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The Essential Spectral Radius and Asymptotic Properties of Transfer Operators

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The Essential Spectral Radius and Asymptotic Properties of Transfer Operators†

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Abstract

The statistical behavior of deterministic and stochastic dynamical systems may be described using transfer operators, which generalize the notion of Frobenius–Perron and Koopman operators. Since numerical techniques to analyse dynamical systems based on eigenvalues problems for the corresponding transfer operator have emerged, bounds on its essential spectral radius became of interest. This article shows that they are also of great theoretical interest. We give an analytical representation of the essential spectral radius in $L^1(\mu)$, which then is exploited to analyse the asymptotical properties of transfer operators by combining results from functional analysis, Markov operators and Markov chain theory. In particular, it is shown that an essential spectral radius less than 1, uniform constrictiveness and some "weak form" of the so–called Doeblin condition are equivalent. Finally, we apply the results to study three main problem classes: deterministic systems, stochastically perturbed deterministic systems and stochastic systems.

Keywords. uniformly constrictive, asymptotically stable, exact, asymptotically periodic, ergodic, aperiodic, Frobenius–Perron operator, Koopman operator, Markov operator, transfer operator, propagator, Doeblin condition, irreducible, uniformly ergodic, deterministic dynamical system, stochastic dynamical system, stochastic perturbation, statistical behavior, eigenvalue cycle

1 Introduction

Recently, efficient techniques for the numerical approximation of the essential statistical behavior of deterministic as well as stochastic dynamical systems have been proposed [1, 2, 17]. They are based on the observation that certain aspects of the dynamical behavior are related to eigenvalues on and near the unit circle of some corresponding transfer operators which generalize the notion of Frobenius–Perron operators. Furthermore, these statistical aspects may be

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identified exploiting the corresponding eigenfunctions. As a necessary condition for approximating the statistical behavior in a numerically reliable way, the essential spectral radius has to be bounded away from 1, allowing for finitely many isolated eigenvalues of finite multiplicity on and near the unit circle. We show that bounds on the essential spectral radius are also of theoretical interest.

This article brings together aspects from rather isolated mathematical branches. We use a functional analytic approximation result based on weakly compact operators to get an analytic representation of the essential spectral radius including upper bounds. Furthermore, we link properties known from Frobenius–Perron and, more general, Markov operator theory, such as ergodicity, constrictiveness, asymptotic periodicity and asymptotic stability with concepts known from the theory of Markov chains, such as irreducibility, uniform ergodicity and the so–called Doeblin condition. We especially emphasize the result that uniform constrictiveness, some "weak form" of the Doeblin condition and an essential spectral radius less than 1 are equivalent, which, to the author's knowledge, is new.

In our analysis, stochastic transition functions play a key role. On the one hand, they allow to define transfer operators for both the deterministic and the stochastic case in a common setting. On the other hand, they permit to "translate" results for Markov chains to Markov operators and vice versa. We emphasize that in the former theory, results are most often stated for bounded functions, whereas in the latter theory, more frequently essentially bounded functions are involved. Since essentially bounded functions are also the type of functions considered in the deterministic case, we focus on this Banach space. Nevertheless, it should be possible to gain similar result for the Banach space of bounded functions.

In Section 1 we introduce the general setting and define the stochastic transition function and the transfer operators induced by them. Section 2 states the results about the essential spectral radius involving weakly compact operators and decomposition results of the transition function. In Section 3 results about Markov operators and Markov chains are applied to analyse the asymptotic properties of transfer operators. Finally, the last section is devoted to the exemplary application to three main problem classes: deterministic systems, stochastically perturbed deterministic systems and stochastic systems.

2 Transfer Operators

Throughout the article, we fix a measure space $(X, \mathcal{B}(X), \mu)$, where $X \subset \mathbf{R}^n$, $\mathcal{B}(X)$ denotes the Borel σ–algebra of X and μ is a probability measure on $\mathcal{B}(X)$. Define the Banach spaces

$$L^1(\mu) \quad = \quad \left\{ u : X \to \mathbf{C} : \int_X |u(x)| \mu(\mathrm{d}x) < \infty \right\}. \tag{1}$$

and

$$L^\infty(\mu) \quad = \quad \left\{ u : X \to \mathbf{C} : \mu\text{-}\operatorname*{ess\,sup}_{x \in X} |u(x)| < \infty \right\}$$

with corresponding norms $\|\cdot\|_1$ and $\|\cdot\|_\infty$, respectively. Note that $L^\infty(\mu) \subset L^1(\mu)$, which is due to Hölder's inequality.

A *stochastic transition function* is a map

$$\begin{aligned} p : X \times \mathcal{B}(X) &\rightarrow [0,1] \\ (x, A) &\mapsto p(x, A) \end{aligned}$$

with the properties

(i) $x \mapsto p(x, A)$ is measurable for every $A \in \mathcal{B}(X)$,

(ii) $A \mapsto p(x, A)$ is a probability measure for every $x \in X$.

We recursively define the m–step transition function $p^m(x, \mathrm{d}y)$ via the *Chapman–Kolmogorov* equation

$$p^m(x, \mathrm{d}y) = \int_X p^{m-1}(z, \mathrm{d}y)\, p(x, \mathrm{d}z) \tag{2}$$

for all $x \in X$, $m > 1$ and $p^1(x, \mathrm{d}y) = p(x, \mathrm{d}y)$. *We will assume throughout the article that the probability measure μ is* stationary *w.r.t. the stochastic transition function*, i.e.,

$$\int_X p(x, \mathrm{d}y)\mu(\mathrm{d}x) = \mu(\mathrm{d}y),$$

where the above identity stands for $\int_X p(x, A)\mu(\mathrm{d}x) = \mu(A)$ for every $A \in \mathcal{B}(X)$. In the theory of Markov chains [14, 15] it is shown that with every stochastic transition function one may associated a *homogeneous Markov chain* $\{X_n\}_{n \in \mathbf{N}}$ satisfying $p^n(x, A) = \mathbf{P}[X_n \in A | X_0 = x]$. Thus, $p(x, A)$ describes the conditional probability that the Markov chain moves within one step to A when initially started in x.

Our point of view will be the other way around. We will see that a dynamical system gives rise to a stochastic transition function, which, via associable operators, allows to study its statistical behavior. In our setting the following two operators are commonly associated with a stochastic transition function: the *forward transfer operator* or *propagator* P acting on $L^1(\mu)$ and the *backward transfer operator* T acting on the space of essentially bounded functions $L^\infty(\mu)$. For a deterministic dynamical system, the propagator and the backward transfer operator are identical with the *Frobenius–Perron* and the *Koopman operator*, respectivly.

The forward transfer operator or propagator $P : L^1(\mu) \rightarrow L^1(\mu)$ is defined via

$$Pv(y)\mu(\mathrm{d}y) = \int_X v(x)p(x, \mathrm{d}y)\mu(\mathrm{d}x) \tag{3}$$

for every $v \in L^1(\mu)$. As a consequence of the stationarity of μ, the indicator function of the entire space χ_X is a *stationary density* of P, i.e., $P\chi_X = \chi_X$. Furthermore, P is a *Markov operator*, i.e., P preserves norm $\|Pv\|_1 = \|v\|_1$ and positivity $Pv \geq 0$ if $v \geq 0$, which is a simple consequence of the definition.

The backward transfer operator $T : L^\infty(\mu) \rightarrow L^\infty(\mu)$ is defined via

$$Tu(x) = \int_X u(y)p(x, \mathrm{d}y) \tag{4}$$

for every $u \in L^\infty(\mu)$. As a consequence of the second property of the stochastic transition function, we have $T\chi_X = \chi_X$. Both operators are closely connected via the duality bracket

$$\langle v, u\rangle_\mu = \int_X v(x)u(x)\mu(\mathrm{d}x)$$

for all $v \in L^1(\mu)$ and $u \in L^\infty(\mu)$, namely $\langle u, Pv\rangle_\mu = \langle Tu, v\rangle_\mu$. Thus, the backward transfer operator is the adjoint of the propagator: $P^* = T$. For examples, see the applications at the end of this article.

3 The Essential Spectral Radius

This section analyses the essential spectral radius of an arbitrary propagator in terms of its stochastic transition function. After specifying the term "essential spectrum", we characterize the essential spectral radius using some quantity $\Delta(P)$ that then will be related to weakly compact operators. This will enable us to finally reach our goal.

Denote the spectrum of P by $\sigma(P)$; for some eigenvalue $\lambda \in \sigma(P)$ the *multiplicity* of λ is defined as the dimension of the generalized eigenspace; see e.g., [10, Chap. III.6]; eigenvalues of multiplicity 1 are called *simple.* The set of all eigenvalues $\lambda \in \sigma(P)$ that are isolated[1] and of finite multiplicity will be called the *discrete spectrum* of P, denoted by $\sigma_{\mathrm{discr}}(P)$. The complement of $\sigma_{\mathrm{discr}}(P)$ in $\sigma(P)$ will be called the *essential spectrum* of P, denoted by $\sigma_{\mathrm{ess}}(P)$. The *essential spectral radius* r_{ess} of P is defined as the smallest upper bound for all elements of $\sigma_{\mathrm{ess}}(P)$, thus $\sup_{\lambda\in\sigma_{\mathrm{ess}}(P)} |\lambda| = r_{\mathrm{ess}}$. It may be characterized in the following way:

Theorem 3.1 ([19]) *Let $P : L^1(\mu) \to L^1(\mu)$ denote a bounded linear operator. Define the quantity $\Delta(P)$ according to*

$$\Delta(P) = \limsup_{\mu(A)\to 0} \|\chi_A \circ P\|_1, \tag{5}$$

where the limit is understood to be taken over all sequences of subsets whose μ–measure converges to zero and χ_A is interpreted as a multiplication operator: $\chi_A f(x) = \chi_A(x)f(x)$. Then, the essential spectral radius of P is equal to

$$r_{\mathrm{ess}}(P) = \lim_{n\to\infty} \Delta(P^n)^{1/n}. \tag{6}$$

In particular, $r_{\mathrm{ess}}(P) \le \Delta(P)$.

Note the strong analogy to the *spectral radius* $r(P)$ of P, defined as the smallest upper bound for all elements of the spectrum, thus $\sup_{\lambda\in\sigma(P)} |\lambda| = r(P)$. In terms of the operator norm $\|\cdot\|_1$, the representation $r(P) = \lim_{n\to\infty} \|P^n\|_1^{1/n}$ is known [7, Chap. VII.3.5]. Loosely speaking, while $\|\cdot\|_1$ is sensitive to all elements of $\sigma(P)$, the quantity $\Delta(\cdot)$ is sensitive only to those of $\sigma_{\mathrm{ess}}(P)$. Using

[1] There exists some $\epsilon > 0$ such that the intersection of $\sigma(P)$ with the ball of radius ϵ at center λ just contains λ.

weakly compact operators, this will be made more precise in the following.

A subset $A \subset L^1(\mu)$ is called *relatively weakly compact*, if its closure is compact in the weak topology [7, 13]. There is an important characterization of relatively weak compactness in terms of the underlying probablity measure μ:

Lemma 3.2 (Dunford–Pettis,[6, 13]) *A bounded subset $B \subset L^1(\mu)$ is relatively weakly compact if and only if*

$$\lim_{\mu(A)\to 0} \sup_{w\in B} \|\chi_A w\|_1 = 0. \tag{7}$$

We are now ready to introduce the class of weakly compact operators and give a useful characterization based on Lemma 3.2; denote by $B_1(X)$ the closed unit ball in $L^1(\mu)$.

Definition 3.3 ([7, 13]) *A bounded linear operator $S : L^1(\mu) \to L^1(\mu)$ is called* weakly compact *if $S(B_1(X))$ is relatively weakly compact, i.e., the closure of $S(B_1(X))$ is compact in the weak topology.*

Obviously, every compact operator is weakly compact; furthermore:

Lemma 3.4 ([13]) *A bounded linear operator $S : L^1(\mu) \to L^1(\mu)$ is weakly compact, if and only if $\Delta(S) = 0$.*

Using this fact we are now ready to justify the initially made interpretation of $\Delta(P)$:

Theorem 3.5 ([19]) *Let $P : L^1(\mu) \to L^1(\mu)$ denote a bounded linear operator. Then*

(i) the essential spectrum of P is invariant under weakly compact perturbations

$$\sigma_{\text{ess}}(P) \quad = \quad \sigma_{\text{ess}}(P - S), \tag{8}$$

where S is an arbitrary weakly compact operator.

(ii) $\Delta(P) = \min\{\|P - S\|_1 : S$ *is weakly compact* $\}$.

In particular, there exists some best approximation S_0 in the space of weakly compact operators with $\Delta(P) = \|P - S_0\|_1$.

Theorem 3.5 states that $\Delta(P)$ measures the non–weakly compact part of P. Since $\sigma_{\text{ess}}(S_0) \subset \{0\}$ for weakly compact S_0 due to (8), $\Delta(P)$ can be interpreted as the spectral radius of $P - S_0$, which is related to the essential spectrum of P only. Note that while the definition (5) of $\Delta(P)$ involves sequences of subsets whose μ–measure converges to 0, the characterization in Theorem 3.5(ii) is only in terms of weakly compact operators. We will exploit this fact in the following by analysing the relation between weak compactness of P and properties of the stochastic transition function p. As a result, we will see that absolutely continuous stochastic transition functions may give rise to weakly compact operators, while transition functions that are singular w.r.t. μ never do so.

Corollary 3.6 *Consider the propagator $S : L^1(\mu) \to L^1(\mu)$ defined by*

$$Sv(y) \quad = \quad \int_X v(x)p(x,y)\mu(\mathrm{d}x) \tag{9}$$

with absolutely continuous *stochastic transition function* $p(x, \mathrm{d}y) = p(x,y)\mu(\mathrm{d}y)$. *Then S is weakly compact if for some $s > 1$ the inequality*

$$\operatorname*{ess\,sup}_{x\in X} \int_X p(x,y)^s \mu(\mathrm{d}y) \quad < \quad \infty$$

holds. In particular, S is weakly compact if $\operatorname{ess\,sup}_{x,y\in X} p(x,y) < \infty$.

Proof: For $A \in \mathcal{B}(X)$, we have

$$\|\chi_A \circ S\|_1 \quad = \quad \sup_{\|v\|_1 \le 1} \int_A \int_X v(x)p(x,y)\mu(\mathrm{d}x)\mu(\mathrm{d}y).$$

Applying Hölder's inequality twice, we finally get

$$\|\chi_A \circ S\|_1 \quad \le \quad \operatorname*{ess\,sup}_{x\in X} \left| \int_A p(x,y)\mu(\mathrm{d}y) \right| \ \le \ \|\chi_A\|_r \ \ \operatorname*{ess\,sup}_{x\in X} \|p(x,\cdot)\|_s$$

with $1 \le r, s \le \infty$ and $1/s + 1/r = 1$. For $1 < s$, the limit of $\|\chi_A \circ S\|_1$ for $\mu(A) \to 0$ tends to zero, since $\|\chi_A\|_r = \sqrt[r]{\mu(A)}$. □

Assume that the Lebesgue decomposition of the stochastic transition function p is given by $p(x, \mathrm{d}y) = p_a(x,y)\mu(\mathrm{d}y) + p_s(x, \mathrm{d}y)$, where p_a and p_s denote the absolutely continuous and the singular part w.r.t. μ, respectively [11]. Furthermore, define the (not necessarily stochastic) transition function

$$r_n(x,y) = \begin{cases} p_a(x,y) & \text{if } p_a(x,y) \ge n \\ 0 & \text{otherwise} \end{cases}$$

With this notation, we are ready to state the following

Theorem 3.7 (**[20]**) *For an arbitrary propagator $P : L^1(\mu) \to L^1(\mu)$ the equality*

$$\Delta(P) \quad = \quad \inf_{n\in\mathbf{N}} \ \operatorname*{ess\,sup}_{x\in X} \{r_n(x,X) + p_s(x,X)\}$$

holds.

In view of Theorem 3.5, the above theorem states that the weakly compact part of P can be approximated by weakly compact operators defined in terms of μ–essentially bounded transition functions. In the particular case, where p_a gives rise to a weakly compact operator, Theorem 3.7 states that

$$\Delta(P) \quad = \quad \operatorname*{ess\,sup}_{x\in X} p_s(x,X) \ = \ 1 - \operatorname*{ess\,inf}_{x\in X} \int_X p_a(x,y)\mu(\mathrm{d}y).$$

If only some decomposition $P = R + S$ with weakly compact S is known, we can still apply Theorem 3.5 to get an upper bound on $\Delta(P)$. Assume that the stochastic transition function can be decomposed according to $p(x, \mathrm{d}y) = p_R(x, \mathrm{d}y) + p_S(x, \mathrm{d}y)$ such that S, defined via $Sv(y) = \int_X v(x)p_S(x, \mathrm{d}y)$, is weakly compact. Then

$$\Delta(P) \;\leq\; \operatorname*{ess\,sup}_{x\in X} p_R(x, X) \;\leq\; 1 - \operatorname*{ess\,inf}_{x\in X} p_S(x, X).$$

Using one of the above inequalities involving $\Delta(P)$, one is able to bound the essential spectral radius due to Theorem 3.1.

4 Asymptotic Properties

This section analyses the asymptotic properties of transfer operators. It profits from the fact that the analytical representation of r_{ess} enables us to combine results from different mathematical branches, in particular, results about Markov operators and the theory of Markov chains. We will see that transfer operators with essential spectral radius less than 1 play an important role, since they admit to prove results quite similar to the finite dimensional case. Before going into the detail, we state

Lemma 4.1 *Let $P : L^1(\mu) \to L^1(\mu)$ denote an arbitrary propagator and $T : L^\infty(\mu) \to L^\infty(\mu)$ the adjoint backward transfer operator. Then*

$$\|\chi_A \circ P^n\|_1 \;=\; \|T^n \chi_A\|_\infty$$

holds for every $A \in \mathcal{B}(X)$.

Proof: For arbitrary $A \in \mathcal{B}(X)$ we have: $\|\chi_A \circ P^n\|_1 = \|T^n \circ \chi_A\|_\infty = \|T^n\chi_A\|_\infty$, since the multiplication operator χ_A is adjoint to χ_A. □

An important property for Markov operators is *constrictiveness* [12]; it rules out the possibility that for some initial density v the iterates $P^n v$ eventually concentrate on a set of very small or vanishing measure.

Definition 4.2 *A propagator $P : L^1(\mu) \to L^1(\mu)$ is called* constrictive *if there exist constants $\epsilon > 0$ and $\delta > 0$ such that for every* density *$v \in L^1(\mu)$ there is an $m = m(v) \in \mathbf{N}$ with*

$$\mu(A) \leq \epsilon \quad\Rightarrow\quad \int_A P^n v(y)\mu(\mathrm{d}y) \leq 1 - \delta, \tag{10}$$

for all $n \geq m$. We call a propagator uniformly constrictive *if there exists an $m \in \mathbf{N}$ such that Eq. (10) holds for every $v \in L^1(\mu)$ and $n \geq m$.*

For arbitrary $v \in L^1(\mu)$, uniform constrictivenes can be stated as $\mu(A) \leq \epsilon \Rightarrow \|\chi_A \circ P^n\|_1 \leq 1 - \delta$. Moreover, it is sufficient to assume that condition (10) hold for $n = m$ only, since—due to $\|P^k\|_1 = 1$ for $k \in \mathbf{N}$—this already implies (10) for all $n \geq m$.

In view of (5) and the general version of (10), uniform constrictiveness seems to be closely related to $\Delta(P) < 1$ and thus to some bound on the essential spectral radius of P. This is indeed the case, as we will see below. Furthermore, Lemma 4.1 indicates that there should exist a similar condition involving the backward transfer operator T. This, in turn, is closely related to the *Doeblin condition*, known in the theory of Markov chains [14, 15]. It states that there exists a probability measure ν, constants $\epsilon > 0$, $\delta > 0$ and $m \in \mathbf{N}$ such that $\nu(A) \le \epsilon$ with $A \in \mathcal{B}(X)$ implies $\sup_{x\in X} \; p^m(x,A) \le 1-\delta$. Following the strategy of REVUZ (see remark preceding Def. 4.10), we introduce some "almost everywhere version" of the Doeblin condition:

Definition 4.3 *A stochastic transition function fulfills the* μ-a.e. Doeblin condition *if there exist constants $\epsilon > 0$, $\delta > 0$ and $m \in \mathbf{N}$, such that*

$$\mu(A) \le \epsilon \quad \Rightarrow \quad \operatorname*{ess\,sup}_{x\in X} \; p^m(x,A) \le 1-\delta, \tag{11}$$

for all $A \in \mathcal{B}(X)$.

Using the backward transfer operator, we deduce that (11) is equivalent to $\mu(A) < \epsilon \Rightarrow \|T^m\chi_A\|_\infty \le 1-\delta$. In fact, the condition is true for all $n \ge m$, since for $k \ge 1$ the inequality $\|T^{m+k}\chi_A\|_\infty \le \|T^k\|_\infty \|T^m\chi_A\|_\infty$ holds.

The next theorem states an important equivalence from which we will benefit in the sequel.

Theorem 4.4 *Let $P : L^1(\mu) \to L^1(\mu)$ denote the propagator defined in terms of the stochastic transition function $p : X \times \mathcal{B}(X) \to [0,1]$. Then, the following statements are equivalent:*

(i) The essential spectral radius of P is less than one: $r_{\text{ess}}(P) < 1$.

(ii) The propagator P is uniformly constrictive.

(iii) The μ-a.e. Doeblin condition holds for p.

If conditions (ii) or (iii) are satisfied for some $\epsilon, \delta > 0$ and $m \in \mathbf{N}$, then condition (i) holds with $r_{\text{ess}}(P) \le 1-\delta$.

Proof: Assume (i) holds, i.e., $r_{\text{ess}}(P) < 1$. Due to Eqs. (5) and (6), there exists an $m \in \mathbf{N}$ such that $\Delta(P^m) < 1$, which implies the μ-a.e. Doeblin condition (4.3) by Lemma 4.1. Now, (iii) is equivalent to (ii) according to Lemma 4.1. Using the note following (10), it is obvious that (ii) and (i) are equivalent. The bound on $r_{\text{ess}}(P)$ follows from (5) and (6). □

In view of the established equivalence, the essential spectral radius is related to the possibility of the system to eventually concentrate on a set of small or vanishing measure. In other words, the more the dynamics is smeared over the entire state space, the less is the essential spectral radius. In REVUZ [15, Chapter 6] it is shows that for so–called Harris recurrent Markov chains the Doeblin condition is equivalent to *quasi–compactness*[2] of some corresponding transfer operator T acting on the Banach space of bounded measurable functions. Due to HEUSER[3] [9, Sec. 104], this implies $r_{\text{ess}}(T) < 1$. In view of the above established equivalence, it is likely that the converse is also true.

[2]The operator T is called quasi–compact if there exist some $m \in \mathbf{N}$ and a compact operator S such that $\|T^m - S\| < 1$.

[3]The following implication holds if T is considered to act on the *complex* Banach space of bounded functions.

Uniform constrictiveness can be defined for arbitrary Markov operators. Using the characterization of $r_{\mathrm{ess}}(P)$ in (6), one can still show that unifom constrictiveness is equivalent to $r_{\mathrm{ess}}(P) < 1$. As a consequence, every uniform constrictive Markov operator has at least one stationary density.

Now, we want to analyse the spectral structure of *uniformly constrictive* propagators satisfying $P\chi_X = \chi_X$. Let $\omega = \exp(2\pi i/m)$ for some $m \in \mathbf{N}$; we call $\sigma_{\mathrm{cycle}}(\omega) = \{\omega, \omega^2, \ldots, \omega^m\}$ an *eigenvalue cycle* associated with ω if $\sigma_{\mathrm{cycle}}(\omega) \subset \sigma_{\mathrm{discr}}$. A subset $E \subset X$ is called *non–null* if $\mu(E) > 0$. A non–null subset $E \subset X$ is called invariant or *ergodic* if $P\chi_E = \chi_E$. A further subdecomposition of an ergodic subset $E = E_1 \cup \cdots \cup E_m$ into m mutually disjoint, non–null subsets is called an *ergodic cycle* of length m if $P\chi_{E_j} = \chi_{E_{j+1}}$ for $j = 1, \ldots, m$, where we set $E_{m+1} = E_1$ for simplicity.

Parts of the following two theorems are scattered over the literature, see e.g., [7, 12, 21].

Theorem 4.5 (Ergodic Decomposition) *Let $P : L^1(\mu) \to L^1(\mu)$ be a uniformly constrictive propagator satisfying $P\chi_X = \chi_X$. Then*

(i) there are only finitely many eigenvalues $\lambda \in \sigma_{\mathrm{discr}}(P)$ with $|\lambda| = 1$, each being a root of unity. The dimension of each eigenspace is finite and equal to the multiplicity of the corresponding eigenvalue;

(ii) the eigenvalue $\lambda = 1$ is of multiplicity d if and only if there exists a decomposition of the state space

$$X \quad = \quad E_1 \cup \cdots \cup E_d \cup F$$

into d mutually disjoint ergodic subsets E_j and a set $F = X \setminus \bigcup_j E_j$ of μ measure zero.

Proof: Use the equivalence in Thm. 4.4 of this article and Thm. 3 of [7, VIII.8] to prove the first part. For the second statement we exploit the fact that $Pv = v$ implies $Pv^+ = v^+$ and $Pv^- = v^-$, where $v^{+/-}$ denote the positive and negative part of v, respectively [12]. Assume that the multiplicity of $\lambda = 1$ is d. Then, as a consequence of the first part, there exist d linear independent eigenfunctions $v_1, \ldots, v_d$. Due to the decomposition result for v, we can also choose d linear independent *densities*, which we again denote by $v_1, \ldots, v_d$, with $Pv_j = v_j$.

We now show that the densities can be chosen in such a way that their supports $E_j = \mathrm{supp}(v_j)$ are mutually disjoint, i.e., $\mu(E_j \cap E_k) = 0$ for $j \neq k$. If for some choice of linear independent densities $v_1, \ldots, v_d$ there exist v_j, v_k such that $\mu(E_j \cap E_k) > 0$, we simply substitue v_j, v_k by $(v_j - v_k)^+, (v_j - v_k)^-$. This is possible, since $\mathrm{span}\{(v_j - v_k)^+, (v_j - v_k)^-\} = \mathrm{span}\{v_j, v_k\}$ and $\mathrm{span}\{(v_j - v_k)^+, (v_j - v_k)^-, v_j, v_k\} > 2$ would be in contradiction to the fact that the multiplicity of $\lambda = 1$ is d. Due to $P\chi_X = \chi_X$, we have $v_j = 1/\mu(E_j)\chi_{E_j}$ and $\sum_j \mu(E_j) = 1$ Finally, define $F = X \setminus \bigcup_j E_j$. Since any decomposition into d mutually disjoint ergodic subsets results in a multiplicity of $\lambda = 1$ of at least d, the second statement is proved. □

The above decomposition of the state space is unique up to μ–equivalence. There is an analogous decomposition result for the stochastic transition function

p, since for every ergodic subset E

$$\mu(E) \;=\; \int_E \chi_E(y)\mu(\mathrm{d}y) \;=\; \int_E P\chi_E(y)\mu(\mathrm{d}y) \;=\; \int_E p(x,E)\mu(\mathrm{d}x)$$

implies $p(x,E)=1$ for μ–almost every $x \in E$. Thus, the ergodic decomposition of Theorem 4.5 induces a decomposition of the stochastic transition function which is unique up to μ–equivalence. For a "strong" decomposition holding everywhere see, e.g., [21]. As a consequence, the characteristic function χ_E of some ergodic set E is also an eigenfunction of T corresponding to $\lambda = 1$.

Each ergodic subset E can further be decomposed if some associable eigenvalue cycle is of length $m > 1$. For the next theorem, an eigenvalue of multiplicity ν is interpreted as ν equal eigenvalues $\lambda_1, \ldots, \lambda_\nu$ of multiplicity 1.

Theorem 4.6 (Ergodic Cycle Decomposition) *Let $P : L^1(\mu) \to L^1(\mu)$ be a uniformly constrictive propagator satisfying $P\chi_X = \chi_X$. Then*

(i) each eigenvalue $\lambda \in \sigma_{\mathrm{discr}}(P)$ of unit modulus is part of some eigenvalue cycle, i.e., there exists some constant $m \geq 1$ such that $\lambda \in \sigma_{\mathrm{cycle}}(\omega) \subset \sigma_{\mathrm{discr}}(P)$ for $\omega = \exp(2\pi i/m)$;

(ii) there is a one–to–one correspondence between eigenvalue cycles and ergodic cycles. More precisely, let d denote the multiplicity of $\lambda = 1$. Then set of all eigenvalues of unit modulus can be decomposed into d eigenvalue cycles $\{\lambda_{j\,1}, \ldots, \lambda_{j\,m_j}\}$ with $j = 1, \ldots, d$ and $m_j \geq 1$ if and only if the state space can be decomposed into d ergodic cycles $\{E_{j\,1}, \ldots, E_{j\,m_j}\}$ of length m_j for $j = 1, \ldots, d$.

Proof: Mimic the proof of Theorem 11 in [21] and use the Ergodic Decomposition Theorem in order to show that each ergodic subset E can be decomposed into an ergodic cycles $\{E_1, \ldots, E_m\}$ of length m. Note that the length m is equal to the multiplicity of $\lambda = 1$ of ${P_E}^m$ for the restricted propagator $P_E = \chi_E \circ P \circ \chi_E$, which is well–defined by Theorem 4.5. Thus, it remains to show that $\sigma(P_E) \cap \{|\lambda| = 1\} = \sigma_{\mathrm{cycle}}(\omega)$ with $\omega = \exp(2\pi i/m)$. But every ergodic cycle $\{E_1, \ldots, E_m\}$ of P is also an ergodic cycle of P_E and allows us to define m linear independent eigenfunctions $v_k = \sum_{j=1}^m \omega^{kj} P_E^j \chi_{E_1}$, see e.g. [1], which correspond to the eigenvalues ω^k for $k = 1, \ldots, m$. □

Due to the above two theorems, a uniformly constrictive propagator is sometimes called *asymptotically periodic* [12]. From a functional analytic point of view, the above decomposition results are related to a partial spectral decomposition of P.

Theorem 4.7 ([7, Chapter VIII]) *Let $P : L^1(\mu) \to L^1(\mu)$ denote a uniformly constrictive propagator satisfying $P\chi_X = \chi_X$ and let Π_λ denote the projection on the eigenspace corresponding to the discrete eigenvalue λ. Then, for all $n \in \mathbf{N}$,*

$$P^n \;=\; \sum_{\lambda \in \sigma(P), |\lambda|=1} \lambda^n \Pi_\lambda + D^n$$

with some strict contraction $D : L^1(\mu) \to L^1(\mu)$ satisfying $\|D^n\|_1 \le Mq^n$ for some constants $M > 0$ and $0 < q < 1$. Furthermore, the projections fulfill

$$\Pi_\lambda \quad = \quad \lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} 1/\lambda^n P^n, \tag{12}$$

where the limit is understood to be uniform.

In the sequel, we will use the above results to analyse the asymptotic properties of P.

Definition 4.8 *Let $P : L^1(\mu) \to L^1(\mu)$ denote a uniformly constrictive propagator satisfying $P\chi_X = \chi_X$. Then we say:*

(i) The operator P is ergodic *if every ergodic subset E is of measure 1. Equivalently, $P\chi_E = \chi_E$ implies $\mu(E) = 0$ or $\mu(E) = 1$.*

(ii) The operator P is periodic with period *p if it is ergodic and p is the largest integer for which an ergodic cycle of length p occurs. If $p = 1$, then P is called* aperiodic.

Some remarks are in order. An arbitrary Markov operator $P : L^1(\mu) \to L^1(\mu)$ satisfying $P\chi_X = \chi_X$ is said to be ergodic if $P^n v$ converges weakly to χ_X in the sense of Cesàro[4] for all densities $v \in L^1(\mu)$ [12]. Anticipating the results of the next corollary and using Thm. 5.5.1 from [12, Sec. 5.5], it can easily be shown that for uniformly constrictive propagators this definition is equivalent to Def. 4.8(i). In Markov chain theory, the term "ergodicity" is used in a different way, since it implies aperiodicity; Corollary 4.9 may used to establish the relation. We now turn to the question how these properties are related to the decomposition results obtained in the previous two theorems.

Corollary 4.9 *Let $P : L^1(\mu) \to L^1(\mu)$ be a uniformly constrictive propagator satisfying $P\chi_X = \chi_X$. Then*

(i) P is ergodic if and only if the eigenvalue $\lambda = 1$ is simple.

(ii) P is aperiodic if and only if the eigenvalue $\lambda = 1$ is simple and dominant, i.e., $\eta \in \sigma_{\mathrm{discr}}(P)$ with $|\eta| = 1$ implies $\eta = 1$.

Ergodicity is related to the fact that it is impossible to decompose the state space into independent parts. The analogue in the theory of Markov chains is *μ–irreducibility* expressing that it is possible to move from every state to every "relevant" subset within a finite time. More precisely, $\mu(A) > 0$ implies $p^m(x, A) > 0$ for some $m \in \mathcal{M}$ and every $x \in X$, $A \in \mathcal{B}(X)$. Revuz introduces the following "μ–almost everywhere version" of irreducibility, which fits perfectly to our context.

Definition 4.10 ([15, Chap. 3.2]) *A stochastic transition function p is called* μ-a.e. irreducible *if for μ–almost every $x \in X$ and $A \in \mathcal{B}(X)$*

$$\mu(A) > 0 \quad \Rightarrow \quad p^m(x, A) > 0$$

for some $m \in \mathbf{N}$ possibly depending on both x and A.

[4] This means that $\lim_{n\to\infty} 1/n \sum_{k=1}^{n} \langle P^k v, u\rangle = \langle \chi_X, u\rangle$ for all $u \in L^\infty(\mu)$ [12].

The next theorem states the relation between the two characterizations of indecomposability:

Theorem 4.11 *Let $P : L^1(\mu) \to L^1(\mu)$ be a uniformly constrictive propagator that corresponds to the stochastic transition function p and satisfies $P\chi_X = \chi_X$. Then P is ergodic if and only if p is μ-a.e. irreducible.*

Proof: Due to the remark following Def. 4.8, P is ergodic if and only if $P(\chi_B/\mu(B))$ converges to χ_X in the sense of Cesàro for every $B \in \mathcal{B}(X)$ with $\mu(B) > 0$. For arbitrary $A \in \mathcal{B}(X)$ with $\mu(A) > 0$ this is equivalent to

$$\begin{aligned}
& \lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} \int_X P^k \chi_B(y) \chi_A(y)\, \mu(\mathrm{d}y) = \mu(A)\, \mu(B) \\
\Leftrightarrow \quad & \lim_{n\to\infty} \int_B \frac{1}{n} \sum_{k=1}^{n} p^k(x, A) \mu(\mathrm{d}y) = \int_B \mu(A) \mu(\mathrm{d}y) \\
\Leftrightarrow \quad & \lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} p^k(x, A) = \mu(A); \qquad \mu\text{–a.e.},
\end{aligned}$$

where we used Lebesgue's dominated convergence theorem. Since $\mu(A) > 0$ by assumption, this is equivalent to μ-a.e. irreducibility according to Def. 4.10. □

Often, one is interested in dynamical systems—deterministic or stochastic—that exhibit a *unique* stationary density and guarantee that for every initial density v the iterates $P^n v$ converge to the stationary density. In view of Corollary 4.9, these systems are necessarily connected to ergodic propagators, but due to the possible cyclic behavior, ergodicity is no sufficient condition. As we will see below, one has to require aperiodicity.

Definition 4.12 ([12, Chap. 5.6]) *A propagator $P : L^1(\mu) \to L^1(\mu)$ is called* asymptotically stable *if $P\chi_X = \chi_X$ and*

$$\lim_{n\to\infty} \|P^n v - \chi_X\|_1 \quad = \quad 0 \tag{13}$$

for every density $v \in L^1(\mu)$.

Define the limit propagator $P_\infty : L^1(\mu) \to L^1(\mu)$ by

$$P_\infty v(y) \quad \equiv \quad \int_X v(x) \mu(\mathrm{d}x) \tag{14}$$

for arbitrary $v \in L^1(\mu)$, which corresponds to the projection on the eigenspace spanned by χ_X. In terms of P_∞ we can state (13) in the equivalent form: $\lim_{n\to\infty} \|P^n v - P_\infty v\|_1 = 0$ for $v \in L^1(\mu)$. Applying Thm. 4.7, we get

Corollary 4.13 *Let $P : L^1(\mu) \to L^1(\mu)$ be a uniformly constrictive propagator satisfying $P\chi_X = \chi_X$. Then P is asymptotically stable if and only if P is aperiodic. In either case,*

$$\|P^n - P_\infty\|_1 \quad \leq \quad M q^n \quad \longrightarrow \quad 0 \tag{15}$$

as $n \to \infty$ with some constants $M > 0$ and $0 < q < 1$.

An analogous result to Cor. 4.13 is well established in the theory of Markov chains [14]. It is related to a property of the stochastic transition function called *uniform ergodicity*: $\sup_{x\in X} \|p^n(x,\cdot) - \mu\|_{\mathrm{TV}} \to 0$ for $n \to \infty$ in the total variation norm

$$\|\nu\|_{\mathrm{TV}} \quad = \quad \sup_{|u|\leq 1} \int_X u(y)\nu(\mathrm{d}y).$$

We will show that a corresponding result holds if we impose a "μ–almost everywhere version" of uniform ergodicity on p. Note that $\|\mu\|_{\mathrm{TV}} = \|T_\infty\|_\infty$ holds for the limit backward transfer operator $T_\infty : L^\infty(\mu) \to L^\infty(\mu)$ defined by

$$T_\infty u(x) \quad \equiv \quad \int_X u(y)\mu(\mathrm{d}y);$$

the two limit operators are related via $P_\infty^* = T_\infty$.

Definition 4.14 *A stochastic transition function p is called* μ-a.e. uniformly ergodic *if*

$$\operatorname*{ess\,sup}_{x\in X} \|p^n(x,\cdot) - \mu\|_{\mathrm{TV}} \quad \longrightarrow \quad 0 \tag{16}$$

for $n \to \infty$.

In terms of the backward transfer operator and its limit operator, Eq. (16) is equivalent to $\lim_{n\to\infty} \|T^n - T_\infty\|_\infty = 0$. We summarize the relation between asymptotically stable propagators and μ-a.e. uniformly ergodic stochastic transition functions.

Corollary 4.15 *A propagator $P : L^1(\mu) \to L^1(\mu)$ satisfying $P\chi_X = \chi_X$ is asymptotically stable if and only if the corresponding stochastic transition function p is μ-a.e. uniformly ergodic.*

5 Applications

Discrete dynamical systems. Consider the discrete dynamical system

$$X_{n+1} \quad = \quad f(X_n), \quad n = 1, 2, \dots, \tag{17}$$

where $f : X \to X$ is a measurable diffeomorphism[5] on the probability space $(X, \mathcal{B}(X), \mu)$ with $X \subset \mathbf{R}^d$. Denote by δ_y the Dirac measure supported on $y \in X$. Then, we may write the stochastic transition function defined by (17) as $p(x, \mathrm{d}y) = \delta_{f(x)}(\mathrm{d}y)$. For $n > 1$, we obtain via the Chapman–Kolmogorov equation

$$p^n(x, \mathrm{d}y) \quad = \quad \delta_{f^n(x)}(\mathrm{d}y). \tag{18}$$

Assume that μ is stationary w.r.t. p, which holds if and only if f is measure preserving, i.e., $\mu(A) = \mu(f^{-1}(A))$ for all $A \in \mathcal{B}(X)$ [12]. Then, the propagator

[5] We assume that both f and f^{-1} are measurable.

$P : L^1(\mu) \to L^1(\mu)$ defined in terms of $p(x, \mathrm{d}y)$ is the well–known Frobenius–Perron operator associated with f [12]; it satisfies

$$\int_A P^n v(y)\, \mu(\mathrm{d}y) \quad = \quad \int_{f^{-n}(A)} v(x)\mu(\mathrm{d}x) \quad = \quad \int_A v(f^{-n}y)\, \mu(\mathrm{d}x)$$

for all $v \in L^1(\mu)$ and $A \in \mathcal{B}(X)$, hence $P^n v = v \circ f^{-n}$. Without any further knowledge about the stationary probability measure μ, little can be said about the essential spectral radius. However, it is shown in [12, Remark 4.3.1] that a propagator corresponding to some *invertible* measure preserving transformation cannot be asymptotically stable. Furthermore, using a result from DING [4], one can show that the entire discrete spectrum lies *on* the unit circle.

If, for instance, it is known that the stationary measure μ is absolutely continuous w.r.t. the Lebesgue measure, then, due to (18), we have $\Delta(P^n) = 1$ for all $n \geq 0$ and therefore, $r_{\text{ess}}(P) = 1$ according to Theorem 3.1.

Remark: There do exist non–invertible measure preserving transformations that give rise to asymptotically stable propagators that are not constrictive, e.g., the dyadic transformation on the interval $[0,1]$ (see [12] for details). Furthermore, results for transfer operators on the Banach space of functions of bounded variation may be quite different from ours. Ding and Li [5] report about a discrete dynamical system with a piecewise stretching mapping f on $[0,1]$, where the corresponding transfer operator has $r_{\text{ess}} < 1$ in the space of functions of bounded variation, whereas $r_{\text{ess}} = 1$ in L^1.

Stochastically perturbed discrete dynamical systems. Consider now some stochastic perturbation of the above dynamical system

$$X_{n+1} \quad = \quad f(X_n) + \xi_n, \quad n = 1, 2, \dots, \tag{19}$$

where $\{\xi_n\}_{n \in \mathbf{N}}$ is an i.i.d. sequence of random vectors, each having the same density g w.r.t. μ, i.e., $\mathbf{P}(\xi_n \in A) = \int_A g(x)\mu(\mathrm{d}x)$ for all $A \in \mathcal{B}(X)$ [12]. The stochastic transition function is given by

$$p(x, \mathrm{d}y) \quad = \quad g(x - f(y))\mu(\mathrm{d}y) \tag{20}$$

and the corresponding propagator $P : L^1(\mu) \to L^1(\mu)$ admits the simple representation

$$Pv(y) \quad = \quad \int_X v(x) g(x - f(y))\mu(\mathrm{d}x).$$

For arbitrary $g \in L^\infty(\mu)$, we have $r_{\text{ess}}(P) = 0$ by Cor. 3.6. Under a suitable Lyapunov condition on the stochastic transition function, it is shown in [12] that P is asymptotically stable and thus uniformly ergodic according to Cor. 4.15.

Although the unperturbed transfer operator corresponding to the deterministic dynamical system may have more than one stationary density (even infinitely many), the stochastically perturbed transfer operator possesses a unique stationary density under suitable conditions on the perturbation, i.e., the distribution of g, and a Lyapunov condition on p.

In [12], the relation between the two transfer operators is studied for the limit of vanishing perturbation: Denote by P and P_ϵ the transfer operators corresponding to the unperturbed and the perturbed system, respectively, where the random vectors in (19) possess the common density $g_\epsilon(x) = 1/\epsilon\, g(x/\epsilon)$. If for all $0 < \epsilon < \epsilon_0$ the operators P_ϵ have a stationary density f_ϵ and furthermore, the limit $f_* = \lim_{\epsilon\to 0} f_\epsilon$ exists, then f_* is a stationary density of the unperturbed transfer operator P. The proof is based on the fact that $\lim_{\epsilon\to 0} \|P_\epsilon f - Pf\|_1 = 0$ for all $f \in L^1(\mu)$. This result allows the following intriguing interpretation: Suppose that for all $0 < \epsilon < \epsilon_0$, the density f_ϵ is the *unique* stationary density of P_ϵ. Then, the process of decreasing the "amplitude" ϵ of the stochastic perturbation can be used to "select" a *specific* stationary density of P, namely f, since f_ϵ approximates f for small ϵ. This procedure is used by DELLNITZ and JUNGE in [1] to approximate SRB measures for hyperbolic dynamical systems.

Stochastic dynamical systems. For a differentiable potential function $V : X \subset \mathbf{R}^d \to \mathbf{R}$, the *Hamiltonian equations of motion* are given by

$$\begin{aligned} \dot{q} &= M^{-1}p \\ \dot{p} &= -\nabla_q V(q) \end{aligned} \tag{21}$$

where q and p denote the states and the momenta of the system, respectively and M the diagonal mass matrix [8]. Let Φ^t denote the flow associated with (21). It is well–known that the *canonical measure*

$$\mu_{\text{can}}(\mathrm{d}q\mathrm{d}p) = \underbrace{\frac{1}{Z_q}\exp(-\beta V(q))\mathrm{d}q}_{\mu_Q(\mathrm{d}q)} + \underbrace{\frac{1}{Z_p}\exp(-\frac{\beta}{2}p^t M^{-1}p)\mathrm{d}p}_{\mu_P(\mathrm{d}p)}$$

corresponding to the so–called inverse temperature β is invariant w.r.t. the flow Φ^t. In the following, we restrict our attention to potential functions V that allow to normalize μ_{can} to a probability measure.

Aiming at the identification of molecular conformations, DEUFLHARD et al. [2] considered the Hamiltonian flow modeling the molecular dynamics for some *fixed* observation time span $\tau > 0$

$$X_{n+1} = \Phi^\tau(X_n), \quad n = 1, 2, \dots, \tag{22}$$

with $X_n = (Q_n, P_n)$. Obviously, X_n is equal to the solution of the Hamiltonian equation of motion for the initial values X_0 at $t = n\tau$. According to our first example, the essential spectral radius of the propagator P associated with (22) is equal to 1. Furthermore, since Φ^τ is invertible, P cannot be asymptotically stable.

Upon keeping a clear orientation towards an analysis of biomolecular systems, the computational techniques based on the above model appeared to be unsatisfactory [18]. Guided by concepts of statistical physics and numerical efficiency, Schütte remodelled the problem and introduced in [17, 16] the *Hamiltonian stochastic system*

$$Q_{n+1} = \Pi_Q \Phi^\tau(Q_n, P_n), \quad n = 1, 2, \dots, \tag{23}$$

where $\Pi_Q : \mathbf{R}^{2d} \to \mathbf{R}^d$ is the projection on the state space variable Q and $\{P_n\}_{n\in\mathbf{N}}$ is an i.i.d. sequence of random variables, each distributed according to

μ_P, i.e., $\mathbf{P}[P_n \in A] = \mu_P(A)$. The stochastic transition function corresponding to (23) is given by

$$p(q, A) \quad = \quad \int_{\mathbf{R}^d} \chi_A(\Pi_Q \Phi^\tau(q,p))\, \mu_P(\mathrm{d}p)$$

for all $A \in \mathcal{B}(X)$; in [16] it is shown that μ_Q is stationary w.r.t. p. Exploiting properties of the Hamiltonian equation of motion, the corresponding propagator $P : L^1(\mu) \to L^1(\mu)$ may be written as

$$Pv(y) \quad = \quad \int_{\mathbf{R}^d} v(\Pi_Q \Phi^{-\tau}(q,p))\, \mu_P(\mathrm{d}p).$$

for $v \in L^1(\mu)$ [17, 16].

Assume that for μ_Q–almost every $q \in X$ the mapping $p \mapsto \Pi_Q\Phi^\tau(q,p)$ is invertible in an open set $U(q)$. If for μ_Q–almost every q we have $\mu_P(U(q)) \geq \eta > 0$, then the stochastic transition function decomposes into an absolutely continuous and a singular part w.r.t. μ_Q [16]. If the corresponding density is shown to be in $L^\infty(\mu)$, this yields $r_{\text{ess}}(P) \leq 1 - \eta$ due to Thm. 3.7.

Asymptotic stability of the Hamiltonian stochastic system can be shown under some additionally *mixing condition* [16]: For every pair of open sets $A, B \in \mathcal{B}(X)$ there exists some $m \in \mathbf{N}$ such that $\int_A p^m(x,B)\mu_Q(\mathrm{d}x) > 0$. The mixing condition can be interpreted as some open set accessibility of the system, since it states that it is possible to move from the open set A to B within m steps. Under the above mixing condition, the propagator P is asymptotically stable. Applying Cor. 4.15, we finally get μ-a.e. uniform ergodicity.

For the most significant application class of periodic boundary conditions—implying some compact state space X—Schütte showed in [16] that the above conditions are indeed satisfied.

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References

[1] M. Dellnitz and O. Junge. On the approximation of complicated dynamical behavior. *SIAM J. Num. Anal.*, 36(2):491–515, 1999.

[2] P. Deuflhard, M. Dellnitz, O. Junge, and C. Schütte. Computation of essential molecular dynamics by subdivision techniques. In *[3]*, pages 98–115, 1999.

[3] P. Deuflhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, and R. D. Skeel, editors. *Computational Molecular Dynamics: Challenges, Methods, Ideas*, volume 4 of *Lecture Notes in Computational Science and Engineering*. Springer, 1999.

[4] J. Ding. The point spectrum of Frobenius–Perron and Koopman operators. *Proc. Amer. Math. Soc.*, 126(5):1355–1361, 1998.

[5] J. Ding and T. Y. Li. A convergence rate analysis for Markov finite approximations to a class of Frobenius-Perron operators. *Nonlinear Anal. Theory Methods Appl.*, 31(5-6):765–776, 1998.

[6] N. Dunford and B. J. Pettis. Linear operator on summable functions. *Trans. Amer. Math. Soc.*, 47:323–392, 1940.

[7] N. Dunford and J. T. Schwartz. *Linear Operators, Part I: General Theory*, volume VII of *Pure and Applied Mathematics*. Interscience, 1957.

[8] R. Haberlandt, S. Fritzsche, G. Peinel, and K. Heinzinger. *Molekulardynamik - Grundlagen und Anwendungen.* Vieweg, 1995.

[9] H. Heuser. *Funktionalanalysis.* Teubner, 1986.

[10] T. Kato. *Perturbation Theory for Linear Operators.* Springer, 1995. Reprint of the 1980 edition.

[11] K. Lange. Decomposition of substochastic transition functions. *Proc. Amer. Math. Soc.*, 37:575–580, 1973.

[12] A. Lasota and M. C. Mackey. *Chaos, Fractals and Noise*, volume 97 of *Applied Mathematical Sciences.* Springer, New York, 2nd edition, 1994.

[13] L. Maligranda. Weakly compact operators and interpolation. *Acta Appl. Math.*, 72:79–89, 1992.

[14] S. Meyn and R. Tweedie. *Markov Chains and Stochastic Stability.* Springer, Berlin, Heidelberg, New York, Tokyo, 1993.

[15] D. Revuz. *Markov Chains.* North–Holland, Amsterdam, Oxford, 1975.

[16] C. Schütte. *Conformational Dynamics: Modelling, Theory, Algorithm, and Application to Biomolecules.* Habilitation Thesis, Fachbereich Mathematik und Informatik, Freie Universität Berlin, 1998. Available as Report SC-99-18 via http://www.zib.de/bib/pub/pw/.

[17] C. Schütte, A. Fischer, W. Huisinga, and P. Deuflhard. A direct approach to conformational dynamics based on hybrid Monte Carlo. *J. Comput. Phys., Special Issue on Computational Biophysics*, 151:146–168, 1999.

[18] C. Schütte, W. Huisinga, and P. Deuflhard. Transfer operator approach to conformational dynamics in biomolecular systems. Preprint SC-99-36, Konrad–Zuse–Zentrum, Berlin. Available via http://www.zib.de/MDGroup, 1999.

[19] L. Weis. Decompostions of positive operators and some of their applications. In K. D. Bierstedt and B. Fuchssteiner, editors, *Functional Analysis: Surveys and Recent Results III*, pages 95–115. North–Holland, 1983.

[20] L. Weis. Approximation by weakly compact operators in L_1. *Math. Nachr.*, 118:321–326, 1984.

[21] K. Yoshida and S. Kakutani. Operator–theoretical treatment of Markoff's process and mean ergodic theorem. *Annals of Mathematics*, 42(1):188–228, 1941.

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