}^d \to \mathbb{R}$ is the potential energy function, $\gamma > 0$ is the damping parameter, and W_t is a d-dimensional Brownian motion.

In practice, these dynamics are metastable, meaning that the process spends most of its time in some regions of the phase space, called metastable states. Metastable states typically correspond to some macroscopic states of the system, and studying the transitions between them is thus of first importance to understand the molecular mechanisms associated with these transitions.

As an example, one could think of a system consisting of a protein and a ligand, in which case studying the transition from the bound state (when the ligand is within a pocket of the protein) to the unbound state (when the ligand is detached from the protein) is key for some applications in drug design [36, 20]. Indeed, computing the mean reaction time

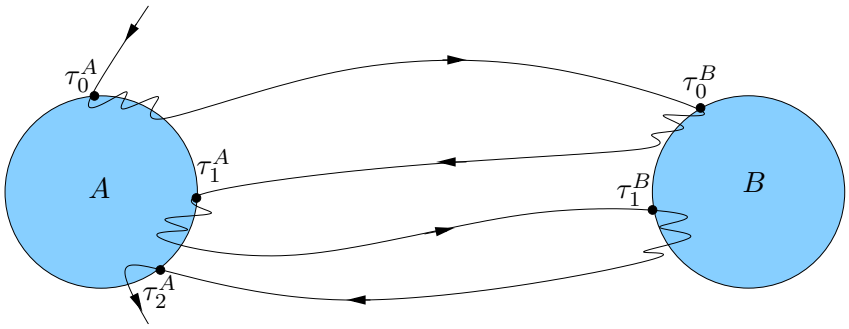

Figure 1: Reactive entrance times in the sets A and B.

from the bound state to the unbound state is crucial to rank the efficiencies of ligands for a given target pocket.

However, transitions between metastable states are rare events, which make the simulation of these transitions very difficult. This is related to a timescale problem: for example, the typical timestep for the discretisation of the Langevin dynamics is of the order of $10^{-15}s$, while transitions between metastable states can occur over timescales of order $10^{-6}s$ to $10^{2}s$. This explains why naive algorithms cannot be used to simulate such events.

To formalize the problem, let us denote by $X_t = (q_t, p_t)$ (resp. $X_t = q_t$) the Markov process of interest for the Langevin (resp. overdamped Langevin) dynamics and A and B two disjoint sets which define the metastable states of interest. Notice that, in practice, these states are typically defined in the position space only, so that in the context of the Langevin dynamics, $A = A_q \times \mathbb{R}^d$ and $B = B_q \times \mathbb{R}^d$ where A_q and B_q are two disjoint subsets of the position space $\mathbb{R}^d$. As illustrated on Figure 1, let us also introduce the successive reactive entrance times in A and B as $\tau_0^A = \inf\{t > 0,\, X_t \in \bar{A}\}$, $\tau_0^B = \inf\{t > \tau_0^A,\, X_t \in \bar{B}\}$ and, for all $n \geq 0$,

$$\tau_{n+1}^A = \inf\{t > \tau_n^B,\, X_t \in \bar{A}\} \text{ and } \tau_{n+1}^B = \inf\{t > \tau_{n+1}^A,\, X_t \in \bar{B}\}.$$

We use the qualifier "reactive" in reactive entrance time to indicate that the times (τ_n^A) are entrance times in A for trajectories coming from B, and the times (τ_n^B) are entrance times in B for trajectories coming from A.

One is then interested in computing the mean reaction time from A to B at equilibrium

$$T_{AB} := \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} (\tau_n^B - \tau_n^A),$$

which is the equilibrium average duration of the path from A to B. A path from A to B is a trajectory that starts from the boundary of A coming from B and goes to B: such a trajectory performs many visits to A before going to B. The last part from the boundary of A to B without going back to A is called a reactive trajectory. More generally, a reactive trajectory is a trajectory which leaves A and goes to B without going back to A, or leaves B and goes to A without going back to B.

Many techniques have been proposed to estimate this quantity, relying on more or less aggressive assumptions. We do not intend here to give an exhaustive list of numerical methods. Specifically, we are interested in techniques which are based on the introduction

of a source in A and a sink in B in order to create a non-steady state flux from A to B, and which approximate the reaction time by measuring the non-equilibrium flux. This idea dates back to [24, 30], and has been used in the weighted ensemble technique [40, 5], milestoning [39, 23, 4], and Transition Interface Sampling [38]. We also have in mind multilevel splitting techniques [29, 15] such as Forward Flux Sampling [2], Non Equilibrium Umbrella Sampling [21, 37] or Adaptive Multilevel Splitting [12, 14]. In particular, we will show why the Hill relation is a cornerstone to analyse the error introduced by these methods.

The objective of this work is to give rigorous mathematical foundations to such computations, by clarifying the error introduced when applying the Hill relation, depending on the distribution used to re-inject the process in A after hitting B. In particular, we identify the ideal probability measure that should be considered so that no error is introduced: this is the reactive entrance distribution. In addition, we explain why, when A is metastable, it is possible to use a "local equilibrium within A" (namely, a quasi-stationary distribution) to re-inject the process in A, while keeping a small error. This is crucial because this local equilibrium is widely used in practice since it is easy to sample, contrary to the reactive entrance distribution. The sharpness of our error estimate is illustrated on various examples.

The paper is organized as follows. In Section 2, we present in more details the motivation of this work, namely the computation of mean reaction times for diffusion processes. We show that this question is equivalent to computing a quantity of the form

$$\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] \tag{1.3}$$

for some test function f and a discrete-time Markov process (Y_n) with values in a domain $\mathcal{A} \cup \mathcal{B}$, where $\mathcal{A}$ and $\mathcal{B}$ are disjoint sets. In (1.3), ν_{E} is the so-called reactive entrance distribution in $\mathcal{A}$ and $T_{\mathcal{B}} := \inf\{n \geq 0,\, Y_n \in \mathcal{B}\}$ is the hitting time of $\mathcal{B}$. This setting is detailed in Section 3, where the problem is stated in a rather general framework. Section 3 also gives the main assumptions as well as the definitions of auxiliary Markov chains needed to perform the analysis. The Hill relation is stated and proved in Section 4 in a general setting. Section 5 analyses the error introduced when replacing ν_{E} in (1.3) by a quasi-stationary distribution: we show that under a timescale separation assumption, this error is small (see Theorem 5.6, which is the main mathematical result of this work). Returning to the setting of Section 2, Section 6 discusses the applicability of the theory to the computation of reaction times for diffusion processes. Finally, Appendix A demonstrates on simple toy models the sharpness of the error estimator of Section 5, Appendix B shows that the reversibility may not be conserved for the reactive entrance process, while Appendix C gives details about the Birkhoff's approach to prove existence and convergence to a QSD under the so-called two-sided condition.

2 Motivation: how to compute mean reaction times?

The purpose of this section is to motivate by the following question the discrete-time setting that will be at the core of Section 3: how to compute reaction times from one metastable state to another for a diffusion process? This section can be easily skipped if one is only interested in the mathematical results we have obtained, forgetting about this motivation.

2.1 The diffusion process and reaction time

Let $(X_t) \in \mathbb{R}^d$ be the solution of the stochastic differential equation

$$dX_t = f(X_t)dt + g(X_t)dW_t, \tag{2.1}$$

where (W_t) denotes a k-dimensional standard Wiener process. Here we assume that $f : \mathbb{R}^d \to \mathbb{R}^d$ and $g : \mathbb{R}^d \to \mathbb{R}^{d\times k}$ are smooth and satisfy conditions that guarantee the ergodicity of the Markov process (X_t) with respect to a unique invariant probability distribution. For example, one could keep in mind the Langevin and overdamped Langevin dynamics (1.1) and (1.2).

Let $A, B \subset \mathbb{R}^d$ be two open sets with smooth boundaries such that $\bar{A}$ and $\bar{B}$ are disjoint, and with non-zero measure for the invariant probability distribution of (2.1). Since the process is ergodic, (X_t) will visit A and B infinitely often. We are interested in the paths from A to B, namely the pieces of the trajectory $t \mapsto X_t$ that, coming from B, pass from A to B (see Figure 1).

For this, let us recall the definition of the reactive entrance times: $\tau_0^A = \inf\{t > 0,\, X_t \in \bar{A}\}$, $\tau_0^B = \inf\{t > \tau_0^A,\, X_t \in \bar{B}\}$ and, for all $n \geq 0$,

$$\tau_{n+1}^A = \inf\{t > \tau_n^B,\, X_t \in \bar{A}\} \text{ and } \tau_{n+1}^B = \inf\{t > \tau_{n+1}^A,\, X_t \in \bar{B}\},$$

and the associated empirical entrance distribution in A:

$$\mu_{A,N}^+ = \frac{1}{N}\sum_{n=1}^{N} \delta_{X_{\tau_n^A}}.$$

The reactive entrance distribution ν_{E} in A is defined as the weak limit of $\mu_{A,N}^+$ as $N \to \infty$ (see [33, Proposition 1.5] where ν_{E} is denoted η_A^+), meaning that for any continuous and bounded $f : \partial A \to \mathbb{R}$, one has

$$\int_{\partial A} f(x)\mu_{A,N}^+(dx) \xrightarrow[N\to\infty]{a.s.} \int_{\partial A} f(x)\nu_{\mathrm{E}}(dx). \tag{2.2}$$

Note that the reactive entrance distribution ν_{E} is not the restriction of the stationary measure of (X_t) to the boundary ∂A since ν_{E} only takes into account the paths that reach A coming from B. In general, even if the original process has an explicit invariant measure, ν_{E} does not admit a simple analytical expression, see [33] for more details.

As already mentioned, the quantity of interest in the present article is the expected reaction time T_{AB} from A to B, that is

$$T_{AB} := \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N}(\tau_n^B - \tau_n^A) = \mathbb{E}^{\nu_{\mathrm{E}}}[\tau_B]\,, \tag{2.3}$$

where τ_B is the hitting time of $\bar{B}$. The last equality is expected using the ergodicity of the original process and the strong Markov property. It is for example rigorously proved in [33], see Equation (1.32) and Proposition 1.8, in the case where A and B are bounded smooth, and gg^T is bounded from above and from below by strictly positive constants. The proof in [33] uses an ergodicity result (Doeblin's minorization condition) on the sequence of paths $((X_{(\tau_n^A+t)\wedge\tau_n^B})_{t\geq 0})$ seen as a Markov chain indexed by n, see the proof of [33, Theorem 1.7].

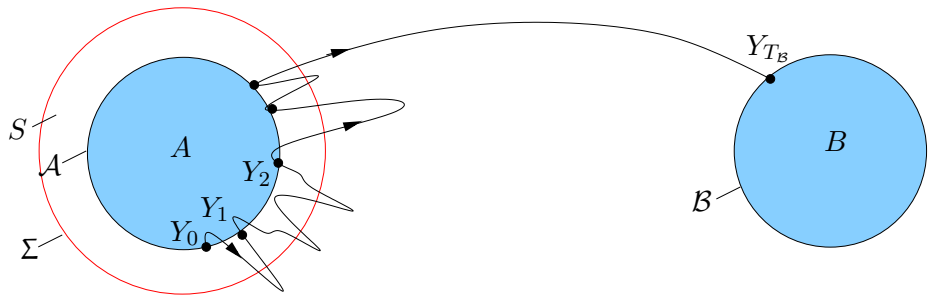

Figure 2: The Markov chain (Y_n).

2.2 From a diffusion (X_t) to a Markov chain (Y_n)

As explained in the introduction, to estimate the expected reaction time T_{AB}, many algorithms rely on the following construction. The path from A to B is divided into two parts: the so-called loops, namely the pieces of the trajectory between successive visits of A without visiting B, and the so-called reactive trajectory, namely the last part of the trajectory, which leaves A and go to B without going back to A. The idea is then to estimate the reaction time by multiplying the average number of loops by their mean duration, and then adding the expected duration of the reactive trajectory. However, because of the irregularity of the paths, the successive entrances in A do not define in general a countable set: one thus needs to define the loops and the successive entrances in A in a different way. This is why a separation surface Σ between A and B is introduced.

Let Σ be a smooth submanifold of codimension 1, such that the probability starting from A to reach B without crossing Σ is zero and such that $\bar{\Sigma} \cap \bar{A} = \varnothing$ and $\bar{\Sigma} \cap \bar{B} = \varnothing$. For example, as illustrated in Figure 2, such a submanifold can be constructed as the boundary of a smooth compact set S which contains $\bar{A}$ and does not intersect $\bar{B}$. Denote $\mathcal{A} = \partial A$, $\mathcal{B} = \partial B$ and $\mathcal{E} = \mathcal{A} \cup \mathcal{B}$. Considering a trajectory (X_t) with initial condition $X_0 \in \mathcal{E}$, the hitting times are defined inductively by $\tau_{Y,0} = 0$ and, for all $k \geq 0$,

$$\tau_{\Sigma,k+1} = \inf\{t > \tau_{Y,k},\, X_t \in \Sigma\} \text{ and } \tau_{Y,k+1} = \inf\{t > \tau_{\Sigma,k+1},\, X_t \in A \cup B\}.$$

Let us then introduce the sequence (see Figure 2)

$$\forall n \geq 0,\, Y_n = X_{\tau_{Y,n}} \tag{2.4}$$

of successive intersections of the sample path (X_t) with $A \cup B$, with intermediate hits to Σ before returning to $A \cup B$. The strong Markov property implies that the law of Y_{n+1} given Y_n is independent of n and of the past trajectory $(Y_m)_{m<n}$. In other words, (Y_n) forms a time-homogeneous Markov chain on $\mathcal{E}$. We thus obtain a discrete-time continuous-space Markov chain with transition kernel K defined by

$$K(x, \mathcal{C}) = \mathbb{P}^x(Y_1 \in \mathcal{C})$$

for any $x \in \mathcal{E}$ and any Borel set $C \in \mathscr{B}(\mathcal{E})$.

Remark 2.1 (Reversibility of (Y_n))**.** In general, the Markov chain (Y_n) defined by (2.4) is not reversible even if this is the case for the original process (X_t), and its stationary distribution does not have an analytic expression. For a related discussion, we refer to Remarks 3.11 and 3.12, and Appendix B. ◊

2.3 Expressing the mean reaction time T_{AB} as a function of (Y_n)

It turns out that the mean reaction time $T_{AB} = \mathbb{E}^{\nu_{\mathrm{E}}}[\tau_B]$ in (2.3) can be expressed in terms of the Markov chain (Y_n). To make this connection, let us define the function $\Delta : \mathcal{E} \mapsto \mathbb{R}^+$ by

$$\Delta(x) = \begin{cases} \mathbb{E}^x[\tau_{Y,1}] & \text{for } x \in \mathcal{A}, \\ 0 & \text{for } x \in \mathcal{B}. \end{cases} \tag{2.5}$$

Denoting $T_{\mathcal{B}} = \inf\{n \geq 0,\, Y_n \in \mathcal{B}\}$, the reaction time can then be reformulated as

$$T_{AB} = \mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{\infty} (\tau_{Y,n+1} - \tau_{Y,n}) \mathbf{1}_{n<T_{\mathcal{B}}}\right]$$

or, thanks to the strong Markov property,

$$T_{AB} = \mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} \Delta(Y_n)\right]. \tag{2.6}$$

The latter is the quantity of interest that will be considered in the following. Notice that, even though the process (Y_n) and the function Δ depend on the submanifold Σ, the left-hand side T_{AB} is independent of Σ. Accordingly, Σ can be seen as a tuning parameter. In the three upcoming sections we will discuss the computation of quantities of the form (2.6) for a Markov chain (Y_n). Eventually, we will return to the application of our results to the diffusive case in Section 6.

Notice that by considering other functions Δ, one can thus have access to different equilibrium properties over the ensemble of paths entering A and going to B at equilibrium. These are the paths $((X_{(\tau_n^A+t)\wedge\tau_n^B})_{t\geq 0})$ at equilibrium, sometimes also called transition paths [11], not to be confused with the reactive paths introduced above, even though there is no consensus on this denomination in the literature: transition path is sometimes used as a synonym of reactive path, as for example in [33, 22].

Remark 2.2 (Generalisation to other Markov processes)**.** We wrote everything starting from a diffusion process, but all this can be generalised to other Markov processes: jump processes, discrete-time Markov processes, etc. In particular, one should keep in mind that in the context of molecular dynamics, only a time-discretized version of the (overdamped) Langevin dynamics is used in practice, which means that the original process is actually a Markov chain in this context. ♢

Remark 2.3 (The case of the Langevin dynamics)**.** For the Langevin dynamics (1.1), it is possible to define the successive entrance times in $A_q \cup B_q$ as

$$\tau_{Y,k+1} = \inf\{t > \tau_{Y,k}, q_t \in A_q \text{ and } p_t \cdot n_{A_q} < 0, \text{ or } q_t \in B_q \text{ and } p_t \cdot n_{B_q} < 0\},$$

where n_{A_q} and n_{B_q} are the unit outward normals to A_q and B_q. These successive times are indeed such that $\lim_{k\to\infty} \tau_{Y,k} = \infty$ almost surely, under some smoothness assumption on A_q and B_q. There is thus no need to introduce the intermediate submanifold Σ in this context. In addition, it is possible in this case to identify an analytical formula for the equilibrium distribution π_0 of (Y_n) (see [32, Chapter 3] for related considerations). This yields to alternative numerical methods based on the exact Hill relation (see Equation (4.3) in Section 4.2 below), without having to replace ν_{E} by the quasi-stationary distribution ν_{Q}.

Nevertheless, in practice, this does not seem to be used by practitioners. We will investigate in future works the interest of such an approach compared to the usual method which consists in introducing the intermediate submanifold Σ. Likewise, we do not prove in this work that the relations (2.3) as well as the Assumptions on (Y_n) stated below hold for the Langevin dynamics (for the sake of simplicity, we indeed check that they hold only for elliptic diffusions and compact domains $\mathcal{A}$ and $\mathcal{B}$, see Section 6). Again, this will be the subject of a future work. $\Diamond$

3 The discrete-time setting

In this section, we detail the Markov chain setting we have in mind. After the introduction of the main notation and assumptions in Section 3.1, we present related Markov chains that play a central role in our context. First, the reactive entrance process is studied in Section 3.2. Then, the process killed when leaving $\mathcal{A}$, or killed process, is defined in Section 3.3. The latter allows us to introduce the notion of quasi-stationary distribution in $\mathcal{A}$, which is the formalization of the "local equilibrium within $\mathcal{A}$" reached by the process when it is trapped in the initial metastable state. Finally, the π-return process presented in Section 3.4 is the formalization of the source-sink process discussed in the introduction, and is required to establish the Hill relation which is at the core of Section 4.

3.1 Notation and assumptions

The purpose of this section is to introduce notation and assumptions on the Markov chain (Y_n) that we will consider throughout this article.

The Markov chain (Y_n). Let $\mathcal{A}$ and $\mathcal{B}$ be two disjoint compact sets of a separable metric space E, typically $\mathbb{R}^d$ or a discrete set such as $\mathbb{Z}^d$. Let us denote by $\mathscr{B}(E)$ the corresponding Borel-σ-algebra. Consider a Markov chain (Y_n) on $\mathcal{E} := \mathcal{A} \cup \mathcal{B}$ with transition kernel K, meaning that for any $x \in \mathcal{E}$ and any $\mathcal{C} \in \mathscr{B}(\mathcal{E})$, we have

$$K(x, \mathcal{C}) = \mathbb{P}^x(Y_1 \in \mathcal{C}) \, .$$

As usual, K^n stands for the n-step transition kernel defined by $K^0(x, \mathcal{C}) = \delta_x(\mathcal{C}) = \mathbf{1}_{x \in \mathcal{C}}$ and, for all $n \geq 1$,

$$K^n(x, \mathcal{C}) = \mathbb{P}^x(Y_n \in \mathcal{C}) = \int_{\mathcal{E}} K^{n-1}(x, dz) K(z, \mathcal{C}).$$

The Markov kernel K induces two Markov semi-groups in the standard way: the probability measure πK defined for any $\mathcal{C} \in \mathscr{B}(\mathcal{E})$ by

$$\pi K(\mathcal{C}) = \int_{\mathcal{E}} \pi(x) K(x, \mathcal{C}) = \mathbb{P}^\pi(Y_1 \in \mathcal{C})$$

is associated with any probability measure π on $\mathcal{E}$, while for any test (i.e., bounded measurable) function $f : \mathcal{E} \to \mathbb{R}$, one can also consider the test function Kf, defined for any $x \in \mathcal{E}$ by

$$Kf(x) = \int_{\mathcal{E}} K(x, dy) f(y) = \mathbb{E}^x[f(Y_1)] \, .$$

We recall some concepts for Markov chains on general spaces that will prove useful in the following (see for example [27, Section 4.2] and [34, Chapter 9]). For any $\mathcal{C} \in \mathscr{B}(\mathcal{E})$, the hitting and return times for the Markov chain (Y_n) are respectively defined by

$$T_{\mathcal{C}} = \inf\{n \geq 0,\, Y_n \in \mathcal{C}\} \text{ and } T_{\mathcal{C}}^+ = \inf\{n \geq 1,\, Y_n \in \mathcal{C}\}.$$

If π denotes a probability measure on $(\mathcal{E}, \mathscr{B}(\mathcal{E}))$, a Markov chain (Y_n) is called π-*irreducible* if, for all $x \in \mathcal{E}$ and all $\mathcal{C} \in \mathscr{B}(\mathcal{E})$ such that $\pi(\mathcal{C}) > 0$, one has

$$\mathbb{E}^x\left[\sum_{n=1}^{\infty} \mathbf{1}_{\{Y_n \in \mathcal{C}\}}\right] = \sum_{n=1}^{\infty} \mathbb{P}^x(Y_n \in \mathcal{C}) = \sum_{n=1}^{\infty} K^n(x, \mathcal{C}) > 0,$$

or, equivalently, if

$$\mathbb{P}^x\big(T_{\mathcal{C}}^+ < \infty\big) > 0. \tag{3.1}$$

It is called *recurrent* if there exists a probability measure π such that

$$\mathbb{E}^x\left[\sum_{n=1}^{\infty} \mathbf{1}_{\{Y_n \in \mathcal{C}\}}\right] = \infty, \qquad \forall x \in \mathcal{E}, \forall \mathcal{C} \in \mathscr{B}(\mathcal{E}) \text{ such that } \pi(\mathcal{C}) > 0. \tag{3.2}$$

It is called *Harris recurrent* if there exists a probability measure π such that

$$\mathbb{P}^x\left(\sum_{n=1}^{\infty} \mathbf{1}_{\{Y_n \in \mathcal{C}\}} = \infty\right) = 1, \qquad \forall x \in \mathcal{E}, \forall \mathcal{C} \in \mathscr{B}(\mathcal{E}) \text{ such that } \pi(\mathcal{C}) > 0.$$

Clearly, Harris recurrence implies recurrence, which itself implies π-irreducibility. If a (Harris) recurrent Markov chain admits an invariant probability measure, then it is called positive (Harris) recurrent. We recall [27, Proposition 4.2.11]:

Proposition 3.1. *A (Harris) recurrent Markov chain admits (up to a multiplicative constant) a unique invariant measure. Hence, if the invariant measure happens to be a probability measure, then the Markov chain is positive (Harris) recurrent.*

The following assumptions will be of constant use throughout this work. As usual, $C_b(\mathcal{E}, \mathbb{R})$ stands for continuous and bounded functions from $\mathcal{E}$ to $\mathbb{R}$.

Assumption A. [A1] $\mathcal{A}$ and $\mathcal{B}$ are compact disjoint sets and $\mathcal{E} = \mathcal{A} \cup \mathcal{B}$.

[A2] K is weak-Feller, meaning that $Kf \in C_b(\mathcal{E}, \mathbb{R})$ whenever $f \in C_b(\mathcal{E}, \mathbb{R})$.

[A3] The kernel K is positive Harris recurrent, and π_0 denotes its unique stationary probability measure.

[A4] $\pi_0(\mathcal{A}) > 0$ and $\pi_0(\mathcal{B}) > 0$.

Remark 3.2 (Assumptions in the case of a diffusion)**.** Returning to the setting of Section 2, one can exhibit conditions on the diffusion (X_t) solution to (2.1) so that Assumption A is satisfied, see Section 6. ♢

Norms and operators. For any test function $f : \mathcal{E} \to \mathbb{R}$, the supremum norm is as usual $\|f\|_\infty := \sup_{x\in\mathcal{E}} |f(x)|$. The total variation norm of a finite signed measure μ on $(\mathcal{E}, \mathscr{B}(\mathcal{E}))$ is defined by $\|\mu\| := \sup_{\|f\|_\infty\le 1} \mu f$. Accordingly, given two finite signed measures π and ν, the total variation distance between π and ν is

$$\|\pi - \nu\| = \sup_{\|f\|_\infty\le 1} (\pi f - \nu f). \tag{3.3}$$

Beware that a classic convention in probability is to define the total variation distance between two probability measures as half of the latter quantity. In the sequel, the operator norm of a finite kernel K acting on test functions is denoted by $\|\cdot\|_\infty$, i.e.,

$$\|K\|_\infty = \sup_{\|f\|_\infty\le 1} \|Kf\|_\infty = \sup_{x\in\mathcal{E}} \sup_{\|f\|_\infty\le 1} |Kf(x)| = \sup_{x\in\mathcal{E}} \|K(x,\cdot)\|. \tag{3.4}$$

Finally, for any $\mathcal{C} \in \mathscr{B}(\mathcal{E})$, $\mathrm{id}_\mathcal{C}$ is the identity operator on $\mathcal{C}$, that is

$$\pi\,\mathrm{id}_\mathcal{C}\, f = \pi f, \qquad \forall \pi \text{ measure on } \mathcal{C}, \forall f : \mathcal{C} \to \mathbb{R} \text{ bounded measurable},$$

and $\mathbb{1}_\mathcal{C} : \mathcal{C} \to \mathbb{R}$ denotes the function defined on $\mathcal{C}$ and identically equal to one on $\mathcal{C}$.

Markov and sub-Markov kernels. For what follows, we need to consider some restrictions of the Markov kernel K to subsets of $\mathcal{E}$. Specifically, for any $\mathcal{C}, \mathcal{D} \in \mathscr{B}(\mathcal{E})$, we introduce the nonnegative sub-Markov kernel $K_{\mathcal{C}\mathcal{D}}$ defined for all $x \in \mathcal{C}$ and all $D \in \mathscr{B}(\mathcal{D})$ by

$$K_{\mathcal{C}\mathcal{D}}(x, D) = \int_D K(x, dy).$$

In other words, for any probability π on $\mathcal{C}$ and any test function f on $\mathcal{D}$, one simply has $\pi K_{\mathcal{C}\mathcal{D}} f = \pi K f$. If $\mathcal{D} = \mathcal{C}$, we just write $K_\mathcal{C}$. Using this notation, the transition kernel K can be decomposed as a two-block kernel on $\mathcal{E} = \mathcal{A} \cup \mathcal{B}$ as

$$K = \begin{bmatrix} K_\mathcal{A} & K_{\mathcal{A}\mathcal{B}} \\ K_{\mathcal{B}\mathcal{A}} & K_\mathcal{B} \end{bmatrix}. \tag{3.5}$$

Note that for all $x \in \mathcal{A}$ and all $n \ge 0$,

$$\mathbb{P}^x(T_\mathcal{B} > n) = \mathbb{P}^x(Y_1 \in \mathcal{A}, \dots, Y_n \in \mathcal{A}) = K_\mathcal{A}^n \mathbb{1}_\mathcal{A}(x). \tag{3.6}$$

Besides, for all $x \in \mathcal{A}$, it is readily seen that

$$K_\mathcal{A}\mathbb{1}_\mathcal{A}(x) + K_{\mathcal{A}\mathcal{B}}\mathbb{1}_\mathcal{B}(x) = \mathbb{1}_\mathcal{A}(x),$$

which amounts to saying that

$$(\mathrm{id}_\mathcal{A} - K_\mathcal{A})\mathbb{1}_\mathcal{A} = K_{\mathcal{A}\mathcal{B}}\mathbb{1}_\mathcal{B}. \tag{3.7}$$

Accordingly, we also have, for any probability distribution π on $\mathcal{A}$,

$$\mathbb{P}^\pi(Y_1 \in \mathcal{B}) = \pi K_{\mathcal{A}\mathcal{B}}\mathbb{1}_\mathcal{B}. \tag{3.8}$$

Preliminary results on the Markov chain (Y_n). We give here some important consequences of our assumptions.

Lemma 3.3. *Under Assumption A,*

$$\sup_{x\in\mathcal{A}} \mathbb{P}^x(Y_1 \in \mathcal{B}) > 0 \qquad \text{and} \qquad \sup_{x\in\mathcal{B}} \mathbb{P}^x(Y_1 \in \mathcal{A}) > 0.$$

Moreover, there exists an integer n such that

$$\inf_{x\in\mathcal{A}} \mathbb{P}^x(T_{\mathcal{B}} \leq n) > 0 \qquad \text{and} \qquad \inf_{x\in\mathcal{B}} \mathbb{P}^x(T_{\mathcal{A}} \leq n) > 0. \tag{3.9}$$

Proof. The fact that $\sup_{x\in\mathcal{A}} \mathbb{P}^x(Y_1 \in \mathcal{B}) > 0$ is a direct consequence of Assumptions [A3] and [A4]. Next, suppose that for all $n \in \mathbb{N}$, we have $\inf_{x\in\mathcal{A}} \mathbb{P}^x(T_{\mathcal{B}} \leq n) = 0$. Then, one could exhibit a sequence $(x_n) \in \mathcal{A}$ such that, for all n, we would have $\mathbb{P}^{x_n}(T_{\mathcal{B}} \leq n) \leq 1/n$. Hence, for all $m \leq n$, $\mathbb{P}^{x_n}(T_{\mathcal{B}} \leq m) \leq 1/n$. By compactness of $\mathcal{A}$ (see Assumption [A1]), up to extracting a subsequence of (x_n), there exists $\overline{x} \in \mathcal{A}$ such that $x_n \to \overline{x}$. Now, as $\mathcal{A}$ and $\mathcal{B}$ are disjoint compact sets, the mapping $x \mapsto \mathbf{1}_{\mathcal{A}}(x)$ is continuous and so is $x \mapsto K\mathbf{1}_{\mathcal{A}}(x)$ by Assumption [A2]. Since $K = K_{\mathcal{A}}$ on $\mathcal{A}$ and $(x_n) \in \mathcal{A}$, we deduce from (3.6) that the mapping $x \mapsto \mathbb{P}^x(T_{\mathcal{B}} \leq m) = 1 - K_{\mathcal{A}}^m \mathbb{1}_{\mathcal{A}}(x)$ is continuous on $\mathcal{A}$, so that

$$\forall m \in \mathbb{N}, \qquad \mathbb{P}^{\overline{x}}(T_{\mathcal{B}} \leq m) \leq \lim_{n\to\infty} \frac{1}{n} = 0.$$

Thus $\mathbb{P}^{\overline{x}}(T_{\mathcal{B}} < \infty) = 0$, which is in contradiction with the π_0-irreducibility Assumption [A3] and Equation (3.1). Thus, we can conclude that there exists an integer n such that $\inf_{x\in\mathcal{A}} \mathbb{P}^x(T_{\mathcal{B}} \leq n) > 0$. □

A simple but crucial consequence of this result is the well-posedness of Poisson equations associated with $K_{\mathcal{A}}$ and $K_{\mathcal{B}}$. By convention, an empty sum is equal to zero. Recall that the space $B(\mathcal{A}, \mathbb{R})$ of test (i.e., bounded and measurable) functions equipped with the supremum norm is a Banach space.

Corollary 3.4. *Under Assumption A, the operator $(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})$ is invertible in the following sense: for any test function g on $\mathcal{A}$, the unique test function solution of the Poisson boundary value problem*

$$\begin{cases} (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})r(x) = g(x), & x \in \mathcal{A} \\ r(x) = 0, & x \in \mathcal{B} \end{cases} \tag{3.10}$$

is given by

$$r(x) = \mathbb{E}^x\left[\sum_{n=0}^{T_{\mathcal{B}}-1} g(Y_n)\right]. \tag{3.11}$$

Mutatis mutandis, the same result holds for the operator $(\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})$.

Proof. Let us first prove that the operator $(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})$ is invertible. By (3.9), let n be such that $\inf_{x\in\mathcal{A}} \mathbb{P}^x(T_{\mathcal{B}} \leq n) > 0$. Then, by definition of the operator norm defined in (3.4) and thanks to (3.6), we are led to

$$\|K_{\mathcal{A}}^n\|_\infty = \sup_{x\in\mathcal{A}} K_{\mathcal{A}}^n \mathbb{1}_{\mathcal{A}}(x) = \sup_{x\in\mathcal{A}} \mathbb{P}^x(T_{\mathcal{B}} > n) < 1.$$

Hence, the series $\sum_n \|K_{\mathcal{A}}^n\|_\infty$ converges and $(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})$ is indeed invertible as an operator on the Banach space $(B(\mathcal{A}, \mathbb{R}), \|\cdot\|_\infty)$. The uniqueness of the solution to (3.10) is then immediate since the operator $(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})$ is invertible. Moreover,

$$r(x) = (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} g(x) = \sum_{n \geq 0} K_{\mathcal{A}}^n g(x) = \sum_{n \geq 0} \mathbb{E}^x [g(Y_n) \mathbf{1}_{T_{\mathcal{B}} > n}] .$$

To deduce (3.11), it remains to apply Fubini's theorem, which is possible since

$$\sum_{n \geq 0} \mathbb{E}^x [|g(Y_n) \mathbf{1}_{T_{\mathcal{B}} > n}|] \leq \|g\|_\infty \sum_{n \geq 0} K_{\mathcal{A}}^n \mathbb{1}_{\mathcal{A}}(x) \leq \|g\|_\infty \sum_n \|K_{\mathcal{A}}^n\|_\infty < \infty.$$

□

Hence, for any test function g and all $x \in \mathcal{A}$, one has

$$(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} g(x) = \mathbb{E}^x \left[\sum_{n=0}^{T_{\mathcal{B}}-1} g(Y_n) \right],$$

or more generally, for any probability measure π on $\mathcal{A}$,

$$\pi (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} g = \mathbb{E}^\pi \left[\sum_{n=0}^{T_{\mathcal{B}}-1} g(Y_n) \right]. \tag{3.12}$$

Taking $g = \mathbb{1}_{\mathcal{A}}$ yields the next result.

Corollary 3.5. *For all $x \in \mathcal{A}$,*

$$\mathbb{E}^x [T_{\mathcal{B}}] = (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} \mathbb{1}_{\mathcal{A}}(x). \tag{3.13}$$

And similarly, for all $x \in \mathcal{B}$, $\mathbb{E}^x [T_{\mathcal{A}}] = (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} \mathbb{1}_{\mathcal{B}}(x)$.

Restricted and conditional stationary measures. Given a probability measure π on $\mathcal{E}$ and a Borel set $\mathcal{C} \in \mathscr{B}(\mathcal{E})$ such that $\pi(\mathcal{C}) > 0$, we denote by $\pi^{\mathcal{C}}$ the measure restricted to $\mathcal{C}$:

$$\pi^{\mathcal{C}}(\mathcal{D}) = \pi(\mathcal{D} \cap \mathcal{C}), \quad \forall \mathcal{D} \in \mathscr{B}(\mathcal{E}),$$

and by $\pi_{|\mathcal{C}}$ the measure conditioned to $\mathcal{C}$:

$$\pi_{|\mathcal{C}}(\mathcal{D}) = \frac{\pi(\mathcal{D} \cap \mathcal{C})}{\pi(\mathcal{C})}, \quad \forall \mathcal{D} \in \mathscr{B}(\mathcal{E}). \tag{3.14}$$

In the sequel, we will need various relations involving these restricted and conditional measures. Recall that, under Assumption A, π_0 denotes the unique stationary probability measure of (Y_n).

Proposition 3.6. *Under Assumption A, we have*

$$\pi_0^{\mathcal{A}} (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}}) = \pi_0^{\mathcal{B}} K_{\mathcal{B}\mathcal{A}} \tag{3.15}$$

as well as

$$\pi_{0|\mathcal{A}} = \pi_{0|\mathcal{A}} K_{\mathcal{A}} + \pi_{0|\mathcal{A}} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}}. \tag{3.16}$$

Proof. Since $\pi_0 K = \pi_0$, one just has to consider the two-block decomposition (3.5) to deduce that

$$\pi_0^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}}) = \pi_0^{\mathcal{B}} K_{\mathcal{B}\mathcal{A}}.$$

From this, by switching the roles of $\mathcal{A}$ and $\mathcal{B}$ and taking into account that $(\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})$ is invertible, we immediately get

$$\pi_0^{\mathcal{B}} = \pi_0^{\mathcal{A}} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1},$$

so that putting all things together yields

$$\pi_0^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}}) = \pi_0^{\mathcal{A}} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}}.$$

Since $\pi_0(\mathcal{A}) > 0$, it suffices to divide both terms by $\pi_0(\mathcal{A})$ to obtain (3.16). □

3.2 The reactive entrance process

Under Assumption A, the Markov chain (Y_n) is positive Harris recurrent, hence it will visit the sets $\mathcal{A}$ and $\mathcal{B}$ infinitely often. Remind that, in fine, we are interested in the transitions of the Markov chain from $\mathcal{A}$ to $\mathcal{B}$ at equilibrium. In this aim, we first introduce the reactive entrance process.

Definition of the reactive entrance process. From the Markov chain (Y_n) living on $\mathcal{E} = \mathcal{A} \cup \mathcal{B}$, one can also define a process in $\mathcal{A}$ monitored only when visiting $\mathcal{A}$ after having reached $\mathcal{B}$. We call it the reactive entrance process in $\mathcal{A}$ and denote it by (Y_n^{E}). We recall that $T_{\mathcal{B}}^+ = \inf\{n \geq 1,\, Y_n \in \mathcal{B}\}$ and define

$$T^{\mathcal{A}} = \inf\{n > T_{\mathcal{B}}^+, Y_n \in \mathcal{A}\},$$

which is the hitting time of $\mathcal{A}$ after having reached $\mathcal{B}$.

Definition 3.7 (Reactive entrance process)**.** *The reactive entrance process associated with the process (Y_n) is the Markov chain (Y_n^{E}) on $\mathcal{A}$ with transition kernel*

$$K^{\mathrm{E}}(x, \mathcal{C}) = \mathbb{P}^x(Y_{T^{\mathcal{A}}} \in \mathcal{C}) \qquad \forall x \in \mathcal{A}, \forall \mathcal{C} \in \mathscr{B}(\mathcal{A}),$$

or, equivalently,

$$K^{\mathrm{E}} = (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}}.$$

Let us check that both definitions coincide. Using the strong Markov property, one obtains that for all $x \in \mathcal{A}$ and all $\mathcal{C} \in \mathscr{B}(\mathcal{A})$

$$\mathbb{P}^x(Y_{T^{\mathcal{A}}} \in \mathcal{C}) = \int_{\mathcal{B}} \mathbb{P}^x\left(Y_{T_{\mathcal{B}}^+} \in dy\right) \mathbb{P}^y\left(Y_{T_{\mathcal{A}}^+} \in \mathcal{C}\right).$$

The first term in this integral can be decomposed as

$$\mathbb{P}^x\left(Y_{T_{\mathcal{B}}^+} \in dy\right) = \sum_{n=0}^{\infty} \int_{\mathcal{A}} K_{\mathcal{A}}^n(x, dx') K_{\mathcal{A}\mathcal{B}}(x', dy),$$

which amounts to saying that

$$\mathbb{P}^x\left(Y_{T_{\mathcal{B}}^+} \in dy\right) = \left[(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} K_{\mathcal{A}\mathcal{B}}\right](x, dy).$$

In the same vein, we may write

$$\mathbb{P}^y\Big(Y_{T_{\mathcal{A}}^+} \in \mathcal{C}\Big) = \left[(\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}}\right](y, \mathcal{C}),$$

so that, finally,

$$\mathbb{P}^x(Y_{T^{\mathcal{A}}} \in \mathcal{C}) = \left[(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}}\right](x, \mathcal{C}).$$

This shows the equivalence between the formulations of K^{E} in Definition 3.7.

Some properties of the reactive entrance process. Recall that π_0 is the unique invariant probability measure of (Y_n) and, $\forall \mathcal{D} \in \mathscr{B}(\mathcal{E})$,

$$\pi_{0|\mathcal{A}}(\mathcal{D}) = \frac{\pi_0(\mathcal{D} \cap \mathcal{A})}{\pi_0(\mathcal{A})} = \frac{\pi_0^{\mathcal{A}}(\mathcal{D})}{\pi_0(\mathcal{A})}.$$

Proposition 3.8. *Under Assumption A, the reactive entrance process (Y_n^{E}) is positive Harris recurrent with unique invariant probability measure*

$$\nu_{\mathrm{E}} := \frac{\pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})}{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}. \tag{3.17}$$

Equivalently, we have

$$\pi_{0|\mathcal{A}} = \frac{\nu_{\mathrm{E}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]}. \tag{3.18}$$

Proof. The chain (Y_n^{E}) inherits the positive Harris recurrent property from the original Markov chain (Y_n). Indeed, assuming that (Y_n), starting from $x \in \mathcal{A}$, is positive Harris recurrent with π_0 as its unique invariant probability measure implies that for all $\mathcal{C} \in \mathcal{B}(\mathcal{A})$ such that $\pi_0(\mathcal{C}) > 0$, there exists $\Omega_x^{\mathcal{C}}$ such that $\mathbb{P}(\Omega_x^{\mathcal{C}}) = 1$ and

$$\forall \omega \in \Omega_x^{\mathcal{C}},\ \forall n_0 \in \mathbb{N}, \exists n = n(\omega) > n_0,\ Y_n \in \mathcal{C}.$$

Denote $\Omega_x^{\mathcal{B}}$ accordingly and remark that $\pi_0(\mathcal{B}) > 0$ by Assumption A. Then $\mathbb{P}(\Omega_x^{\mathcal{B}} \cap \Omega_x^{\mathcal{C}}) = 1$ and, obviously,

$$\forall \omega \in \Omega_x^{\mathcal{B}} \cap \Omega_x^{\mathcal{C}},\ \forall n_0 \in \mathbb{N}, \exists n = n(\omega) > n_0,\ Y_n^{\mathrm{E}} \in \mathcal{C},$$

which shows that (Y_n^{E}) is positive Harris recurrent. Therefore, by Proposition 3.1, it admits, up to a multiplicative constant, a unique invariant measure. Since

$$K^{\mathrm{E}} = (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}},$$

and, by (3.16),

$$\pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}}) = \pi_{0|\mathcal{A}} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} K_{\mathcal{B}\mathcal{A}},$$

we see that this invariant measure is $\pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})$. To normalize it, just notice that, via (3.7),

$$\pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})\mathbb{1}_{\mathcal{A}} = \pi_{0|\mathcal{A}} K_{\mathcal{A}\mathcal{B}} \mathbb{1}_{\mathcal{B}} = \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\,.$$

To deduce (3.18) from (3.17), it suffices to apply (3.13). ∎

Starting from $Y_0 = x \in \mathcal{A}$, we define the reactive entrance times by setting $T_0^{\mathcal{A}} = 0$ and, for all $n \geq 0$,

$$T_{n+1}^{\mathcal{B}} = \inf\{m > T_n^{\mathcal{A}},\, Y_m \in \mathcal{B}\} \text{ and } T_{n+1}^{\mathcal{A}} = \inf\{m > T_{n+1}^{\mathcal{B}},\, Y_m \in \mathcal{A}\}.$$

Hence we have $Y_0^{\mathrm{E}} = x$ and, for all $n \geq 1$, $Y_n^{\mathrm{E}} = Y_{T_n^{\mathcal{A}}}$. The following sample-path ergodic property is a consequence of the previous result and of [27, Theorem 4.2.13]. It can be seen as the equivalent of (2.2) for a fixed initial condition x and a broader class of test functions.

Corollary 3.9. *Under Assumption A, for every initial condition $Y_0 = Y_0^{\mathrm{E}} = x \in \mathcal{A}$ and every function $f \in L^1(\nu_{\mathrm{E}})$, one has*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(Y_n^{\mathrm{E}}) = \int_{\mathcal{A}} f(x)\nu_{\mathrm{E}}(dx) \qquad \mathbb{P}_x - \textit{almost surely.}$$

Remark 3.10 (From the reactive entrance distributions to the original stationary distribution)**.** Switching the roles of $\mathcal{A}$ and $\mathcal{B}$, the reactive entrance process in $\mathcal{B}$ also admits a unique stationary distribution. Denoting $\nu_{\mathrm{E}}^{\mathcal{B}}$ the stationary distribution of the reactive entrance process in $\mathcal{B}$, and $\nu_{\mathrm{E}}^{\mathcal{A}}$ the stationary distribution of the reactive entrance process in $\mathcal{A}$, (3.17), (3.15), and (3.18) imply that

$$\nu_{\mathrm{E}}^{\mathcal{B}} = \frac{\nu_{\mathrm{E}}^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} K_{\mathcal{AB}}}{\nu_{\mathrm{E}}^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} K_{\mathcal{AB}} \mathbb{1}_{\mathcal{B}}}.$$

Moreover, assuming that both reactive entrance processes are positive Harris recurrent with stationary distributions $\nu_{\mathrm{E}}^{\mathcal{A}}$ and $\nu_{\mathrm{E}}^{\mathcal{B}}$, then the original process (Y_n) is also positive Harris recurrent and its unique stationary distribution satisfies for all $\mathcal{C} \in \mathscr{B}(\mathcal{E})$

$$\pi_0(\mathcal{C}) = \frac{1}{\mathbb{E}^{\nu_{\mathrm{E}}^{\mathcal{A}}}[T_{\mathcal{B}}] + \mathbb{E}^{\nu_{\mathrm{E}}^{\mathcal{B}}}[T_{\mathcal{A}}]} \Big(\nu_{\mathrm{E}}^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} \mathbb{1}_{\mathcal{A}\cap\mathcal{C}} + \nu_{\mathrm{E}}^{\mathcal{B}}(\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} \mathbb{1}_{\mathcal{B}\cap\mathcal{C}} \Big). \tag{3.19}$$

Let us give the proof of (3.19). Notice first that

$$\pi_0(\mathcal{C}) = \pi_{0|\mathcal{A}}(\mathcal{C})\pi_0(\mathcal{A}) + \pi_{0|\mathcal{B}}(\mathcal{C})\pi_0(\mathcal{B}).$$

From Equation (3.17), we also know that

$$\pi_{0|\mathcal{A}}(\mathcal{C}) = \left(\nu_{\mathrm{E}}^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} \mathbb{1}_{\mathcal{A}\cap\mathcal{C}}\right) \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\,.$$

We thus have

$$\pi_0(\mathcal{C}) = \left(\nu_{\mathrm{E}}^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} \mathbb{1}_{\mathcal{A}\cap\mathcal{C}}\right) \mathbb{P}^{\pi_0^{\mathcal{A}}}(Y_1 \in \mathcal{B}) + \left(\nu_{\mathrm{E}}^{\mathcal{B}}(\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} \mathbb{1}_{\mathcal{B}\cap\mathcal{C}}\right) \mathbb{P}^{\pi_0^{\mathcal{B}}}(Y_1 \in \mathcal{A})\,.$$

In addition, one can check that $\mathbb{P}^{\pi_0^{\mathcal{A}}}(Y_1 \in \mathcal{B}) = \mathbb{P}^{\pi_0^{\mathcal{B}}}(Y_1 \in \mathcal{A})$. Indeed, from Equations (3.7), (3.8) and (3.15),

$$\mathbb{P}^{\pi_0^{\mathcal{A}}}(Y_1 \in \mathcal{B}) = \pi_0^{\mathcal{A}} K_{\mathcal{AB}} \mathbb{1}_{\mathcal{B}} = \pi_0^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})\mathbb{1}_{\mathcal{A}} = \pi_0^{\mathcal{B}} K_{\mathcal{BA}} \mathbb{1}_{\mathcal{A}} = \mathbb{P}^{\pi_0^{\mathcal{B}}}(Y_1 \in \mathcal{A})\,.$$

Therefore,

$$\pi_0(\mathcal{C}) = c^{-1} \Big(\nu_{\mathrm{E}}^{\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} \mathbb{1}_{\mathcal{A}\cap\mathcal{C}} + \nu_{\mathrm{E}}^{\mathcal{B}}(\mathrm{id}_{\mathcal{B}} - K_{\mathcal{B}})^{-1} \mathbb{1}_{\mathcal{B}\cap\mathcal{C}} \Big)$$

where

$$c^{-1} = \mathbb{P}^{\pi_0^{\mathcal{A}}}(Y_1 \in \mathcal{B}) = \mathbb{P}^{\pi_0^{\mathcal{B}}}(Y_1 \in \mathcal{A})$$

is independent of $\mathcal{C}$ and, necessarily, $c = \mathbb{E}^{\nu_{\mathrm{E}}^{\mathcal{A}}}[T_{\mathcal{B}}] + \mathbb{E}^{\nu_{\mathrm{E}}^{\mathcal{B}}}[T_{\mathcal{A}}]$ by considering $\mathcal{C} = \mathcal{E}$ and (3.18) since $\pi_0(\mathcal{E}) = 1$. ◊

Remark 3.11 (Reversibility of the reactive entrance process)**.** The fact that K is reversible with respect to π_0 does not imply that K^{E} is reversible with respect to ν_{E}. An example of such a situation is given in Appendix B. $\Diamond$

Remark 3.12 (Back to the case of a diffusion process)**.** Returning to the setting of Section 2, (Y_n) can be seen as the reactive entrance process in $\bar{A} \cup \bar{B}$ after visiting Σ, associated with the original diffusion process (X_t). In connection with Remarks 2.1 and 3.11, the fact that (X_t) is reversible does not imply that (Y_n) is reversible. In addition, notice that (Y_n^{E}) can be seen as the reactive entrance process of (X_t) in $\mathcal{A}$ after visiting $\mathcal{B}$, and it does not depend on Σ. Accordingly, as already mentioned, ν_{E} does not depend on Σ either. $\Diamond$

As already mentioned, since the Markov chain (Y_n) is positive Harris recurrent, it will visit the sets $\mathcal{A}$ and $\mathcal{B}$ infinitely often. We are interested in the transitions of the Markov chain from $\mathcal{A}$ to $\mathcal{B}$ at equilibrium.

The reactive entrance distribution at equilibrium. Let us now introduce the reactive entrance distribution at equilibrium in $\mathcal{A}$, simply called "reactive entrance distribution" in the following. When we refer to an average quantity over the paths from A to B at equilibrium, we thus refer to the law of the paths from A to B starting from the reactive entrance distribution in $\mathcal{A}$. For a given test function $f : \mathcal{A} \to \mathbb{R}$, the aim of this work is to estimate the following equilibrium quantity:

$$\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right], \tag{3.20}$$

where $T_{\mathcal{B}} = \inf\{n \geq 0, Y_n \in \mathcal{B}\}$. As explained in Section 2, for an appropriate choice of f and (Y_n), the quantity (3.20) is the mean reaction time at equilibrium of a diffusion process, see (2.5) and (2.6).

When the sets $\mathcal{A}$ and $\mathcal{B}$ are metastable, simulating directly (3.20) is very challenging for two reasons: first, $T_{\mathcal{B}}$ is very large and, second, ν_{E} is difficult to sample, and not known analytically in general. However, since $\mathcal{A}$ is metastable, the process (Y_n) reaches a "local equilibrium within $\mathcal{A}$" (namely a quasi-stationary distribution) before transitioning to $\mathcal{B}$. The objective of this work is twofold:

- first, to explain why, when replacing ν_{E} by a quasi-stationary distribution, the quantity (3.20) can be efficiently approximated using the Hill relation and rare event sampling methods such as those mentioned in the introduction (see Section 4 and Section 6.2);
- second, to quantify the error introduced when replacing ν_{E} by a quasi-stationary distribution (see Section 5).

Before proceeding, we need to detail the notions of killed process and π-return process. We refer the reader to Table 1 at the end of Section 3.4 for a summary of the various processes at stake in this paper.

3.3 The killed process

From the process (Y_n) living on $\mathcal{E} = \mathcal{A} \cup \mathcal{B}$, one can define the process (Y_n^{Q}) killed when leaving $\mathcal{A}$ (or, equivalently, killed when hitting $\mathcal{B}$).

Definition 3.13 (Killed process)**.** *The killed process when leaving $\mathcal{A}$ associated with the process (Y_n) is the discrete-time process (Y_n^{Q}) on $\mathcal{A}$ with transition kernel*

$$K_{\mathcal{A}}(x,\mathcal{C}) = \mathbb{P}^x\Big(Y_1^{\mathrm{Q}} \in \mathcal{C}\Big) = \mathbb{P}^x(Y_1 \in \mathcal{C}, T_{\mathcal{B}} > 1) \quad \forall x \in \mathcal{A}, \forall \mathcal{C} \in \mathscr{B}(\mathcal{A}).$$

Assumption A implies that this process does not admit a stationary distribution. Indeed, suppose that π is such a distribution, then from (3.9), there exists an n such that

$$\pi K_{\mathcal{A}}^n \mathbb{1}_{\mathcal{A}} \leq \|K_{\mathcal{A}}^n\|_\infty = \sup_{x\in\mathcal{A}} \mathbb{P}^x(T_{\mathcal{B}} > n) < 1,$$

which contradicts the stationarity because $\pi \mathbb{1}_{\mathcal{A}} = 1$. Nevertheless, we may consider the notion of quasi-stationary distribution, which extends the idea of stationary distribution to such sub-Markov kernels.

Definition 3.14 (Quasi-stationary distribution)**.** *A probability distribution π on $\mathcal{A}$ is a quasi-stationary distribution (QSD) for the killed process (Y_n^{Q}) if for every measurable set $\mathcal{C} \in \mathscr{B}(\mathcal{A})$,*

$$\mathbb{P}^\pi(Y_n \in \mathcal{C}, T_{\mathcal{B}} > n) = \mathbb{P}^\pi(T_{\mathcal{B}} > n)\, \pi(\mathcal{C}), \quad \forall n \geq 0. \tag{3.21}$$

It turns out that our framework ensures the existence of such a QSD.

Lemma 3.15. *Under Assumption A, the killed process (Y_n^{Q}) admits a QSD. Specifically, a probability measure π on $\mathcal{A}$ is a QSD for (Y_n^{Q}) if and only if there exists $\theta \geq 0$ such that*

$$\pi K_{\mathcal{A}} = \theta \pi,$$

in which case $\theta = \mathbb{P}^\pi(T_{\mathcal{B}} > 1)$.

Proof. Recall that, for all $n \geq 0$, (3.6) gives

$$\mathbb{P}^\pi(Y_n \in \mathcal{C}, T_{\mathcal{B}} > n) = \pi K_{\mathcal{A}}^n(\mathcal{C}). \tag{3.22}$$

In particular, one has for any probability measure π on $\mathcal{A}$ and any $\mathcal{C} \in \mathscr{B}(\mathcal{A})$

$$\pi K_{\mathcal{A}}(\mathcal{C}) = \mathbb{P}^\pi(Y_1 \in \mathcal{C}, T_{\mathcal{B}} > 1)\,.$$

Thus, in view of (3.21), if π is a quasi-stationary distribution, this leads to

$$\pi K_{\mathcal{A}} = \mathbb{P}^\pi(T_{\mathcal{B}} > 1)\, \pi,$$

which shows that a quasi-stationary distribution is a left probability eigenmeasure associated to the eigenvalue $\mathbb{P}^\pi(T_{\mathcal{B}} > 1)$. Conversely, let us assume that there exists a probability measure π on $\mathcal{A}$ and a real number $\theta \geq 0$ such that $\pi K_{\mathcal{A}} = \theta \pi$. Then, for any n, (3.22) yields

$$\mathbb{P}^\pi(Y_n \in \mathcal{C}, T_{\mathcal{B}} > n) = \pi K_{\mathcal{A}}^n(\mathcal{C}) = \theta^n \pi(\mathcal{C})$$

and π satisfies (3.21) with $\mathbb{P}^\pi(T_{\mathcal{B}} > n) = \theta^n$. As a consequence, showing the existence of a QSD amounts to asserting the existence of a left probability eigenmeasure for the kernel $K_{\mathcal{A}}$. Under Assumption A, the existence of such a QSD is ensured from [19, Proposition 2.10] since $\mathcal{A}$ is compact and K is weak-Feller. □

Remark 3.16 (Degenerate case)**.** Although theoretically possible, the case $\theta = 0$ is of no interest in our context. It occurs when there exists $x \in \mathcal{A}$ such that $\mathbb{P}^x(T_{\mathcal{B}} > 1) = 0$, meaning that if $Y_0 = x$ then $Y_1 \in \mathcal{B}$ almost surely. Therefore, from now on, we assume that

$$\forall x \in \mathcal{A}, \qquad \mathbb{P}^x(T_{\mathcal{B}} > 1) > 0, \tag{3.23}$$

which in turn ensures that $\theta > 0$ in Lemma 3.15. ◊

Remark 3.17 (On the uniqueness of the QSD)**.** As stated in Lemma 3.15, Assumption A implies the existence of a quasi-stationary distribution, but as shown in [7, Section 3.1] there may exist several quasi-stationary distributions. Conditions to ensure the uniqueness can be found for example in [18]. A simple sufficient condition to get uniqueness is the following so-called two-sided estimate (see for example [18, Section 7.1] or [8]): if for some $n \geq 1$, there exist a constant $C \geq 1$, a probability measure π on $\mathcal{A}$, and a measurable function $s : \mathcal{A} \to (0, 1]$ such that, for all $x \in \mathcal{A}$,

$$s(x)\pi(dy) \leq K_{\mathcal{A}}^n(x, dy) \leq Cs(x)\pi(dy), \tag{3.24}$$

then the killed Markov chain admits a unique QSD. ◊

In the sequel, a quasi-stationary distribution for the process (Y_n^{Q}) will be denoted by ν_{Q}. We remind that, by (3.23), this implicitly implies that $\mathbb{P}^{\nu_{\mathrm{Q}}}(T_{\mathcal{B}} = 1) < 1$.

Lemma 3.18. *Starting from a quasi-stationary distribution ν_{Q}, the killing time $T_{\mathcal{B}}$ is geometrically distributed with parameter*

$$p = \mathbb{P}^{\nu_{\mathrm{Q}}}(T_{\mathcal{B}} = 1) \in (0, 1).$$

Notice that $p = \nu_{\mathrm{Q}} K_{\mathcal{AB}} \mathbb{1}_{\mathcal{B}}$ and $1 - p = \nu_{\mathrm{Q}} K_{\mathcal{A}} \mathbb{1}_{\mathcal{A}}$.

Proof. For all $m, n \in \mathbb{N}$, (3.22) gives

$$\mathbb{P}^{\nu_{\mathrm{Q}}}(T_{\mathcal{B}} > m + n) = \nu_{\mathrm{Q}} K_{\mathcal{A}}^{m+n} \mathbb{1}_{\mathcal{A}}.$$

Taking into account that ν_{Q} is a QSD, Lemma 3.15 tells us that

$$\mathbb{P}^{\nu_{\mathrm{Q}}}(T_{\mathcal{B}} > m + n) = \mathbb{P}^{\nu_{\mathrm{Q}}}(T_{\mathcal{B}} > 1)^{m+n},$$

which is the desired result. □

3.4 The π-return process

The π-return process was introduced in [6] in the context of population genetics. In words, the π-return process in $\mathcal{A}$ is a process which evolves exactly like (Y_n) until it hits $\mathcal{B}$, and is then instantaneously redistributed on $\mathcal{A}$ according to some probability measure π supported on $\mathcal{A}$. As a consequence, the π-return process can be seen as a process with a sink in $\mathcal{B}$ and a source in $\mathcal{A}$.

For any nonnegative test function $f : \mathcal{E} \to \mathbb{R}_+$ and any probability measure π, the outer product $f \otimes \pi$ is the nonnegative operator defined by $(f \otimes \pi)(x, \mathcal{C}) = f(x)\pi(\mathcal{C})$. Here is the formal definition of the π-return process.

Definition 3.19 (π-return process)**.** *Let π and (Y_n) denote respectively a probability measure on $\mathcal{A}$ and a Markov chain on $\mathcal{A} \cup \mathcal{B}$. The π-return process associated to (Y_n) is the Markov chain (Y_n^π) on $\mathcal{A}$ with transition kernel*

$$K^\pi(x, \mathcal{C}) = \mathbb{P}^x(Y_1 \in \mathcal{C}, T_\mathcal{B} > 1) + \mathbb{P}^x(Y_1 \in \mathcal{B})\, \pi(\mathcal{C}) \qquad \forall x \in \mathcal{A}, \forall \mathcal{C} \in \mathscr{B}(\mathcal{A}),$$

or, equivalently,

$$K^\pi = K_\mathcal{A} + (K_{\mathcal{A}\mathcal{B}} \mathbb{1}_\mathcal{B}) \otimes \pi.$$

The next result shows that the π-return process admits a unique stationary distribution.

Proposition 3.20. *Under Assumption A, the π-return process admits a unique stationary distribution, that is*

$$R(\pi) = \frac{\pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1}}{\mathbb{E}^\pi[T_\mathcal{B}]}.$$

Proof. Let us show that under Assumption A, the π-return process is π-recurrent. Since

$$\mathbb{E}^x\left[\sum_{n=1}^\infty \mathbf{1}_{\{Y_n^\pi \in \mathcal{C}\}}\right] = \sum_{n=1}^\infty \mathbb{P}^x(Y_n^\pi \in \mathcal{C}) \geq \sum_{n=1}^\infty \mathbb{P}^x(T_\mathcal{B} = n)\, \pi(\mathcal{C}),$$

with $\sum_{n=1}^\infty \mathbb{P}^x(T_\mathcal{B} = n) = \infty$ by (3.2) and the fact that (Y_n) is π_0-recurrent with $\pi_0(\mathcal{B}) > 0$, one obtains

$$\mathbb{E}^x\left[\sum_{n=1}^\infty \mathbf{1}_{\{Y_n^\pi \in \mathcal{C}\}}\right] = \infty, \qquad \forall x \in \mathcal{A}, \forall \mathcal{C} \in \mathscr{B}(\mathcal{A}) \text{ such that } \pi(\mathcal{C}) > 0.$$

Thus the π-return process is π-recurrent. Therefore, by Proposition 3.1, it admits, up to a multiplicative constant, a unique invariant measure. To check that $\pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1}$ is invariant, just notice that

$$\pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K^\pi = \pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K_\mathcal{A} + (\pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K_{\mathcal{A}\mathcal{B}} \mathbb{1}_\mathcal{B})\pi.$$

Using (3.7), the right hand side can be simplified as

$$\pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K^\pi = \pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K_\mathcal{A} + \pi.$$

Therefore, one has

$$\pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K^\pi = \pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1}(K_\mathcal{A} - \mathrm{id}_\mathcal{A}) + \pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} + \pi = \pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1}.$$

Since (3.13) shows that $\mathbb{E}^\pi[T_\mathcal{B}] = \pi(\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} \mathbb{1}_\mathcal{A}$, the proof is complete. □

Before going further, Table 1 recaps the various Markov chains introduced so far. Note that ν_Q is not an invariant distribution for the killed process but a quasi-stationary distribution.

Markov chain	State Space	Transition kernel	Invariant Measure
(Y_n): Initial process	$\mathcal{A} \cup \mathcal{B}$	K	π_0
(Y_n^Q): Process killed when leaving $\mathcal{A}$	$\mathcal{A}$	$K_\mathcal{A}$	ν_Q (QSD)
(Y_n^E): Reactive entrance process	$\mathcal{A}$	$K^\mathrm{E} = (\mathrm{id}_\mathcal{A} - K_\mathcal{A})^{-1} K_{\mathcal{A}\mathcal{B}} (\mathrm{id}_\mathcal{B} - K_\mathcal{B})^{-1} K_{\mathcal{B}\mathcal{A}}$	ν_E
(Y_n^π): π-Return process	$\mathcal{A}$	$K^\pi = K_\mathcal{A} + (K_{\mathcal{A}\mathcal{B}} \mathbb{1}_\mathcal{B}) \otimes \pi$	$R(\pi)$

Table 1: Summary of the different Markov chains.

4 The Hill relation

Considering a source-sink process at equilibrium, the Hill relation is an equality between the mean reaction time from the source to the sink and the inverse of the probability flux. The probability flux is the proportion of trajectories starting from one state and reaching the other state within one unit of time. This relation was introduced in biochemistry, see [28, Section 8]. Variations exist depending on how the source-sink process is precisely defined.

4.1 The general Hill relation

In our context, we derive a Hill relation for the π-return process of Section 3.4, in a more general form than the standard one which only considers the mean reaction time.

Proposition 4.1. *Under Assumption A, let π be a probability distribution on $\mathcal{A}$ and consider the π-return process together with its stationary distribution $R(\pi)$. Then, for any test function $f : \mathcal{A} \to \mathbb{R}$,*

$$\mathbb{E}^{\pi}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] = \frac{R(\pi)f}{\mathbb{P}^{R(\pi)}(Y_1 \in \mathcal{B})}. \tag{4.1}$$

The classical Hill relation is obtained by setting $f = \mathbb{1}_{\mathcal{A}}$, that is

$$\mathbb{E}^{\pi}[T_{\mathcal{B}}] = \frac{1}{\mathbb{P}^{R(\pi)}(Y_1 \in \mathcal{B})}.$$

Proof. Since $R(\pi)$ is the stationary distribution of the π-return process with transition kernel $K^{\pi} = K_{\mathcal{A}} + (K_{\mathcal{A}\mathcal{B}}\mathbb{1}_{\mathcal{B}}) \otimes \pi$, (3.8) implies

$$R(\pi)(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}}) = (R(\pi)K_{\mathcal{A}\mathcal{B}}\mathbb{1}_{\mathcal{B}})\pi = \mathbb{P}^{R(\pi)}(Y_1 \in \mathcal{B})\,\pi,$$

so that

$$\frac{R(\pi)}{\mathbb{P}^{R(\pi)}(Y_1 \in \mathcal{B})} = \pi(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}.$$

The Hill relation is then just a consequence of (3.12). □

Remark 4.2 (On other source-sink processes)**.** For related results, we refer to [3, Theorem A.1] where a Hill relation is derived for a slightly different source-sink process than the π-return process (Y_n^{π}) considered here. ♢

To compute the quantity of interest, namely

$$\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right], \tag{4.2}$$

it is natural to apply the Hill relation to $\pi = \nu_{\mathrm{E}}$, where ν_{E} is the reactive entrance distribution in $\mathcal{A}$. However, this requires to identify $R(\nu_{\mathrm{E}})$. This is the purpose of the next section.

4.2 The Hill relation and the reactive entrance distribution

Thanks to the explicit formulas obtained previously for $R(\pi)$ and ν_{E}, the Hill relation applied to the reactive entrance distribution yields a first useful expression to compute (4.2). Putting Proposition 3.20 and (3.18) together indeed provides the following result. Recall that $\pi_{0|\mathcal{A}}$ was defined in (3.14).

Corollary 4.3. *The stationary distribution of the ν_{E}-return process is the stationary distribution π_0 conditioned to $\mathcal{A}$:*

$$R(\nu_{\mathrm{E}}) = \pi_{0|\mathcal{A}}.$$

In particular, the Hill relation yields

$$\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] = \frac{\pi_{0|\mathcal{A}} f}{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}. \tag{4.3}$$

From a numerical point of view, the interest of the Hill formula is that the right-hand side of (4.3) does not involve $T_{\mathcal{B}}$ (which is typically very large) anymore. Accordingly, in the framework of Section 2, there is no need to simulate a whole path, but only reactive trajectories starting from $\pi_{0|\mathcal{A}}$.

However, sampling according to $\pi_{0|\mathcal{A}}$ can be a very difficult task since, in general, no analytical formula for $\pi_{0|\mathcal{A}}$ is known (see however Remark 2.3 on the Langevin process). Therefore, it requires to sample the stationary state of the initial process, which is computationally demanding when $\mathcal{A}$ and $\mathcal{B}$ are metastable.

Nevertheless, considering the metastability of $\mathcal{A}$, it seems intuitively sensible that a good approximation of $\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]$ is $\mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]$ where ν_{Q} is a QSD of the original process in $\mathcal{A}$, as introduced in Section 3.3 above. We will see in the next section that this leads to a formula which is even easier to use numerically.

4.3 The Hill relation and quasi-stationary distributions

Let us first establish a connection between a QSD ν_{Q} in $\mathcal{A}$ and the stationary law of a ν_{Q}-return process.

Proposition 4.4. *A probability measure π is a quasi-stationary distribution for the process (Y_n^{Q}) killed when leaving $\mathcal{A}$ if and only if π is a stationary distribution of the π-return process, i.e.,*

$$\pi = R(\pi).$$

Therefore, under Assumption A, there exists a (not necessarily unique) probability measure π such that $\pi = R(\pi)$. In particular, if ν_{Q} is a QSD, then for any test function $f : \mathcal{A} \mapsto \mathbb{R}$ the Hill relation writes

$$\mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] = \frac{\nu_{\mathrm{Q}} f}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})}. \tag{4.4}$$

Proof. The transition kernel of the π-return process is $K^{\pi} = K_{\mathcal{A}} + (K_{\mathcal{A}\mathcal{B}}\mathbb{1}_{\mathcal{B}}) \otimes \pi$, so one has $\pi = \pi K^{\pi}$ if and only if

$$\pi = \pi K_{\mathcal{A}} + (\pi K_{\mathcal{A}\mathcal{B}}\mathbb{1}_{\mathcal{B}})\pi = \pi K_{\mathcal{A}} + \mathbb{P}^{\pi}(T_{\mathcal{B}} = 1)\,\pi,$$

which is equivalent to say that $\pi K_{\mathcal{A}} = \mathbb{P}^{\pi}(T_{\mathcal{B}} > 1)\,\pi$ or, by Lemma 3.15, that π is a QSD for the process (Y_n^{Q}) killed when leaving $\mathcal{A}$. The Hill relation (4.4) is then a consequence of (4.1).

□

Remark 4.5 (Connection with Wald's equation)**.** A general version of Wald's identity is the following: consider a sequence of integrable random variables (X_n) with same mean, a nonnegative integer-valued and integrable random variable N, and assume that for all $n \geq 0$, $\mathbb{E}[X_n \mathbf{1}_{N \geq n}] = \mathbb{E}[X_n]\mathbb{P}(N \geq n)$ and $\sum_{n=1}^{\infty} \mathbb{E}[|X_n|\mathbf{1}_{N \geq n}] < \infty$, then

$$\mathbb{E}\left[\sum_{n=1}^{N} X_n\right] = \mathbb{E}[N]\mathbb{E}[X_1].$$

Interestingly, (4.4) might be regarded as a consequence of this identity, while the general Hill relation (4.1) can be considered as a similar relation in a different setting. ◊

If one admits, as will be justified in Section 5, that ν_{Q} is a good approximation of ν_{E} when $\mathcal{A}$ is metastable, the right-hand side of (4.4) is then a very efficient way to approximate the quantity of interest (4.2), that is

$$\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right].$$

Compared to (4.3), the interest is that ν_{Q} is easier to sample than $\pi_{0|\mathcal{A}}$ since it does not require to observe transitions to $\mathcal{B}$. To illustrate the practical interest of (4.4), Section 6.2 provides some insights on how this can be used for estimating reaction times for diffusions.

5 On the error introduced when replacing ν_{E} by ν_{Q}

As explained in the previous section, for numerical purposes, it is natural to approximate the quantity of interest $\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]$ by $\mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]$, where ν_{Q} is a QSD as introduced in Section 3.3. The objective of this section is thus to quantify the error introduced by this approximation. More precisely, we would like a sharp estimate of the relative error between these two quantities. Using the Hill relations (4.3) and (4.4), the relative error satisfies, for any test function $f : \mathcal{A} \to \mathbb{R}$,

$$\left|\frac{\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] - \mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]}{\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]}\right| = \left|1 - \frac{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\,\nu_{\mathrm{Q}} f}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})\,\pi_{0|\mathcal{A}} f}\right|. \tag{5.1}$$

Intuitively, one expects that the relative error will be small if the time needed to reach $\mathcal{B}$ is much longer than the time needed to relax to a local equilibrium within $\mathcal{A}$, namely the time for the process conditioned to stay in $\mathcal{A}$ to reach the quasi-stationary distribution.

Therefore, the main idea is to introduce two timescales: the timescale to observe a transition from $\mathcal{A}$ to $\mathcal{B}$, and the timescale to reach the QSD starting from ν_{E}, denoted by $T_{\mathrm{Q}}^{\mathrm{E}}$. This is the subject of Sections 5.1 and 5.2. Once this is done, we show in Section 5.3 that the error (5.1) is small when the former is much larger than the latter. Finally, Section 5.4 proposes two ways to estimate $T_{\mathrm{Q}}^{\mathrm{E}}$.

5.1 A lower bound for the reaction time

Let us introduce

$$p^+ = \sup_{x\in\mathcal{A}} \mathbb{P}^x(Y_1 \in \mathcal{B}). \tag{5.2}$$

Under Assumption A, we know from Lemma 3.3 that $p^+ > 0$.

Lemma 5.1. *Under Assumption A, for all $x \in \mathcal{A}$, one has*

$$\frac{1}{p^+} \le \mathbb{E}^x[T_{\mathcal{B}}]\,.$$

Proof. Since $\mathbb{E}^x[T_{\mathcal{B}}] = \sum_{k=0}^{\infty} \mathbb{P}^x(T_{\mathcal{B}} > k)$, and

$$\mathbb{P}^x(T_{\mathcal{B}} > k) = \prod_{\ell=1}^{k} \mathbb{P}^x(T_{\mathcal{B}} > \ell | T_{\mathcal{B}} > \ell - 1) = \prod_{\ell=1}^{k} \Big(1 - \mathbb{P}^x(T_{\mathcal{B}} = \ell | T_{\mathcal{B}} > \ell - 1)\Big),$$

one obtains that

$$\mathbb{E}^x[T_{\mathcal{B}}] \ge \sum_{k=0}^{\infty} (1-p^+)^k = \frac{1}{p^+}.$$

□

In the following, we will use $1/p^+$ as a measure of the time for a transition from $\mathcal{A}$ to $\mathcal{B}$. The previous lemma only shows that $1/p^+$ is a lower bound of the mean reaction time to $\mathcal{B}$. In Section A.2, we will check on a simple example that $1/p^+$ indeed yields to a sharp estimate of the error (5.1), as stated in Theorem 5.6, in the sense that it cannot be replaced by $1/\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})$ or $1/\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})$.

5.2 Relaxation time to a QSD

Definition of the relaxation time $T_{\mathrm{Q}}^{\mathrm{E}}$ to a QSD. Let ν_{Q} be a QSD for the process killed when leaving $\mathcal{A}$. We define the relaxation time to ν_{Q} through the ν_{Q}-return process $(Y_n^{\nu_{\mathrm{Q}}})$ starting from ν_{E}.

Proposition 5.2. *Under Assumption A, let ν_{Q} denote a QSD for the process killed when leaving $\mathcal{A}$. Let us define the signed kernel H_{Q} by*

$$H_{\mathrm{Q}} = (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}}), \tag{5.3}$$

or, equivalently, for any test function $f : \mathcal{A} \to \mathbb{R}$ and any $x \in \mathcal{A}$:

$$H_{\mathrm{Q}} f(x) = \mathbb{E}^x\left[\sum_{n=0}^{T_{\mathcal{B}}-1} \{f(Y_n) - \nu_{\mathrm{Q}} f\}\right]. \tag{5.4}$$

Then, denoting $(Y_n^{\nu_{\mathrm{Q}}})$ the ν_{Q}-return process, it also writes

$$H_{\mathrm{Q}} f(x) = \sum_{n=0}^{\infty} \mathbb{E}^x\big[f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}} f\big]\,. \tag{5.5}$$

The relaxation time to the QSD ν_{Q} in $\mathcal{A}$ starting from ν_{E} is then defined as

$$T_{\mathrm{Q}}^{\mathrm{E}} = \|\nu_{\mathrm{E}} H_{\mathrm{Q}}\|. \tag{5.6}$$

Let us also define a uniform relaxation time to the QSD by

$$T_{\mathrm{Q}} = \|H_{\mathrm{Q}}\|_\infty = \sup_{x\in\mathcal{A}} \|H_{\mathrm{Q}}(x,\cdot)\| < \infty. \tag{5.7}$$

One obviously has $T_{\mathrm{Q}}^{\mathrm{E}} \le T_{\mathrm{Q}}$.

Proof. Let us first notice that

$$T_{\mathrm{Q}}^{\mathrm{E}} \le T_{\mathrm{Q}} = \|H_{\mathrm{Q}}\|_\infty = \|(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}})\|_\infty \le 2\|(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}\|_\infty$$

is finite under Assumption A, by Corollary 3.4. The equivalence between (5.3) and (5.4) is again a consequence of Corollary 3.4. Finally, for (5.5), by the same reasoning as in the proof of Corollary 3.4, Fubini's theorem yields

$$\begin{aligned}\mathbb{E}^x\left[\sum_{n=0}^{T_{\mathcal{B}}-1} \{f(Y_n) - \nu_{\mathrm{Q}} f\}\right] &= \sum_{n=0}^{\infty} \mathbb{E}^x[\{f(Y_n) - \nu_{\mathrm{Q}} f\}\mathbf{1}_{T_{\mathcal{B}}>n}] \\ &= \sum_{n=0}^{\infty} \mathbb{E}^x\left[\left\{f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}} f\right\}\mathbf{1}_{T_{\mathcal{B}}>n}\right], \end{aligned} \tag{5.8}$$

where we have used that $\mathbb{E}^x[f(Y_n)\mathbf{1}_{T_{\mathcal{B}}>n}] = \mathbb{E}^x\left[f(Y_n^{\nu_{\mathrm{Q}}})\mathbf{1}_{T_{\mathcal{B}}>n}\right]$. In addition,

$$\sum_{n=0}^{\infty} \mathbb{E}^x\left[\left\{f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}} f\right\}\mathbf{1}_{T_{\mathcal{B}}\le n}\right] = \sum_{n=1}^{\infty} \mathbb{E}^x[f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}} f | T_{\mathcal{B}} \le n]\mathbb{P}^x(T_{\mathcal{B}} \le n) = 0. \tag{5.9}$$

The last equality comes from the strong Markov property: indeed, when the ν_{Q}-return process reaches $\mathcal{B}$, it is instantaneously redistributed according to ν_{Q}, and then starting from the QSD ν_{Q}, one has $\mathbb{E}^{\nu_{\mathrm{Q}}}\left[f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}} f\right] = 0$. Equation (5.5) is then obtained by adding (5.8) and (5.9). □

Why is $T_{\mathrm{Q}}^{\mathrm{E}}$ a sensible measure of the relaxation time to a QSD? The next result shows that the time for the process conditioned to stay in $\mathcal{A}$ to converge to the QSD is closely related to the time for the ν_{Q}-return process to reach its equilibrium.

Lemma 5.3. *For any probability measure μ on $\mathcal{A}$, any test function f, and all $n \ge 0$, one has*

$$\mathbb{E}^\mu\left[f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}} f\right] = \Big(\mathbb{E}^\mu[f(Y_n)|T_{\mathcal{B}} > n] - \nu_{\mathrm{Q}} f\Big)\mathbb{P}^\mu(T_{\mathcal{B}} > n)\,. \tag{5.10}$$

As a consequence, denoting $\mathcal{L}^\mu(\cdot)$ the law of a process with initial distribution μ, we get

$$\|\mathcal{L}^\mu(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}}\| \le \|\mathcal{L}^\mu(Y_n|T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\|.$$

Using these estimates with $\mu = \nu_{\mathrm{E}}$, one obtains in particular

$$T_{\mathrm{Q}}^{\mathrm{E}} \le \sum_{n=0}^{\infty} \|\mathcal{L}^{\nu_{\mathrm{E}}}(Y_n|T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\|.$$

Proof. By definition of the ν_{Q}-return process, we have

$$\mathbb{E}^\mu\left[f(Y_n^{\nu_{\mathrm{Q}}})\mathbf{1}_{T_{\mathcal{B}}>n}\right] = \mathbb{E}^\mu[f(Y_n)\mathbf{1}_{T_{\mathcal{B}}>n}]\,, \tag{5.11}$$

whereas

$$\mathbb{E}^{\mu}\big[f(Y_n^{\nu_{\mathrm{Q}}})\mathbf{1}_{T_{\mathcal{B}}\le n}\big] = \sum_{m=0}^{n} \mathbb{E}^{\mu}\big[f(Y_n^{\nu_{\mathrm{Q}}})\mathbf{1}_{T_{\mathcal{B}}=m}\big]$$
$$= \sum_{m=0}^{n} \mathbb{E}^{\mu}\big[\mathbb{E}^{\nu_{\mathrm{Q}}}\big[f(Y_{n-m}^{\nu_{\mathrm{Q}}})\big]\,\mathbf{1}_{T_{\mathcal{B}}=m}\big] = (\nu_{\mathrm{Q}}f)\mathbb{P}^{\mu}(T_{\mathcal{B}}\le n)\,. \tag{5.12}$$

As a consequence, summing (5.11) and (5.12), one has

$$\begin{aligned}\mathbb{E}^{\mu}\big[f(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}}f\big] &= \mathbb{E}^{\mu}[f(Y_n)\mathbf{1}_{T_{\mathcal{B}}>n}] + (\nu_{\mathrm{Q}}f)\mathbb{P}^{\mu}(T_{\mathcal{B}}\le n) - \nu_{\mathrm{Q}}f\\ &= \mathbb{E}^{\mu}[f(Y_n)\mathbf{1}_{T_{\mathcal{B}}>n}] - (\nu_{\mathrm{Q}}f)\mathbb{P}^{\mu}(T_{\mathcal{B}}>n)\\ &= \Big(\mathbb{E}^{\mu}[f(Y_n)|T_{\mathcal{B}}>n] - \nu_{\mathrm{Q}}f\Big)\mathbb{P}^{\mu}(T_{\mathcal{B}}>n)\,.\end{aligned}$$

This yields the first claim of Lemma 5.3. The second claim is obtained by using the trivial bound $\mathbb{P}^{\mu}(T_{\mathcal{B}}>n)\le 1$. □

Let us comment on the result of Lemma 5.3, see Equation (5.10). It shows that the convergence of the ν_{Q}-return process to ν_{Q} occurs if the process $(Y_n)_{n\ge0}$ conditioned to stay in $\mathcal{A}$ converges to ν_{Q}, or if the process $(Y_n)_{n\ge0}$ reaches $\mathcal{B}$ (all these processes starting from μ). In our context, we consider metastable situations where transitions to $\mathcal{B}$ are rare: $\mathbb{P}^{\mu}(T_{\mathcal{B}}>n)\ge(1-p^{+})^n$ with $p^{+}\ll 1$. In this case, the convergence of the ν_{Q}-return process to ν_{Q} is more related to the distance to ν_{Q} of the process $(Y_n)_{n\ge0}$ conditioned to stay in $\mathcal{A}$, than to the probability for the process $(Y_n)_{n\ge0}$ to reach $\mathcal{B}$.

Remark 5.4 (Interpretation of T_{Q})**.** Let us recall that a randomized stopping time for $(Y_n^{\nu_{\mathrm{Q}}})$ is a stopping time with respect to a possibly enlarged version of the filtration generated by the random variables $(Y_n^{\nu_{\mathrm{Q}}})$. Then, following [1], define for $0<c<1$

$$T_{\mathrm{stop}}(c) = \sup_x \inf_T \{\mathbb{E}^x[T] \text{ where } T \text{ is a randomized stopping time s.t. } \|\mathcal{L}^x(Y_T^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}}\| \le c\}. \tag{5.13}$$

From [1, Theorem 1], it is known that if T_{Q} or $T_{\mathrm{stop}}(c)$ (for some $0<c<1$) is finite then T_{Q} and $T_{\mathrm{stop}}(c)$ are equivalent in the sense that

$$T_{\mathrm{stop}}(c) \le \frac{4}{c^2}T_{\mathrm{Q}} < \frac{8}{c^2(1-c)}T_{\mathrm{stop}}(c). \tag{5.14}$$

As a consequence, T_{Q} quantifies the time for the ν_{Q}-return process to converge to ν_{Q}, uniformly over the initial condition. ◊

5.3 A general bound on the relative error

In this section, we prove Theorem 5.6 which gives an upper bound on the relative error introduced in (5.1) by using the two time scales introduced above: $1/p^{+}$ as a measure of the time to observe a transition from $\mathcal{A}$ to $\mathcal{B}$, and $T_{\mathrm{Q}}^{\mathrm{E}}$ as a measure of the time to relax to the QSD. The proof of Theorem 5.6 relies on the following estimate of the difference between a quasi-stationary distribution and the conditional stationary distribution.

Lemma 5.5. *Let $\pi_{0|\mathcal{A}}$ be the stationary distribution π_0 conditioned to $\mathcal{A}$, and ν_{Q} be a QSD for the killed process (Y_n^{Q}). Then one has*

$$\|\pi_{0|\mathcal{A}} - \nu_{\mathrm{Q}}\| = \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1\in\mathcal{B})\,T_{\mathrm{Q}}^{\mathrm{E}}, \tag{5.15}$$

where $T_{\mathrm{Q}}^{\mathrm{E}}$ denotes the relaxation time defined by (5.6).

Proof. Since $\pi_{0|\mathcal{A}} - \nu_{\mathrm{Q}} = \pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}})$, we get, using (5.3) for H_{Q}:

$$\pi_{0|\mathcal{A}} - \nu_{\mathrm{Q}} = \pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}}) = \pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})H_{\mathrm{Q}}.$$

Now, from (3.17), $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\,\nu_{\mathrm{E}} = \pi_{0|\mathcal{A}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})$, and it follows that

$$\pi_{0|\mathcal{A}} - \nu_{\mathrm{Q}} = \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\,\nu_{\mathrm{E}} H_{\mathrm{Q}}.$$

This yields (5.15) by taking the total variation norm. □

We are now in a position to state the main mathematical result of this work.

Theorem 5.6. *Let ν_{Q} be a QSD for the process killed when leaving $\mathcal{A}$ and let us assume that $p^+ T_{\mathrm{Q}}^{\mathrm{E}} < 1$, where p^+ is defined by (5.2) and $T_{\mathrm{Q}}^{\mathrm{E}}$ by (5.6). Then the relative error introduced in (5.1) is bounded as follows:*

$$\left| \frac{\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] - \mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]}{\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]} \right| \leq \frac{p^+ T_{\mathrm{Q}}^{\mathrm{E}}}{1 - p^+ T_{\mathrm{Q}}^{\mathrm{E}}} \left(1 + \frac{\|f\|_\infty}{|\pi_{0|\mathcal{A}} f|}\right). \tag{5.16}$$

Proof. From (5.1), the relative error is bounded by

$$\begin{aligned} &\left| \frac{\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right] - \mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]}{\mathbb{E}^{\nu_{\mathrm{E}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1} f(Y_n)\right]} \right| \\ &\qquad \leq \left| 1 - \frac{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})} \right| + \frac{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})} \left| 1 - \frac{\nu_{\mathrm{Q}} f}{\pi_{0|\mathcal{A}} f} \right|. \end{aligned}$$

From (5.15), one has, for any test function $f : \mathcal{A} \to \mathbb{R}$,

$$|\mathbb{E}^{\pi_{0|\mathcal{A}}}[f] - \mathbb{E}^{\nu_{\mathrm{Q}}}[f]\,| \leq \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, T_{\mathrm{Q}}^{\mathrm{E}} \|f\|_\infty.$$

Applying this inequality with $f(x) = \mathbb{P}^x(Y_1 \in \mathcal{B})$ gives, since $\|f\|_\infty = p^+$,

$$\left| 1 - \frac{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})}{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})} \right| \leq p^+ T_{\mathrm{Q}}^{\mathrm{E}}.$$

As $p^+ T_{\mathrm{Q}}^{\mathrm{E}} < 1$ by assumption, one deduces that

$$\left| 1 - \frac{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})} \right| \leq \frac{p^+ T_{\mathrm{Q}}^{\mathrm{E}}}{1 - p^+ T_{\mathrm{Q}}^{\mathrm{E}}}.$$

From this equation, we also have

$$\frac{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})} \leq \frac{1}{1 - p^+ T_{\mathrm{Q}}^{\mathrm{E}}}.$$

Finally, using again (5.15), one obtains

$$\left| 1 - \frac{\nu_{\mathrm{Q}} f}{\pi_{0|\mathcal{A}} f} \right| \leq T_{\mathrm{Q}}^{\mathrm{E}} \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, \frac{\|f\|_\infty}{|\pi_{0|\mathcal{A}} f|},$$

and the result follows by bounding $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})$ by p^+. □

The upper bound in (5.16) shows that the relative error is small if $T_{\mathrm{Q}}^{\mathrm{E}} \ll 1/p^+$, namely if the timescale associated with the relaxation time to the QSD in $\mathcal{A}$ is small compared to the timescale associated with the transition time from $\mathcal{A}$ to $\mathcal{B}$. Notice that the result holds for any QSD ν_{Q}, T_Q^{E} being the associated convergence time for the ν_{Q}-return process starting from ν_{E}. We refer to Appendix A for a discussion on the sharpness of the error estimate (5.16), and in particular to Apprendix A.1 for a situation with two QSDs.

5.4 On pratical estimates of $T_{\mathrm{Q}}^{\mathrm{E}}$

We discuss in this section two ways to estimate $T_{\mathrm{Q}}^{\mathrm{E}}$.

Quasi-ergodicity. The first one is based on the notion of quasi-ergodicity.

Assumption B (Quasi-ergodicity)**.** There exist a QSD ν_{Q} in $\mathcal{A}$ and a constant $\eta < \infty$ such that

$$\sum_{n\geq 0} \|\mathcal{L}^{\nu_{\mathrm{E}}}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \eta.$$

Quasi-ergodicity provides an elementary bound on the relaxation time $T_{\mathrm{Q}}^{\mathrm{E}}$.

Proposition 5.7. *Under Assumptions A and B, the relaxation time $T_{\mathrm{Q}}^{\mathrm{E}}$ to the QSD ν_{Q} satisfies*

$$T_{\mathrm{Q}}^{\mathrm{E}} \leq \eta.$$

Proof. Let us consider the QSD ν_{Q} introduced in Assumption B. Let $f : \mathcal{A} \to \mathbb{R}$ be a test function, then for all $x \in \mathcal{A}$, (5.5), (5.8), and (5.9) ensure that

$$\nu_{\mathrm{E}} H_{\mathrm{Q}} f = \sum_{n=0}^{\infty} \mathbb{E}^{\nu_{\mathrm{E}}}[\{f(Y_n) - \nu_{\mathrm{Q}} f\}\mathbf{1}_{T_{\mathcal{B}}>n}]\,.$$

Note that, by conditioning,

$$\begin{aligned}\mathbb{E}^{\nu_{\mathrm{E}}}[\{f(Y_n) - \nu_{\mathrm{Q}} f\}\mathbf{1}_{T_{\mathcal{B}}>n}] &= \mathbb{E}^{\nu_{\mathrm{E}}}[f(Y_n) - \nu_{\mathrm{Q}} f | T_{\mathcal{B}} > n]\mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} > n) \\ &= (\mathbb{E}^{\nu_{\mathrm{E}}}[f(Y_n)|T_{\mathcal{B}} > n] - \nu_{\mathrm{Q}} f)\,\mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} > n)\,.\end{aligned}$$

For all $n \geq 0$, let us introduce

$$I(n) = \sum_{m=0}^{n} (\mathbb{E}^{\nu_{\mathrm{E}}}[f(Y_m)|T_{\mathcal{B}} > m] - \nu_{\mathrm{Q}} f)\,,$$

with the convention $I(-1) = 0$. One has

$$\mathbb{E}^{\nu_{\mathrm{E}}}[f(Y_n)|T_{\mathcal{B}} > n] - \nu_{\mathrm{Q}} f = I(n) - I(n-1).$$

Besides, notice that under Assumption B,

$$|I(n)| \leq \eta \|f\|_{\infty}. \tag{5.17}$$

As a consequence, a summation by parts yields

$$\begin{aligned}\nu_{\mathrm{E}} H_{\mathrm{Q}} f &= \sum_{n\geq 0} \Big(I(n) - I(n-1)\Big)\mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} > n) \\ &= \sum_{n\geq 0} I(n)\Big(\mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} > n) - \mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} > n+1)\Big) \\ &= \sum_{n\geq 0} I(n)\mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} = n+1)\,.\end{aligned}$$

Using (5.17), the result follows by taking the supremum over all test functions f such that $\|f\|_{\infty} \leq 1$ since, under Assumption A, $\sum_{n\geq 0} \mathbb{P}^{\nu_{\mathrm{E}}}(T_{\mathcal{B}} = n+1) = 1$. □

Geometric ergodicity. A stronger assumption is the geometric convergence of the conditioned process starting from ν_{E} to a QSD ν_{Q}. This provides a second manner to estimate $T_{\mathrm{Q}}^{\mathrm{E}}$.

Assumption C (Geometric ergodicity)**.** There exist a QSD ν_{Q}, a constant $\alpha < \infty$, and a constant $\rho \in (0,1)$ such that, for all $n \geq 0$,

$$\|\mathcal{L}^{\nu_{\mathrm{E}}}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \alpha \rho^n.$$

Lemma 5.8. *Under Assumptions A and C, the relaxation time satisfies*

$$T_{\mathrm{Q}}^{\mathrm{E}} \leq \frac{\alpha}{1-\rho}. \tag{5.18}$$

Proof. Lemma 5.3 shows that, under Assumption C,

$$T_{\mathrm{Q}}^{\mathrm{E}} \leq \sum_{n=0}^{\infty} \|\mathcal{L}^{\nu_{\mathrm{E}}}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \frac{\alpha}{1-\rho}.$$

□

Uniform geometric ergodicity. In practice, it may be easier to prove a stronger assumption than Assumption C, namely the uniform geometric ergodicity, which writes:

Assumption D (Uniform geometric ergodicity)**.** There exist a QSD ν_{Q}, a constant $\alpha < \infty$, and a constant $\rho \in (0,1)$ such that, for all $n \geq 0$,

$$\sup_{x \in \mathcal{A}} \|\mathcal{L}^{x}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \alpha \rho^n. \tag{5.19}$$

With our definition (3.3) of the total variation distance, one can prove that necessarily, in Assumption D, one has $\alpha \geq 1$, provided that $\mathcal{A}$ is not reduced to a single point. The uniform geometric ergodicity (5.19) is for example a consequence of the two-sided condition stated in Equation (3.24) as will be illustrated in the upcoming section (see [9], [18, Section 7.1], and Appendix C). One can verify that if (5.19) is satisfied, then for any initial distribution ν on $\mathcal{A}$,

$$\|\mathcal{L}^{\nu}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \alpha \rho^n.$$

In particular, Assumption D implies the unicity of the quasi-stationary distribution as well as Assumption C and thus (5.18). Actually, under (5.19), one can prove the following equivalent of Lemma 5.8:

Lemma 5.9. *Under Assumptions A and D, the relaxation time satisfies*

$$T_{\mathrm{Q}}^{\mathrm{E}} \leq T_{\mathrm{Q}} \leq \min\left\{ \frac{\alpha}{1-\rho}, \inf_{0<c<1} \frac{2}{1-c} \left\lceil \frac{\ln(c\alpha^{-1})}{\ln(\rho)} \right\rceil \right\}.$$

where $\lceil \cdot \rceil$ *denotes the ceiling function. As a consequence,* T_{Q} *is upper-bounded by* $\min(\alpha, 2)$ *when* ρ *tends to* 0.

Remember that T_{Q} defined by (5.7) is an upper-bound of $T_{\mathrm{Q}}^{\mathrm{E}}$.

Proof. First, by the very definition of T_{Q} and Lemma 5.3, one has

$$T_{\mathrm{Q}} = \sup_{x\in\mathcal{A}} \|H_{\mathrm{Q}}(x,\cdot)\| \leq \sup_{x\in\mathcal{A}} \sum_{n=0}^{\infty} \|\mathcal{L}^x(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}}\| \leq \sup_{x\in\mathcal{A}} \sum_{n=0}^{\infty} \|\mathcal{L}^x(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \frac{\alpha}{1-\rho}.$$

Additionally, for any $0 < c < 1$ and the deterministic time $T = \left\lceil \frac{\ln(c\alpha^{-1})}{\ln(\rho)} \right\rceil$, it holds

$$\|\mathcal{L}^x(Y_T | T_{\mathcal{B}} > T) - \nu_{\mathrm{Q}}\| \leq \alpha\rho^T \leq c.$$

Therefore, if $0 < c < 1$, using (5.13) and again the fact that, by Lemma 5.3,

$$\|\mathcal{L}^x(Y_n^{\nu_{\mathrm{Q}}}) - \nu_{\mathrm{Q}}\| \leq \|\mathcal{L}^x(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\|,$$

one has $T_{\mathrm{stop}}(c) \leq T$. By (5.14), the relaxation time satisfies

$$T_{\mathrm{Q}} \leq \frac{2}{1-c} \left\lceil \frac{\ln(c\alpha^{-1})}{\ln(\rho)} \right\rceil.$$

When ρ tends to 0, this upper-bound converges to 2 by considering $c = \alpha\rho$. □

6 Back to the case of a diffusion process

6.1 Verifying assumptions A and D

The setting in this section is the same as in Section 2: the Markov chain (Y_n) is defined by (2.4) from a diffusion process (X_t) satisfying (2.1). Let us recall that the functions f and g in (2.1) are assumed to be smooth (globally Lipschitz is enough to get the Feynman-Kac representations formulas in the proof of Proposition 6.1 below) and such that (X_t) is ergodic with respect to a stationary measure which gives a non-zero probability to the sets A and B. The sets A and B are thus visited infinitely often and the Markov chain (Y_n) is then well defined for all $n \geq 0$.

The objective of this section is to exhibit some sufficient assumptions on the diffusion (X_t) for the associated Markov chain (Y_n) to satisfy Assumptions A and D. Let us emphasize that we stick to a relatively simple set of assumptions (smooth Lipschitz coefficients, elliptic diffusion) for the sake of simplicity, but we expect the result to be true for much more general diffusions, including the Langevin dynamics (1.1), see also Remark 2.3. The objective here is just to illustrate how Assumptions A and D can be obtained in practice in a simple setting.

Proposition 6.1. *Let us assume that the domains A and B are chosen such that Assumption [A1] on $\mathcal{A}$ and $\mathcal{B}$ is satisfied, meaning that $\mathcal{A} = \partial A$ and $\mathcal{B} = \partial B$ are compact disjoint sets and $\mathcal{E} = \mathcal{A} \cup \mathcal{B}$. Let us assume moreover that the infinitesimal generator of (X_t) satisfying* (2.1) *is elliptic, in the sense that*

$$\exists \lambda, \Lambda > 0,\ \forall x \in \mathbb{R}^d,\ \lambda \leq gg^T(x) \leq \Lambda. \tag{6.1}$$

Then, the associated Markov chain (Y_n) defined by (2.4) *satisfies Assumptions A and D.*

Proof. Recall that S is such that $A \subset S$, $B \subset S^c$ and $\partial S = \Sigma$. Let us start with some notation and some classical results to relate the process (X_t) with the solutions to some partial differential equations. Let $\varphi : \Sigma \to \mathbb{R}$ and $\psi : \mathcal{A} \to \mathbb{R}$ be continuous functions. Define for all $x \in \mathbb{R}^d$

$$u(x) = \mathbb{E}^x[\varphi(X_{\tau_\Sigma})] \text{ and } v(x) = \mathbb{E}^x[\psi(X_{\tau_\mathcal{A}})\mathbf{1}_{\tau_\mathcal{A}<\tau_\mathcal{B}}],$$

where $\tau_C = \inf\{t > 0, X_t \in C\}$. Hence, denoting by L the generator of the diffusion process (X_t), u and v satisfy (see for example [25, Theorem 5.1])

$$\begin{cases} Lu(x) = 0 & \text{for } x \in S, \\ u(x) = \varphi(x) & \text{for } x \in \Sigma, \end{cases} \tag{6.2}$$

and

$$\begin{cases} Lv(x) = 0 & \text{for } x \in (A \cup B)^c, \\ v(x) = \psi(x) & \text{for } x \in \mathcal{A}, \\ v(x) = 0 & \text{for } x \in \mathcal{B}. \end{cases} \tag{6.3}$$

In particular, u and v are $\mathcal{C}^\infty$ functions in the interior of their domains of definition, from standard elliptic regularity results (see for example [26, Corollary 8.11]). Then, denoting by $K_{S\Sigma}(x, dy)$ the measure of the first hitting point on Σ for the process (X_t) starting from $x \in S$, and $K_{(A\cup B)^c\mathcal{A}}(x, dy)$ the measure of the first hitting point on $\mathcal{A}$ for the process (X_t) starting from $x \in (A \cup B)^c$ and reaching $\mathcal{A}$ before $\mathcal{B}$, one has

$$u(x) = \int_\Sigma K_{S\Sigma}(x, dy)\varphi(y) \text{ and } v(x) = \int_\mathcal{A} K_{(A\cup B)^c\mathcal{A}}(x, dy)\psi(y). \tag{6.4}$$

We first verify that Assumption [A2] is satisfied. Let us take a bounded continuous function $f : \mathcal{E} \to \mathbb{R}$. One would like to check that $Kf(x) = \mathbb{E}^x[f(Y_1)]$ is a bounded continuous function of x. Let us consider $x \in \mathcal{A}$ (the reasoning is similar if $x \in \mathcal{B}$). Then

$$Kf(x) = \mathbb{E}^x[f(Y_1)\mathbf{1}_{Y_1\in\mathcal{A}}] + \mathbb{E}^x[f(Y_1)\mathbf{1}_{Y_1\in\mathcal{B}}].$$

Considering the first term (the reasoning is similar for the second one), one has

$$\mathbb{E}^x[f(Y_1)\mathbf{1}_{Y_1\in\mathcal{A}}] = \mathbb{E}^x[\varphi(X_{\tau_\Sigma})]$$

where

$$\varphi(x) = \mathbb{E}^x[f(X_{\tau_A})\mathbf{1}_{\tau_A<\tau_B}].$$

Thus φ satisfies (6.3) for the boundary condition $\psi = f\mathbf{1}_\mathcal{A}$. In particular, φ is continuous and bounded on Σ. Then, $\mathbb{E}^x[\varphi(X_{\tau_\Sigma})]$ satisfies (6.2), and is thus again a continuous and bounded function. This concludes the proof of Assumption [A2].

Let us now prove Assumptions [A3] and [A4]. As shown in the proof of [33, Theorem 1.7], the reactive entrance processes in $\mathcal{A}$ and $\mathcal{B}$ are positive Harris recurrent under the ellipticity condition (6.1). Thus, by Remark 3.10, the Markov chain (Y_n) defined by (2.4) is positive Harris recurrent, with an invariant measure π_0 which satisfies (3.19). This yields Assumption [A3]. Assumption [A4] is satisfied because, via (3.18) and (3.19),

$$\pi_0(\mathcal{A}) = \frac{\mathbb{E}^{\nu_{\mathrm{E}}^\mathcal{A}}[T_\mathcal{B}]}{\mathbb{E}^{\nu_{\mathrm{E}}^\mathcal{A}}[T_\mathcal{B}] + \mathbb{E}^{\nu_{\mathrm{E}}^\mathcal{B}}[T_\mathcal{A}]} \qquad \text{and} \qquad \pi_0(\mathcal{B}) = \frac{\mathbb{E}^{\nu_{\mathrm{E}}^\mathcal{B}}[T_\mathcal{A}]}{\mathbb{E}^{\nu_{\mathrm{E}}^\mathcal{A}}[T_\mathcal{B}] + \mathbb{E}^{\nu_{\mathrm{E}}^\mathcal{B}}[T_\mathcal{A}]}$$

are non-zero since $\mathbb{E}^{\nu_{\mathrm{E}}^{\mathcal{A}}}[T_{\mathcal{B}}] = T_{AB}$ and $\mathbb{E}^{\nu_{\mathrm{E}}^{\mathcal{B}}}[T_{\mathcal{A}}] = T_{BA}$ are strictly positive and finite (see [33, Proposition 1.8]).

It remains to establish that Assumption D is fulfilled as well. Let (Y_n^Q) be the process killed when leaving $\mathcal{A}$. Its (sub-Markov) transition kernel is given for $x \in \mathcal{A}$ by

$$K_{\mathcal{A}}(x, dy) = \int_{z\in\Sigma} K_{S\Sigma}(x, dz) K_{(A\cup B)^c\mathcal{A}}(z, dy).$$

Let us show that it satisfies the following two-sided condition: there exists a non-zero positive finite measure $\pi_{\mathcal{A}}$ and a constant $C > 0$ such that

$$\pi_{\mathcal{A}}(dy) \leq K_{\mathcal{A}}(x, dy) \leq C\pi_{\mathcal{A}}(dy). \tag{6.5}$$

Note that by the maximum principle, for any non-zero $\varphi \geq 0$, u (solution to (6.2)) is strictly positive on S. Moreover, by the Harnack inequality for elliptic operators [26, Corollary 9.25] and the compactness of $\mathcal{A}$, we then have

$$0 \leq \sup_{x\in\mathcal{A}} u(x) \leq C \inf_{x\in\mathcal{A}} u(x),$$

where the constant C is independent of $\varphi \geq 0$ (considering (2.1), it only depends on the lower and upper bounds of gg^T and on the maximum of $|f|$ on some compact set $\mathcal{A}' \subset S$ which contains a neighborhood of $\mathcal{A}$). Therefore, by (6.4), for all smooth function $\varphi \geq 0$, one has

$$0 \leq \sup_{x\in\mathcal{A}} \int_\Sigma K_{S\Sigma}(x, dy)\varphi(y) \leq C \inf_{x\in\mathcal{A}} \int_\Sigma K_{S\Sigma}(x, dy)\varphi(y),$$

with equality to 0 if and only if $\varphi = 0$. Let O be a non-empty open subset of $\mathcal{A}$, and let us introduce $\varphi_O(x) = K_{(A\cup B)^c\mathcal{A}}(x, O)$. The function φ_O is smooth in the interior of $(A \cup B)^c$ by standard regularity results on elliptic operators (since it satisfies (6.3) with $\psi = \mathbf{1}_O$), and non-zero (by the maximum principle, since $\mathbf{1}_O$ is nonnegative and non-zero). One thus has:

$$0 < \sup_{x\in\mathcal{A}} \int_{z\in\Sigma} K_{S\Sigma}(x, dz) K_{(A\cup B)^c\mathcal{A}}(z, O) \leq C \inf_{x\in\mathcal{A}} \int_{z\in\Sigma} K_{S\Sigma}(x, dz) K_{(A\cup B)^c\mathcal{A}}(z, O), \tag{6.6}$$

where C is independent of O. Let us now introduce

$$\pi_{\mathcal{A}}(dy) = \inf_{x\in\mathcal{A}} \int_{z\in\Sigma} K_{S\Sigma}(x, dz) K_{(A\cup B)^c\mathcal{A}}(z, dy).$$

This is a nonnegative measure on $\mathcal{A}$ as the infimum of positive measures (see for example [17, Lemma 5.2]) which is non-zero since $\pi_{\mathcal{A}}(O) > 0$ for any non-empty open set $O \subset \mathcal{A}$ thanks to (6.6). Notice also that $\pi_{\mathcal{A}}(\mathcal{A}) \leq 1$. Moreover, from (6.6), one has, for all $x \in \mathcal{A}$,

$$\pi_{\mathcal{A}}(dy) \leq \int_{z\in\Sigma} K_{S\Sigma}(x, dz) K_{(A\cup B)^c\mathcal{A}}(z, dy) \leq C\pi_{\mathcal{A}}(dy)$$

which yields (6.5).

Assumption D is then a consequence of the two-sided condition (6.5), and actually of the more general two-sided condition stated in Equation (3.24). See Appendix C and more precisely Proposition C.7, which yields (5.19) with $\rho = \frac{C-1}{C+1}$. □

6.2 Numerical counterparts of the Hill relation

Returning to the setting and notation of Section 2, see Equation (2.5), let us consider the case where $f = \Delta$ in Equation (4.4) to approximate the reaction time T_{AB} in Equation (2.6). We first rewrite the right-hand side of (4.4) as follows:

$$\mathbb{E}^{\nu_{\mathrm{Q}}}\left[\sum_{n=0}^{T_{\mathcal{B}}-1}\Delta(Y_n)\right] = \frac{\mathbb{E}^{\nu_{\mathrm{Q}}}[\Delta(Y_0)\mathbf{1}_{Y_1\in\mathcal{A}}]}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1\in\mathcal{B})} + \frac{\mathbb{E}^{\nu_{\mathrm{Q}}}[\Delta(Y_0)\mathbf{1}_{Y_1\in\mathcal{B}}]}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1\in\mathcal{B})}$$
$$= \mathbb{E}^{\nu_{\mathrm{Q}}}[\Delta(Y_0)|Y_1\in\mathcal{A}]\left(\frac{1}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1\in\mathcal{B})}-1\right) + \mathbb{E}^{\nu_{\mathrm{Q}}}[\Delta(Y_0)|Y_1\in\mathcal{B}]. \quad (6.7)$$

The terms in (6.7) can be computed as follows:

- $\mathbb{E}^{\nu_{\mathrm{Q}}}[\Delta(Y_0)|Y_1\in\mathcal{A}]$ is the mean time of a loop starting from ν_{Q} on $\mathcal{A}$ to Σ and then back to $\mathcal{A}$. It can be estimated by brute force Monte Carlo, provided that we are able to sample from the QSD ν_{Q}. The latter is also required for the quantities at stake in the next two items.

- $\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1\in\mathcal{B})$ is the probability to observe a trajectory that starts from ν_{Q} on $\mathcal{A}$ and directly goes to $\mathcal{B}$ without going back to $\mathcal{A}$ once Σ is crossed. This probability is typically very small, but can be efficiently estimated using rare event simulation methods such as splitting techniques (FFS or AMS).

- $\mathbb{E}^{\nu_{\mathrm{Q}}}[\Delta(Y_0)|Y_1\in\mathcal{B}]$ is the mean duration of a reactive trajectory that, starting from ν_{Q} on $\mathcal{A}$, crosses Σ and then goes to $\mathcal{B}$ without going back to A. Again, this is a quantity associated to the rare event $\{Y_1\in\mathcal{B}\}$. As such, it can be approximated together with $\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1\in\mathcal{B})$, using the algorithms mentioned in the previous item.

Notice that formula (6.7) is exactly [14, Equation (10)] and very close to [2, Equation (6)] (where the duration of the reactive path is neglected), for example.

As explained in Section 2, the submanifold Σ which is used to define the Markov chain (Y_n) can be seen as a tuning parameter: the reaction time T_{AB} is the same whatever this choice. As Σ is chosen further and further from A, it is expected that the error introduced when replacing ν_{E} by ν_{Q} (analysed in Section 5) gets larger and larger since the underlying assumption that an equilibrium between A and Σ is reached before the transition becomes less justified. Moreover, the sampling of ν_{Q} becomes more costly for the loops between A and Σ are more expensive to simulate. Nonetheless, the probability to observe a transition to B rather than to A becomes larger, and thus easier to estimate, when Σ gets further from A. In this respect, it would be interesting to discuss if some general recommendations on the choice of Σ could be given, taking into account the bias, the variance, and the algorithmic cost of the involved estimators. Concerning the variance of the estimators, we refer to [32, Chapter 3] for a discussion of importance sampling methods which greatly reduce the variance of averages over the reactive path ensemble.

Finally, let us mention that, in (6.7), the first term is typically much larger than the second one in most situations of interest. For example, this is made explicit in [13] for an overdamped Langevin dynamics in dimension 1 when the temperature parameter T goes to zero.

A Sharpness of the relative error bound

In this section, we illustrate the sharpness of the bound in Theorem 5.6 thanks to two discrete-time models.

A.1 A toy example

Setting. Consider the Markov chain (Y_n) on $\{1,2,3\}$ with transition matrix

$$K = \begin{bmatrix} 1-p & 0 & p \\ q & 1-q & 0 \\ 0 & r & 1-r \end{bmatrix}.$$

where the parameters p, q, and r all belong to $(0,1)$. Let $\mathcal{A} := \{1,2\}$ and $\mathcal{B} := \{3\}$, so that $p^+ := \sup_{x\in\mathcal{A}} \mathbb{P}^x(Y_1 \in \mathcal{B}) = p$ and $\nu_{\mathrm{E}} = [0,1]$. $\mathcal{A}$ and $\mathcal{B}$ are metastable if $p \ll 1$ and $r \ll 1$. On this elementary example, a probabilistic reasoning on geometric laws straightforwardly gives $\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] = \frac{1}{p} + \frac{1}{q}$. This may also be checked through direct computation since (3.13) implies that the mean hitting time of $\mathcal{B}$ starting from a law ν on $\mathcal{A}$ can be expressed as

$$\mathbb{E}^{\nu}[T_{\mathcal{B}}] = \nu(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}\mathbb{1}_{\mathcal{A}}.$$

One may also see that

$$\mathcal{L}^1(Y_n | T_{\mathcal{B}} > n) = [1,0],$$

and

$$\mathcal{L}^2(Y_n | T_{\mathcal{B}} > n) = \frac{1}{\frac{q}{q-p}(1-p)^n - \frac{p}{q-p}(1-q)^n} \left[\frac{q}{q-p}\left((1-p)^n - (1-q)^n\right), (1-q)^n \right].$$

The eigenvalues $\lambda_1 = (1-p)$ and $\lambda_2 = (1-q)$ of $K_{\mathcal{A}}$ are respectively associated to the left eigenmeasures $\nu_1 = [1,0]$ and $\nu_2 = [q/p, 1-q/p]$. Consequently, if $0 < p \leq q < 1$, ν_1 is the only quasi-stationary distribution for the process killed when leaving $\mathcal{A}$, and

$$H_1 := (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_1) = \frac{1}{q}\begin{bmatrix} 0 & 0 \\ -1 & 1 \end{bmatrix}.$$

Hence, we get

$$T_1 := \|H_1\|_\infty = \sup_{x\in\mathcal{A}} \|H_1(x,\cdot)\| = \frac{2}{q} = \|\nu_{\mathrm{E}} H_1\| =: T_1^{\mathrm{E}}.$$

On the opposite, if $0 < q < p < 1$, there are two quasi-stationary distributions, namely ν_1 and ν_2. This time, we still have $T_1 := \|H_1\|_\infty = \frac{2}{q} = \|\nu_{\mathrm{E}} H_1\| =: T_1^{\mathrm{E}}$. However, we shall also consider

$$H_2 := (\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_2) = \frac{1}{p}\begin{bmatrix} 1-q/p & q/p-1 \\ -q/p & q/p \end{bmatrix},$$

and deduce

$$T_2 := \|H_2\|_\infty = \sup_{x\in\mathcal{A}} \|H_2(x,\cdot)\| = \frac{2}{p}\max(1-q/p, q/p),$$

whereas $T_2^{\mathrm{E}} := \|\nu_{\mathrm{E}} H_2\| = 2q/p^2$.

The case $0 < p \leq q < 1$**.** In this situation, as just mentioned, ν_1 is the only QSD. Clearly, we have $\mathbb{E}^{\nu_1}[T_{\mathcal{B}}] = \frac{1}{p}$, and the relative error (5.1) is thus simply

$$\frac{|\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}]|}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} = \frac{p}{p+q}.$$

Since $p^+ = p$ and $T_1 = T_1^{\mathrm{E}} = 2/q$, the requirement $p^+ T_1^{\mathrm{E}} < 1$ of Theorem 5.6 is satisfied as soon as $p < q/2$. Accordingly, let us consider the regime $p^+ T_1^{\mathrm{E}} \ll 1$, i.e., $p \ll q$. On the one hand, one gets

$$\frac{|\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_1}[T_{\mathcal{B}}]|}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} \sim \frac{p}{q}.$$

On the other hand, the bound on the relative error given by (5.16) scales like (take $f = \mathbb{1}_{\mathcal{A}}$):

$$2\frac{p^+ T_1}{1 - p^+ T_1} = 4\frac{p}{q-2p} \sim 4\frac{p}{q}.$$

This illustrates the sharpness of the bound in Theorem 5.6, even in a case where ν_{E} differs a lot from the QSD ν_1, meaning that they have disjoint supports.

Additionally, one can verify that Assumption D of uniform geometric ergodicity is fulfilled with $\alpha = 2$ and $\rho = (1-q)/(1-p)$. Indeed, standard computations reveal that, for all $n \geq 0$ and all initial condition $x \in \mathcal{A}$,

$$\|\mathcal{L}^x(Y_n | T_{\mathcal{B}} > n) - \nu_1\| = 2\frac{1}{1 + \frac{q}{q-p}\left(\left(\frac{1-p}{1-q}\right)^n - 1\right)} \leq 2\left(\frac{1-q}{1-p}\right)^n.$$

Considering the upper bound in Lemma 5.9 with $\alpha = 2$ and $\rho = (1-q)/(1-p)$, one can then numerically check that, for any $0 < p < q < 1$,

$$\min\left\{\frac{\alpha}{1-\rho}, \inf_{0<c<1} \frac{2}{1-c}\left\lceil \frac{\ln(c\alpha^{-1})}{\ln(\rho)} \right\rceil\right\} = \frac{\alpha}{1-\rho} = 2\frac{1-p}{q-p}.$$

We retrieve the fact that the latter is always larger than $T_1 = 2/q$. More interestingly, in the regime $p \ll q$, we have

$$\frac{\alpha}{1-\rho} = 2\frac{1-p}{q-p} \sim \frac{2}{q} = T_1.$$

The case $0 < q < p < 1$**.** This time, ν_1 and ν_2 are the two quasi-stationary distributions of the process killed when leaving $\mathcal{A}$. As such, Assumption D cannot be fulfilled. One may notice that Assumption C is not satisfied for ν_1 because

$$\|\mathcal{L}^{\nu_{\mathrm{E}}}(Y_n | T_{\mathcal{B}} > n) - \nu_1\| = \|\mathcal{L}^2(Y_n | T_{\mathcal{B}} > n) - \nu_1\| \geq 2\frac{p-q}{p},$$

but the inequality

$$\|\mathcal{L}^{\nu_{\mathrm{E}}}(Y_n | T_{\mathcal{B}} > n) - \nu_2\| = 2\frac{p-q}{p}\frac{1}{\frac{p}{q}\left(\frac{1-q}{1-p}\right)^n - 1} \leq 2\frac{q}{p}\left(\frac{1-p}{1-q}\right)^n$$

shows that Assumption C is fulfilled for ν_2 with $\alpha = 2q/p$ and $\rho = (1-p)/(1-q)$. This is consistent with Lemma 5.8, which tells us that the relaxation time $T_2^{\mathrm{E}} = 2q/p^2$ to ν_2, starting from the reactive entrance distribution ν_{E}, satisfies

$$T_2^{\mathrm{E}} \leq \frac{\alpha}{1-\rho} = 2\frac{q(1-q)}{p(p-q)},$$

and it is also worth noting that, in the regime $q \ll p$, this bound is tight.

Concerning the relative errors, as before, we have

$$\frac{|\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_1}[T_{\mathcal{B}}]|}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} = \frac{p}{p+q}.$$

Recall that $T_1 = T_1^{\mathrm{E}} = 2/q$, hence the condition $p^+ T_1^{\mathrm{E}} < 1$ is never satisfied when $0 < q < p < 1$. Nevertheless, since $T_2^{\mathrm{E}} = 2q/p^2$, the condition $p^+ T_2^{\mathrm{E}} < 1$ is satisfied as soon as $q < p/2$. Thus, under this condition, Theorem 5.6 yields

$$\frac{|\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_2}[T_{\mathcal{B}}]|}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} = \frac{q}{p+q},$$

and for the right-hand side

$$2\frac{p^+ T_2^{\mathrm{E}}}{1 - p^+ T_2^{\mathrm{E}}} = 4\frac{q}{p-2q}.$$

We can remark that, in the regime $q \ll p$, up to a multiplicative factor equal to 4, the upper-bound is sharp. Finally, since $T_2 = 2\max(1-q/p, q/p)/p$, the condition $p^+ T_2 < 1$ is never fulfilled, and this illustrates the importance of using T_2^{E} rather than T_2 to measure the convergence time to the QSD.

A.2 On the choice of $1/p^+$ to measure the reaction time

The objective of this section is to answer to two questions related to the three quantities: $\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})$, $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})$ and p^+ defined by (5.2), and their use as a measure of the mean reaction time to $\mathcal{B}$. The first question is: Is $\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})$ always larger than $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})$? For the toy model introduced in Appendix A.1 the probability $p = \mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})$ indeed satisfies $p = p^+ > \mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})$. The second and more important question is: Is $1/p^+$ a too pessimistic measure of the reaction time to $\mathcal{B}$, and, in particular, is the relative error proportional to $pT_{\mathrm{Q}}^{\mathrm{E}}$ or $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, T_{\mathrm{Q}}^{\mathrm{E}}$ instead of the upper bound $p^+ T_{\mathrm{Q}}^{\mathrm{E}}$ obtained in Theorem 5.6? It turns out that the answers to both questions are no, as will be shown in this section on a toy example. Finally, Remark A.1 discusses the upper-bound given by Lemma 5.9.

Setting. Consider the Markov chain on $\{1,2,3\}$ with $\mathcal{A} = \{1,2\}$ and $\mathcal{B} = \{3\}$, with transition matrix

$$K = \begin{bmatrix} 1-4a & 3a & a \\ 2b & 1-3b & b \\ a & a & 1-2a \end{bmatrix},$$

where $0 < b < a < 1/4$, so that $p^+ := \sup_{x\in\mathcal{A}} \mathbb{P}^x(Y_1 \in \mathcal{B}) = a$. One can also notice that $\nu_{\mathrm{E}} = [1/2, 1/2]$.

Properties of the killed chain and QSD. Consider the process killed when leaving $\mathcal{A}$, whose sub-stochastic transition matrix is given by

$$K_{\mathcal{A}} = \begin{bmatrix} 1-4a & 3a \\ 2b & 1-3b \end{bmatrix}.$$

The eigenvalues of $K_{\mathcal{A}}$ are $\lambda_{1/2} = 1 - \frac{4a+3b\mp\sqrt{16a^2+9b^2}}{2}$, with $\lambda_2 < \lambda_1$. Computing the left eigenvectors associated to these eigenvalues, one can check that the Markov chain admits a unique quasi-stationary distribution in $\mathcal{A}$, namely

$$\nu_{\mathrm{Q}} = \frac{1}{a-b}[p-b, a-p], \tag{A.1}$$

which is associated to the largest eigenvalue $\lambda_1 = 1-p$, where

$$p = \mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B}) = \frac{4a+3b-\sqrt{16a^2+9b^2}}{2}.$$

Indeed, is is readily seen that for $0 < b < a$, ν_{Q} is a probability distribution since $p-b > 0$ and $a-p > 0$. The left eigenvector corresponding to the eigenvalue λ_2 cannot be chosen to be nonnegative so that, according to Lemma 3.15, ν_{Q} is the unique quasi-stationary distribution. Now, using Lemma 3.18, one has

$$\mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}] = \frac{1}{p} > \frac{2}{3b}. \tag{A.2}$$

Properties of $\pi_{0|\mathcal{A}}$. From K we obtain $\pi_0 = [5b, 7a, 6b]/(7a+11b)$ and deduce

$$\pi_{0|\mathcal{A}} = \frac{1}{7a+5b}[5b, 7a].$$

Therefore

$$\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B}) = \frac{12ab}{7a+5b}. \tag{A.3}$$

When $0 < b < a/5$, one always has

$$\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B}) > 3b/2 > \mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B}). \tag{A.4}$$

This answers negatively to the first question asked at the beginning of this section.

Computation of the relative error (5.1)**.** For this Markov chain, the Hill relation with the reactive entrance distribution (using Equation (4.3) with $f = \mathbb{1}_{\mathcal{A}}$) gives

$$\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] = \frac{1}{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})} = \frac{7a+5b}{12ab}.$$

Therefore, if $0 < b < a/5$,

$$\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] < \frac{2}{3b} < \mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}].$$

Since $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B}) > \mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})$, the relative error between mean hitting times satisfies

$$\left|\frac{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}]}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]}\right| = \frac{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})}{\mathbb{P}^{\nu_{\mathrm{Q}}}(Y_1 \in \mathcal{B})} - 1. \tag{A.5}$$

Relaxation time $T_{\mathrm{Q}}^{\mathrm{E}}$. For this Markov chain, one can compute the relaxation time

$$T_{\mathrm{Q}}^{\mathrm{E}} = \|\nu_{\mathrm{E}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}})\|.$$

Indeed, since

$$(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1} = \frac{1}{6ab} \begin{bmatrix} 3b & 3a \\ 2b & 4a \end{bmatrix},$$

and as ν_{Q} is given by (A.1), we are led to

$$(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}}) = \frac{1}{6ab(a-b)} \begin{bmatrix} 6ab - 3p(a+b) & -6ab + 3p(a+b) \\ 6ab - 2p(2a+b) & -6ab + 2p(2a+b) \end{bmatrix} \quad \text{(A.6)}$$

so that, since $\nu_{\mathrm{E}} = [\frac{1}{2}, \frac{1}{2}]$,

$$\nu_{\mathrm{E}}(\mathrm{id}_{\mathcal{A}} - K_{\mathcal{A}})^{-1}(\mathrm{id}_{\mathcal{A}} - \mathbb{1}_{\mathcal{A}} \otimes \nu_{\mathrm{Q}}) = \frac{12ab - p(7a+5b)}{12ab(a-b)} [1, -1]$$

and

$$T_{\mathrm{Q}}^{\mathrm{E}} = \left| \frac{12ab - p(7a+5b)}{6ab(a-b)} \right|.$$

Since $p < 3b/2$ by (A.2), one gets that, when $0 < b < a/5$,

$$T_{\mathrm{Q}}^{\mathrm{E}} = \frac{12ab - p(7a+5b)}{6ab(a-b)} < \frac{2}{a-b}. \quad \text{(A.7)}$$

Is $pT_{\mathrm{Q}}^{\mathrm{E}}$ an upper bound for (5.1)**?** Using (A.2), one obtains

$$\frac{1}{pT_{\mathrm{Q}}^{\mathrm{E}}} > \frac{a-b}{3b}. \quad \text{(A.8)}$$

From (A.3), (A.4), and (A.5), one also deduces

$$\left| \frac{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}]}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} \right| > \frac{12ab}{7a+5b} \frac{2}{3b} - 1 = \frac{a-5b}{7a+5b}. \quad \text{(A.9)}$$

Combining (A.8) and (A.9), one can check that

$$\frac{1}{pT_{\mathrm{Q}}^{\mathrm{E}}} \left| \frac{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}]}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} \right| > \frac{a-b}{3b} \frac{a-5b}{7a+5b} = \frac{a}{3b} \left(1 - \frac{b}{a}\right) \frac{1 - 5\frac{b}{a}}{7 + 5\frac{b}{a}}$$

which is unbounded when $b = o(a)$. Therefore, $pT_{\mathrm{Q}}^{\mathrm{E}}$ is not a bound for the relative error (5.1).

Is $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, T_{\mathrm{Q}}^{\mathrm{E}}$ an upper bound for (5.1)**?** One has

$$\frac{1}{\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, T_{\mathrm{Q}}^{\mathrm{E}}} \left| \frac{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}] - \mathbb{E}^{\nu_{\mathrm{Q}}}[T_{\mathcal{B}}]}{\mathbb{E}^{\nu_{\mathrm{E}}}[T_{\mathcal{B}}]} \right| > \frac{(a-b)(a-5b)}{24ab}$$

and the right-hand side is unbounded when $b = o(a)$. Therefore, $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, T_{\mathrm{Q}}^{\mathrm{E}}$ is not either a bound for the relative error (5.1).

In conclusion, for this Markov chain, the relative error is not proportional to $pT_{\mathrm{Q}}^{\mathrm{E}}$ nor $\mathbb{P}^{\pi_{0|\mathcal{A}}}(Y_1 \in \mathcal{B})\, T_{\mathrm{Q}}^{\mathrm{E}}$ in the regime $b = o(a)$. This answers negatively to the second question asked at the beginning of this section, and illustrates again the sharpness of our error estimate.

Remark A.1 (About Lemma 5.9.)**.** Let $\nu_{1/2}$, $u_{1/2}$ denote respectively left and right eigenvectors of $K_{\mathcal{A}}$ associated with the eigenvalues $\lambda_{1/2}$. We can take

$$\nu_1 = \frac{1}{a-b}\,[p-b, a-p]\,, \qquad u_1 = \frac{1}{2p-(4a+3b)}\,[p-(3a+3b), p-(4a+2b)]^T$$

and

$$\nu_2 = \frac{1}{a-b}\,[(4a+2b)-p, p-(3a+3b)]\,, \qquad u_2 = \frac{1}{2p-(4a+3b)}\,[p-a, p-b]^T$$

so that $\nu_{\mathrm{Q}} = \nu_1$. Next, note that the law of Y_n conditioned to stay in $\mathcal{A}$ with initial distribution μ (row vector) can be written

$$\mathcal{L}^{\mu}(Y_n | T_{\mathcal{B}} > n) = \frac{\mu K_{\mathcal{A}}^n}{\mu K_{\mathcal{A}}^n [1,1]^T}.$$

Using the spectral decomposition

$$K_{\mathcal{A}} = \lambda_1 u_1 \nu_{\mathrm{Q}} + \lambda_2 u_2 \nu_2,$$

one obtains

$$\mathcal{L}^{\mu}(Y_n | T_{\mathcal{B}} > n) = \nu_{\mathrm{Q}} + \frac{1}{1+\left(\frac{\lambda_1}{\lambda_2}\right)^n \frac{\mu u_1}{\mu u_2}}\,(\nu_2 - \nu_{\mathrm{Q}})\,,$$

and, therefore,

$$\|\mathcal{L}^{\mu}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| = \frac{1}{\left|1+\left(\frac{\lambda_1}{\lambda_2}\right)^n \frac{\mu u_1}{\mu u_2}\right|}\|\nu_2 - \nu_{\mathrm{Q}}\|.$$

From now on, let us focus on the case $b = o(a)$. Then, we have in particular that $p \sim 3b/2$, $\lambda_1 \sim 1$, and $\lambda_2 \sim 1 - 4a > 0$, so that $\rho := \frac{\lambda_2}{\lambda_1} \sim 1 - 4a$. One may also notice that

$$\|\nu_2 - \nu_{\mathrm{Q}}\| = \frac{2(4a+3b-2p)}{a-b} \sim 8.$$

Next, let us successively consider the initial conditions $x = 1$ and $x = 2$. On the one hand, if $\mu = \delta_1 = [1, 0]$, then

$$\frac{\mu u_1}{\mu u_2} = \frac{\delta_1 u_1}{\delta_1 u_2} = \frac{(3a+3b)-p}{a-p} \sim 3 > 0,$$

which yields, for all $n \geq 0$,

$$\|\mathcal{L}^{1}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| = \frac{1}{1+\left(\frac{\lambda_1}{\lambda_2}\right)^n \frac{\delta_1 u_1}{\delta_1 u_2}}\|\nu_2 - \nu_{\mathrm{Q}}\| \leq \frac{\delta_1 u_2}{\delta_1 u_1}\|\nu_2 - \nu_{\mathrm{Q}}\|\rho^n.$$

On the other hand, if $\mu = \delta_2 = [0, 1]$, then

$$\frac{\mu u_1}{\mu u_2} = \frac{\delta_2 u_1}{\delta_2 u_2} = \frac{p-(4a+2b)}{p-b} \sim \frac{-8a}{b},$$

which is smaller than -1 in the regime $b = o(a)$ and it is readily seen that, for all $n \geq 0$,

$$\|\mathcal{L}^{2}(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| = \frac{1}{\left(\frac{\lambda_1}{\lambda_2}\right)^n \left|\frac{\delta_2 u_1}{\delta_2 u_2}\right| - 1}\|\nu_2 - \nu_{\mathrm{Q}}\| \leq \frac{1}{\left|\frac{\delta_2 u_1}{\delta_2 u_2}\right| - 1}\|\nu_2 - \nu_{\mathrm{Q}}\|\rho^n.$$

Putting all things together, we conclude that Assumption D is fulfilled, namely

$$\forall x \in \mathcal{A},\, \forall n \geq 0,\, \|\mathcal{L}^x(Y_n | T_{\mathcal{B}} > n) - \nu_{\mathrm{Q}}\| \leq \alpha \rho^n,$$

with $\rho = \frac{\lambda_2}{\lambda_1} \sim 1 - 4a$, and

$$\alpha := \max\left(\frac{1}{\left|\frac{\delta_2 u_1}{\delta_2 u_2}\right| - 1}, \frac{\delta_1 u_2}{\delta_1 u_1}\right) \|\nu_2 - \nu_{\mathrm{Q}}\| = \frac{\delta_1 u_2}{\delta_1 u_1} \|\nu_2 - \nu_{\mathrm{Q}}\| \sim \frac{8}{3}.$$

In particular, considering the upper bound in Lemma 5.9, we have $\frac{\alpha}{1-\rho} \sim \frac{2}{3a} > 2$ since $a < 1/4$, and

$$\inf_{0<c<1} \frac{2}{1-c} \left\lceil \frac{\ln(c\alpha^{-1})}{\ln(\rho)} \right\rceil \xrightarrow[a \to \frac{1}{4}]{} 2.$$

Considering the relaxation times in Lemma 5.9, recall from (A.7) that

$$T_{\mathrm{Q}}^{\mathrm{E}} = \frac{12ab - p(7a + 5b)}{6ab(a-b)} \sim \frac{1}{4a},$$

and, by (A.6),

$$T_{\mathrm{Q}} = \frac{1}{3ab(a-b)} \max\left(|6ab - 3p(a+b)|, |6ab - 2p(2a+b)|\right) \sim \frac{1}{2a} \xrightarrow[a \to \frac{1}{4}]{} 2.$$

This gives an example where the upper-bound in Lemma 5.9 is reached by the right-hand term, and not by $\alpha/(1-\rho)$.

$\Diamond$

B About the reversibility of the reactive entrance process

We consider the situation where $\mathcal{E} = \{1, 2, \ldots, 5\}$ endowed with the discrete topology. Let a, b, c, d be four strictly positive real numbers attached to the edges of the weighted undirected graph G on Figure 3. For i, j in $\mathcal{E}$, the weight w_{ij} is the value of the edge (i, j) if it exists and zero otherwise. From this graph, let us consider the Markov chain on $\mathcal{E}$ with transition probability matrix

$$K_{ij} = \frac{w_{ij}}{\sum_{k=1}^{5} w_{ik}} \quad \forall i, j \in \mathcal{E}.$$

Therefore, the transition matrix is

$$K = \begin{bmatrix} 0 & \frac{a}{a+b+2d} & \frac{b}{a+b+2d} & \frac{d}{a+b+2d} & \frac{d}{a+b+2d} \\ \frac{a}{a+c} & 0 & 0 & 0 & \frac{c}{a+c} \\ \frac{b}{b+c} & 0 & 0 & \frac{c}{b+c} & 0 \\ \frac{d}{c+d} & 0 & \frac{c}{c+d} & 0 & 0 \\ \frac{d}{c+d} & \frac{c}{c+d} & 0 & 0 & 0 \end{bmatrix}.$$

Assumption A is clearly satisfied for this Markov chain which, by construction, is reversible with respect to its invariant distribution π_0 given by

$$\pi_0^i = \frac{\sum_{k=1}^{5} w_{ik}}{\sum_{\ell=1}^{5} \sum_{k=1}^{5} w_{\ell k}} \qquad \forall i \in \mathcal{E}.$$

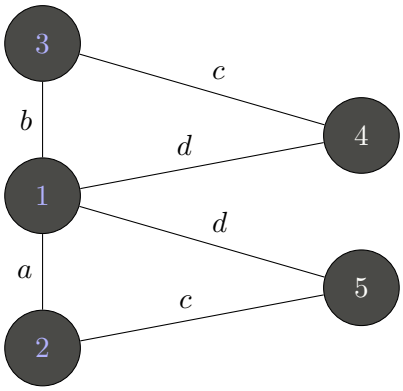

Figure 3: Graph of a reversible Markov chain on $\{1, 2, \dots, 5\}$ which is non-reversible with respect to its reactive entrance distribution in $\mathcal{A} = \{1, 2, 3\}$.

Thus,

$$\pi_0 = \frac{1}{2a + 2b + 4c + 4d} \left[a + b + 2d, a + c, b + c, c + d, c + d\right].$$

Taking $\mathcal{A} = \{1, 2, 3\}$ and $\mathcal{B} = \{4, 5\}$, the reactive entrance distribution given by (3.17) is

$$\nu_{\mathrm{E}} = \frac{1}{2(c + d)} \left[2d, c, c\right].$$

One can check that the process described by (Y_n^{E}) is non-reversible with respect to ν_{E}. Indeed, let us denote by K^{E} its 3×3 transition matrix. To show that the entrance process is non-reversible with respect to ν_{E}, we just have to verify that $K_{32}^{\mathrm{E}} \neq K_{23}^{\mathrm{E}}$, which is true when $a \neq b$ since we deduce from Definition 3.7 that

$$K_{32}^{\mathrm{E}} = \frac{abcd + abc^2 + bc^2d}{(a + b + 2d)(a + c)(b + c)(c + d)},$$

whereas

$$K_{23}^{\mathrm{E}} = \frac{abcd + abc^2 + ac^2d}{(a + b + 2d)(a + c)(b + c)(c + d)}.$$

C Two-sided condition and convergence to the QSD

The objective of this appendix is to rewrite in our specific probabilistic setting the results of [9] to prove existence and convergence to a QSD for a sub-Markov kernel under the so-called two-sided condition (see Equation (6.5) above and Equation (C.15) below). We thus do not claim any originality here, and this appendix is only provided for the sake of completeness. This result is stated in [16], but not proved exactly in the discrete-time setting we consider here, see also [18, Section 7.1]. Notice that Birkhoff's seminal paper [9] is followed by a large body of literature, see in particular [31, 35] and references therein.

This section is organized as follows. After introducing some notation in Section C.1, the Hilbert's projective metric is defined in Section C.2. This is a projective metric on the set of positive (non-zero) measures, which thus defines a metric on the probability measures. In Section C.3, we analyse how the distance between two measures evolves under the application of a sub-Markov kernel K. Section C.4 finally gives the main result, namely the existence and convergence to a QSD under a contraction assumption (in the

spirit of the Banach fixed point theorem), and the fact that this contraction assumption is satisfied under the two-sided condition (C.15).

C.1 The setting

Let us consider the topological vector space $\mathcal{M}$ of Radon measures on a Polish space (X, d) such that

$$\forall \lambda \in \mathcal{M},\ \lambda(X) < \infty, \tag{C.1}$$

equipped with the topology of the convergence in distribution. We denote by $\mathcal{X}$ the ensemble of Borel sets on X. For λ and μ in $\mathcal{M}$, we denote $\lambda \leq \nu$ if for all Borel set $A \in \mathcal{X}$, $\lambda(A) \leq \nu(A)$. This defines a partial ordering such that if $\lim_{n\to\infty} \lambda_n = \lambda$, and $\lambda_n \geq \nu$ for all n, then $\lambda \geq \nu$. Let us now define the convex cone

$$\mathcal{M}_+ = \{\lambda \in \mathcal{M} \text{ s.t. } \lambda \geq 0 \text{ and } \lambda \neq 0\}.$$

For any $\lambda \in \mathcal{M}_+$, one thus has $\lambda(X) > 0$. Notice that $\mathcal{M}_+ \cup \{0\}$ is closed. Let us introduce the equivalence relation:

$$\lambda \sim \nu \iff \exists c > 0, \lambda = c\nu.$$

The quotient of $\mathcal{M}_+$ under $\sim$ is a closed convex set, which, thanks to (C.1), can be identified with the ensemble of probability measures on (X, d), denoted by $\mathcal{M}_1$ in the following.

Let us now consider a non-zero sub-Markov kernel $K : X \times \mathcal{X} \to [0, 1]$:

- for a fixed $A \in \mathcal{X}$, $x \mapsto K(x, A)$ is measurable;
- for a fixed $x \in X$, $A \mapsto K(x, A)$ is a measure with total mass smaller than 1.

Let us denote by

$$\mathcal{T} : \begin{cases} \mathcal{M} \to \mathcal{M} \\ \lambda \mapsto \displaystyle\int_{x\in X} \lambda(dx) K(x, dy) \end{cases}$$

the associated transition kernel on measures. It is a linear map, which is such that

$$\mathcal{T}(\mathcal{M}_+) \subset \mathcal{M}_+ \cup \{0\}.$$

In the notation of Section 3.1, $\mathcal{T}(\lambda) = \lambda K$. Notice that $\mathcal{T}$ is a bounded operator if $\mathcal{M}$ is endowed with the total variation norm, since for any two measures λ and ν, and any Borel set $A \in \mathcal{X}$,

$$|\mathcal{T}(\lambda)(A) - \mathcal{T}(\nu)(A)| = \int_{x\in X} K(x, A)(\lambda - \nu)(dx) \leq \|K(x, A)\|_\infty \|\lambda - \nu\|_{TV} \leq \|\lambda - \nu\|_{TV}.$$

In all the following, it is assumed that

$$\forall \lambda \in \mathcal{M}_+,\ \mathcal{T}(\lambda) \neq 0, \tag{C.2}$$

so that

$$\mathcal{T}(\mathcal{M}_+) \subset \mathcal{M}_+.$$

We will make explicit in Proposition C.7 below a sufficient condition to get (C.2).

C.2 The Hilbert's projective metric

The Hilbert's projective metric Θ on $\mathcal{M}_+$ is defined by

$$\forall \lambda, \nu \in \mathcal{M}_+,\, \Theta(\lambda, \nu) = \ln\left(\frac{C(\lambda,\nu)}{c(\lambda,\nu)}\right),$$

where

$$c(\lambda,\nu) = \sup\{c > 0,\, c\lambda \leq \nu\} \qquad \text{and} \qquad C(\lambda,\nu) = \inf\{C > 0,\, \nu \leq C\lambda\}.$$

We use the standard conventions that $c(\lambda,\nu) = 0$ if $\{c > 0,\, c\lambda \leq \nu\} = \emptyset$ and $C(\lambda,\nu) = \infty$ if $\{C > 0,\, \nu \leq C\lambda\} = \emptyset$. One can check that for any measures $\lambda, \nu, \rho \in \mathcal{M}_+$, $\Theta(\lambda,\nu) = \Theta(\nu,\lambda)$, $\Theta(\lambda,\nu) \leq \Theta(\lambda,\rho) + \Theta(\rho,\nu)$ and $\Theta(\lambda,\nu) = 0$ if and only if $\lambda = t\nu$ for some $t > 0$. Notice that if $\Theta(\lambda,\nu) < \infty$ then λ and ν are equivalent. Finally, remark that this is a projective metric in the sense that for any $t > 0$ and $u > 0$, $\Theta(t\lambda, u\nu) = \Theta(\lambda,\nu)$: it is thus a metric on $\mathcal{M}_1$, and only a pseudo-metric on $\mathcal{M}_+$.

Let us make a link between the Hilbert's projective metric and other more usual metrics. One can read the next two lemmas with the total variation norm in mind, as an example.

Lemma C.1. *Let $\|\cdot\|$ be a norm on $\mathcal{M}$ such that*

$$\forall \lambda, \nu \in \mathcal{M}, \quad -\lambda \leq \nu \leq \lambda \Rightarrow \|\nu\| \leq \|\lambda\|. \tag{C.3}$$

Then, for any λ, ν in $\mathcal{M}_+$ such that $\|\lambda\| = \|\nu\|$, one has

$$\|\lambda - \nu\| \leq (\exp(\Theta(\lambda,\nu)) - 1)\,\|\lambda\|.$$

Proof. We follow [31, Lemma 1.3]. Let $\lambda, \nu \in \mathcal{M}_+$ such that $\|\lambda\| = \|\nu\|$. Notice that necessarily, under (C.3), $c(\lambda,\nu) \leq 1$ and $C(\lambda,\nu) \geq 1$. Indeed $0 \leq \nu - c(\lambda,\nu)\lambda$ and thus $-\nu \leq 0 \leq c(\lambda,\nu)\lambda \leq \nu$ which yields $c(\lambda,\nu)\|\lambda\| \leq \|\nu\|$. The proof is similar to get $C(\lambda,\nu) \geq 1$. Therefore, we have

$$\nu - \lambda \leq (C(\lambda,\nu) - 1)\lambda \leq (C(\lambda,\nu) - c(\lambda,\nu))\lambda,$$

and

$$\nu - \lambda \geq (c(\lambda,\nu) - 1)\lambda \geq -(C(\lambda,\nu) - c(\lambda,\nu))\lambda.$$

This implies

$$\|\nu - \lambda\| \leq (C(\lambda,\nu) - c(\lambda,\nu))\|\lambda\| \leq \frac{(C(\lambda,\nu) - c(\lambda,\nu))}{c(\lambda,\nu)}\|\lambda\| = (\exp(\Theta(\lambda,\nu)) - 1)\,\|\lambda\|.$$

□

Lemma C.2. *Let $\|\cdot\|$ be a norm on $\mathcal{M}$ such that* (C.3) *holds, and such that $\mathcal{M}$ is complete for this norm. Then the set*

$$\mathcal{M}_1^{\|\cdot\|} = \{\lambda \in \mathcal{M}_+,\, \|\lambda\| = 1\}$$

is complete for the Hilbert's projective metric Θ.

Proof. We rely here on [10, Theorem 5] or [9, Lemma 4]. Let $(\lambda_n)_{n\geq 0}$ be a Cauchy sequence for the metric Θ, with values in $\mathcal{M}_1^{\|\cdot\|}$. One can extract a subsequence $\nu_i = \lambda_{n(i)}$ such that for all $i \geq 0$, $\Theta(\nu_i, \nu_{i+1}) \leq 2^{-(i+1)}$. Therefore, for all $i \geq 0$,

$$c(\nu_i, \nu_{i+1})\nu_i \leq \nu_{i+1} \leq C(\nu_i, \nu_{i+1})\nu_i$$

with $\ln(C(\nu_i, \nu_{i+1})/c(\nu_i, \nu_{i+1})) \leq 2^{-(i+1)}$. By the same argument as in the proof of Lemma C.1, one has

$$|\nu_{i+1} - \nu_i| \leq (\exp(\Theta(\nu_i, \nu_{i+1})) - 1)\, \nu_i.$$

Using the fact that

$$\exp(2^{-(i+1)}) - 1 = \int_0^{2^{-(i+1)}} \exp(x)\, dx \leq 2^{-(i+1)} \exp(1/2) \leq 2^{-i},$$

this yields

$$|\nu_{i+1} - \nu_i| \leq \left(\exp(2^{-(i+1)}) - 1\right) \nu_i \leq 2^{-i}\nu_i. \tag{C.4}$$

From this inequality and since $\|\nu_i\| = 1$, one gets

$$\|\nu_{i+1} - \nu_i\| \leq 2^{-i},$$

which implies that ν_i converges to some $\nu_\infty \in \mathcal{M}_1^{\|\cdot\|}$ when $i \to \infty$ in the $\|\cdot\|$-norm because $\mathcal{M}$ is assumed complete for the $\|\cdot\|$-norm. From (C.4), one gets

$$(1 - 2^{-i})\nu_i \leq \nu_{i+1} \leq (1 + 2^{-i})\nu_i,$$

and thus, for $1 \leq i < j$,

$$\prod_{k=i}^{j-1}(1 - 2^{-k})\nu_i \leq \nu_j \leq \prod_{k=i}^{j-1}(1 + 2^{-k})\nu_i.$$

Using Lemma C.3 below, this yields, for $1 \leq i < j$,

$$(1 - 2^{2-i})\nu_i \leq \nu_j \leq (1 + \exp(1)2^{1-i})\nu_i$$

and thus

$$|\nu_j - \nu_i| \leq \exp(1)2^{1-i}\nu_i.$$

By letting $j \to \infty$,

$$|\nu_\infty - \nu_i| \leq \exp(1)2^{1-i}\nu_i.$$

This implies that $\lim_{i\to\infty} \Theta(\nu_i, \nu_\infty) = 0$. Using the triangular inequality, one thus obtains (remember that $\nu_i = \lambda_{n(i)}$)

$$\Theta(\lambda_n, \nu_\infty) \leq \Theta(\lambda_n, \lambda_{n(i)}) + \Theta(\nu_i, \nu_\infty),$$

which goes to zero when n goes to infinity. Indeed, for $\epsilon > 0$, one first chooses n_0 such that for all $m \geq n \geq n_0$, $\Theta(\lambda_n, \lambda_m) \leq \epsilon/2$ and then, for any $n \geq n_0$, one takes i sufficiently large so that $n(i) \geq n$ and $\Theta(\nu_i, \nu_\infty) \leq \epsilon/2$. This yields that for all $n \geq n_0$, $\Theta(\lambda_n, \nu_\infty) \leq \epsilon$. □

Lemmas C.1 and C.2 apply for example to the total variation norm $\|\cdot\|_{TV}$, since the vector space $\mathcal{M}$ of Radon measures is complete for the total variation norm, and since (C.3) is satisfied. In this case $\mathcal{M}_1^{\|\cdot\|_{TV}} = \mathcal{M}_1$ is simply the set of probability measures. Let us conclude this section with a simple technical lemma which has been used in the previous proof.

Lemma C.3. *Let $\alpha \in (0, 1/2]$. Then, for any $1 \leq i \leq j$,*

$$1 - 2\alpha^{i-1} \leq \prod_{k=i}^{j}(1-\alpha^k) \leq \prod_{k=i}^{j}(1+\alpha^k) \leq 1 + \exp(1)\alpha^{i-1}.$$

Proof. Let $1 \leq i \leq j$,

$$\ln\left(\prod_{k=i}^{j}(1+\alpha^k)\right) = \sum_{k=i}^{j}\ln(1+\alpha^k) \leq \sum_{k=i}^{j}\alpha^k \leq \frac{\alpha^i}{1-\alpha} \leq \alpha^{i-1}$$

and thus

$$\prod_{k=i}^{j}(1+\alpha^k) \leq \exp\left(\alpha^{i-1}\right) \leq 1 + \exp(1)\alpha^{i-1}.$$

Likewise, using the fact that for $x \in (0, 1/2)$, $\frac{1}{1-x} \leq 1 + 2x$,

$$\ln\left(\prod_{k=i}^{j}(1-\alpha^k)\right) = -\sum_{k=i}^{j}\ln\left(\frac{1}{1-\alpha^k}\right) \geq -\sum_{k=i}^{j}\ln\left(1+2\alpha^k\right) \geq -2\sum_{k=i}^{j}\alpha^k \geq -2\alpha^{i-1}$$

and thus

$$\prod_{k=i}^{j}(1-\alpha^k) \geq \exp\left(-2\alpha^{i-1}\right) \geq 1 - 2\alpha^{i-1}.$$

□

C.3 The projective metric norm Δ of $\mathcal{T}$

Proposition C.4. *Let us define*

$$\Delta = \sup_{\lambda,\nu\in\mathcal{M}_+} \Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)).$$

Then, for all λ and ν in $\mathcal{M}_+$,

$$\Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)) \leq \tanh\left(\frac{\Delta}{4}\right)\Theta(\lambda, \nu), \tag{C.5}$$

with the convention $\tanh(+\infty) = 1$.

Proof. We here follow [31, Theorem 1.1]. For a geometric interpretation of the computations, we refer to [9]. Let λ and ν in $\mathcal{M}_+$ be two positive (non-zero) measures. If $c(\lambda, \nu) = 0$ or $C(\lambda, \nu) = \infty$, then (C.5) is satisfied. Likewise, if $c(\lambda, \nu) = C(\lambda, \nu)$, which is equivalent to say that ν is proportional to λ, then (C.5) is satisfied. Otherwise, denoting for simplicity

$c = c(\lambda, \nu)$ and $C = C(\lambda, \nu)$, one has, using the continuity property of the partial ordering mentioned in Section C.1,

$$c\lambda \leq \nu \leq C\lambda, \text{ with } C > c > 0$$

and

$$\Theta(\lambda, \nu) = \ln\left(\frac{C}{c}\right) \in (0, \infty).$$

If $\Delta = +\infty$, then (C.5) holds since $\mathcal{T}(\nu - c\lambda) \geq 0$ and $\mathcal{T}(C\lambda - \nu) \geq 0$ implies

$$c\mathcal{T}(\lambda) \leq \mathcal{T}(\nu) \leq C\mathcal{T}(\lambda),$$

so that $c(\mathcal{T}(\lambda), \mathcal{T}(\nu)) \geq c$ and $C(\mathcal{T}(\lambda), \mathcal{T}(\nu)) \leq C$ which yields

$$\Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)) \leq \ln\left(\frac{C}{c}\right) = \Theta(\lambda, \nu).$$

If $\Delta < \infty$, then one has, by assumption,

$$\Theta(\mathcal{T}(\nu - c\lambda), \mathcal{T}(C\lambda - \nu)) \leq \Delta,$$

which implies that there exist two positive real numbers m and M such that

$$m\mathcal{T}(\nu - c\lambda) \leq \mathcal{T}(C\lambda - \nu)) \leq M\mathcal{T}(\nu - c\lambda), \tag{C.6}$$

and

$$\ln\left(\frac{M}{m}\right) \leq \Delta. \tag{C.7}$$

Notice that (C.6) rewrites:

$$\frac{cM + C}{M + 1}\mathcal{T}(\lambda) \leq \mathcal{T}(\nu) \leq \frac{cm + C}{m + 1}\mathcal{T}(\lambda).$$

Therefore,

$$\begin{aligned}
\Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)) &\leq \ln\left(\frac{cm + C}{m + 1}\frac{M + 1}{cM + C}\right) \\
&= \ln\left(\frac{m + \exp(\Theta(\lambda, \nu))}{m + 1}\right) - \ln\left(\frac{M + \exp(\Theta(\lambda, \nu))}{M + 1}\right) \\
&= \int_0^{\Theta(\lambda,\nu)} \frac{\exp(x)}{m + \exp(x)} - \frac{\exp(x)}{M + \exp(x)}\, dx \\
&= \int_0^{\Theta(\lambda,\nu)} \varphi(\exp(x))\, dx \\
&\leq \Theta(\lambda, \nu) \max_{\mathbb{R}_+} \varphi,
\end{aligned} \tag{C.8}$$

where

$$\varphi(y) = \frac{y}{m + y} - \frac{y}{M + y} = -\frac{m}{m + y} + \frac{M}{M + y}.$$

The function φ attains its maximum over $\mathbb{R}_+$ at $y = \sqrt{mM}$, and its maximum value is

$$\max_{\mathbb{R}_+} \varphi = -\frac{m}{m + \sqrt{mM}} + \frac{M}{M + \sqrt{mM}} = \frac{-\sqrt{m} + \sqrt{M}}{\sqrt{m} + \sqrt{M}} = \frac{1 - \sqrt{\frac{m}{M}}}{1 + \sqrt{\frac{m}{M}}},$$

and thus, using the fact that, by (C.7), $\frac{m}{M} \geq \exp(-\Delta)$,

$$\max_{\mathbb{R}_+} \varphi \leq \frac{1-\exp(-\Delta/2)}{1+\exp(-\Delta/2)} = \tanh\left(\frac{\Delta}{4}\right).$$

Plugging this upper bound of $\max_{\mathbb{R}_+} \varphi$ in (C.8) yields (C.5). □

One thus gets a contraction in the Hilbert's projective metric if $\Delta < \infty$. Notice that we implicitly used the fact that $\mathcal{T}(\mathcal{M}_+) \subset \mathcal{M}_+$ to define Δ (otherwise $\Theta(\mathcal{T}\lambda, \mathcal{T}\nu)$ may not be defined). This explains why (C.2) is needed in the first place.

C.4 Fixed point theorem and two-sided condition

For what follows, recall that $\mathcal{T}^0(\lambda) = \lambda$ by convention.

Theorem C.5. *Let us assume that*

$$\Delta = \sup_{\lambda,\nu \in \mathcal{M}_+} \Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)) < \infty, \tag{C.9}$$

and let us introduce $\rho = \tanh\left(\frac{\Delta}{4}\right) \in (0,1)$. *Then, there exists a unique probability measure* $\nu_\infty \in \mathcal{M}_1$ *such that*

$$\mathcal{T}(\nu_\infty) = c\nu_\infty \tag{C.10}$$

for some $c > 0$. *Moreover, for any* $\lambda_0 \in \mathcal{M}_+$, *one has, for all* $n \geq 0$,

$$\Theta(\nu_n, \nu_\infty) \leq \frac{\rho^n}{1-\rho}\Theta(\nu_1, \nu_0) \tag{C.11}$$

where $\nu_n = \frac{\mathcal{T}^n(\lambda_0)}{\mathcal{T}^n(\lambda_0)(X)}$. *This implies in particular: for all* $n \geq 0$,

$$\|\nu_n - \nu_\infty\|_{TV} \leq \frac{\Theta(\nu_1, \nu_0)}{1-\rho} \exp\left(\frac{\Theta(\nu_1, \nu_0)}{1-\rho}\right) \rho^n. \tag{C.12}$$

Proof. We refer to [9, Theorem 1] for a similar reasoning. The uniqueness of a solution to (C.10) is easy to obtain from the assumption $\Delta < \infty$. Indeed, let us assume that two probability measures μ_1 and μ_2 are such that

$$\mathcal{T}(\mu_1) = c_1\mu_1 \text{ and } \mathcal{T}(\mu_2) = c_2\mu_2$$

for some $c_1 > 0$ and $c_2 > 0$. Then, using (C.5), one has

$$\Theta(\mathcal{T}(\mu_1), \mathcal{T}(\mu_2)) \leq \rho\Theta(\mu_1, \mu_2)$$

where $\rho = \tanh\left(\frac{\Delta}{4}\right) \in (0,1)$. Therefore,

$$\Theta(c_1\mu_1, c_2\mu_2) \leq \rho\Theta(\mu_1, \mu_2)$$

and one gets that $\Theta(\mu_1, \mu_2) = 0$ since $\Theta(c_1\mu_1, c_2\mu_2) = \Theta(\mu_1, \mu_2)$. This implies $\mu_1 = \mu_2$ since both are probability measures.

We will now show the existence of a solution to (C.10) using the standard argument of Banach fixed-point theorem. Let $\lambda_0 \in \mathcal{M}_+$, and let us consider, for $n \geq 0$,

$$\lambda_n = \mathcal{T}^n(\lambda_0).$$

Using (C.5), one has, for all $n \geq 1$,

$$\Theta(\lambda_{n+1}, \lambda_n) \leq \rho \Theta(\lambda_n, \lambda_{n-1}).$$

Thus, for all $n \geq 1$,

$$\Theta(\lambda_{n+1}, \lambda_n) \leq \rho^n \Theta(\lambda_1, \lambda_0), \tag{C.13}$$

and the triangular inequality yields, for all $m \geq n \geq 1$,

$$\Theta(\lambda_m, \lambda_n) \leq \left(\sum_{k=n}^{m-1} \rho^k \right) \Theta(\lambda_1, \lambda_0) \leq \frac{\rho^n}{1-\rho} \Theta(\lambda_1, \lambda_0).$$

Let us introduce the probability measures: $\forall n \geq 0$,

$$\nu_n = \frac{\lambda_n}{\lambda_n(X)}.$$

One has that $\Theta(\nu_m, \nu_n) = \Theta(\lambda_m, \lambda_n)$ and thus for all $m \geq n \geq 1$,

$$\Theta(\nu_m, \nu_n) \leq \frac{\rho^n}{1-\rho} \Theta(\nu_1, \nu_0) \tag{C.14}$$

which shows that $(\nu_n)_{n \geq 0}$ is a Cauchy sequence for the Θ-metric. From Lemma C.2, this implies that $\nu_n \in \mathcal{M}_1$ converges to some $\nu_\infty \in \mathcal{M}_1$ as $n \to \infty$ in the Θ-metric, and thus, from Lemma C.1, in total variation norm. From (C.13), one has that

$$\lim_{n \to \infty} \Theta \left(\frac{\mathcal{T}(\nu_n)}{(\mathcal{T}(\nu_n))(X)}, \nu_n \right) = 0$$

and thus, using Lemma C.1,

$$\lim_{n \to \infty} \left\| \frac{\mathcal{T}(\nu_n)}{(\mathcal{T}(\nu_n))(X)} - \nu_n \right\|_{TV} = 0.$$

Since $\lim_{n \to \infty} \nu_n = \nu_\infty$ in total variation norm, then $\lim_{n \to \infty} \mathcal{T}(\nu_n) = \mathcal{T}(\nu_\infty)$ in total variation norm, and thus $\lim_{n \to \infty} (\mathcal{T}(\nu_n))(X) = (\mathcal{T}(\nu_\infty))(X)$. One thus obtains:

$$\frac{\mathcal{T}(\nu_\infty)}{(\mathcal{T}(\nu_\infty))(X)} = \nu_\infty$$

which establishes the existence of the solution to (C.10).

Moreover, by letting $m \to \infty$ in (C.14), one gets (C.11). Using Lemma C.1, one obtains from (C.11): for all $n \geq 0$,

$$\|\nu_n - \nu_\infty\|_{TV} \leq \left(\exp \left(\frac{\Theta(\nu_1, \nu_0)}{1-\rho} \rho^n \right) - 1 \right)$$

which yields (C.12). □

Remark C.6. As usual in a Banach fixed point theorem, it is easy to obtain a similar result assuming that $\mathcal{T}^r$ satisfies both assumptions (C.2) and (C.9) for some positive integer r. ♢

It remains to discuss how to get Assumptions (C.2) and (C.9) in practice. A natural sufficient condition is the so-called two-sided condition (C.15) (notice that in (C.15), s is actually with values in $(0, 1]$ since for all $x \in X$, $s(x) \leq K(x, X)$).

Proposition C.7. *Assume that there exist a measurable function $s : X \to \mathbb{R}_+^*$, a constant $R > 0$, and a probability measure $\pi \in \mathcal{M}_1$ such that for all $x \in X$,*

$$s(x)\pi(dy) \leq K(x, dy) \leq Rs(x)\pi(dy). \tag{C.15}$$

Then, $\mathcal{T}$ satisfies (C.2) *and* (C.9) *(with $\Delta \leq 2 \ln R$). In particular, the results of Theorem C.5 hold and one thus obtains: for all initial condition $\lambda_0 \in \mathcal{M}_+$, for all $n \geq 1$,*

$$\|\nu_n - \nu_\infty\|_{TV} \leq (R+1)(\ln R)R^{R+1}\left(\frac{R-1}{R+1}\right)^{n-1} \tag{C.16}$$

where $\nu_n = \frac{\mathcal{T}^n(\lambda_0)}{\mathcal{T}^n(\lambda_0)(X)}$.

Proof. We refer to [9, Theorem 3] for a similar reasoning. Let us first check that (C.2) holds. Let $\lambda \in \mathcal{M}_+$. Then $\mathcal{T}(\lambda) \geq \left(\int_X s(x)\lambda(dx)\right)\pi$ is a non-zero measure since $\int_X s(x)\lambda(dx) > 0$. Indeed $\int_X s(x)\lambda(dx) = 0$ would imply that $s(x) = 0$ for λ-almost every $x \in X$, which means that

$$\lambda(\{x \in X, s(x) \neq 0\}) = 0$$

which is not possible since $\{x \in X, s(x) \neq 0\} = X$ and $\lambda \neq 0$.

Let us now check (C.9), namely

$$\Delta = \sup_{\lambda,\nu \in \mathcal{M}_+} \Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)) < \infty.$$

Let λ and ν be two measures in $\mathcal{M}_+$. One has

$$\mathcal{T}(\nu) \leq R\left(\int_X s(x)\nu(dx)\right)\pi(dy) \leq R\frac{\int_X s(x)\nu(dx)}{\int_X s(x)\lambda(dx)}\left(\int_X s(x)\lambda(dx)\right)\pi(dy),$$

so

$$\mathcal{T}(\nu) \leq R\frac{\int_X s(x)\nu(dx)}{\int_X s(x)\lambda(dx)}\mathcal{T}(\lambda),$$

which shows that

$$C(\mathcal{T}(\lambda), \mathcal{T}(\nu)) \leq R\frac{\int_X s(x)\nu(dx)}{\int_X s(x)\lambda(dx)} < \infty.$$

Likewise,

$$\mathcal{T}(\nu) \geq \left(\int_X s(x)\nu(dx)\right)\pi(dy) \geq \frac{\int_X s(x)\nu(dx)}{R\int_X s(x)\lambda(dx)}R\left(\int_X s(x)\lambda(dx)\right)\pi(dy),$$

so

$$\mathcal{T}(\nu) \geq \frac{\int_X s(x)\nu(dx)}{R\int_X s(x)\lambda(dx)}\mathcal{T}(\lambda),$$

which shows that

$$c(\mathcal{T}(\lambda), \mathcal{T}(\nu)) \geq \frac{\int_X s(x)\nu(dx)}{R\int_X s(x)\lambda(dx)} > 0.$$

Therefore,

$$\Theta(\mathcal{T}(\lambda), \mathcal{T}(\nu)) = \ln\left(\frac{C(\mathcal{T}(\lambda), \mathcal{T}(\nu))}{c(\mathcal{T}(\lambda), \mathcal{T}(\nu))}\right) \leq \ln(R^2)$$

so that $\Delta \leq \ln(R^2) < \infty$. Thus, using (C.12), one gets: for all $n \geq 1$,

$$\begin{aligned}\|\nu_n - \nu_\infty\|_{TV} &\leq \frac{\Theta(\nu_2,\nu_1)}{1-\rho} \exp\left(\frac{\Theta(\nu_2,\nu_1)}{1-\rho}\right) \rho^{n-1}, \\ &\leq \frac{\Delta}{1-\rho} \exp\left(\frac{\Delta}{1-\rho}\right) \rho^{n-1},\end{aligned}$$

with $\rho = \tanh\left(\frac{\Delta}{4}\right) \leq \tanh\left(\frac{\ln R}{2}\right) = \frac{R-1}{R+1}$, so that $\frac{\Delta}{1-\rho} \leq (\ln R)(R+1)$. This yields (C.16). □

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