

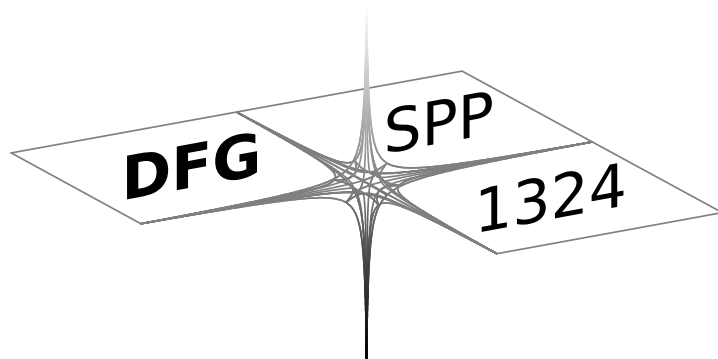
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„Extraktion quantifizierbarer Information aus komplexen Systemen“

Positivity of hit-and-run and related algorithms

D. Rudolf, M. Ullrich

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POSITIVITY OF HIT-AND-RUN AND RELATED ALGORITHMS

DANIEL RUDOLF AND MARIO ULLRICH

ABSTRACT. We prove positivity of the Markov operators that correspond to the hit-and-run algorithm, random scan Gibbs sampler, slice sampler and an Metropolis algorithm with positive proposal. In all of these cases the positivity is independent of the state space and the stationary distribution. In particular, the results show that it is not necessary to consider the lazy versions of these Markov chains. The proof relies on a well known lemma which relates the positivity of the product MTM^* , for some operators M and T , to the positivity of T . It remains to find that kind of representation of the Markov operator with a positive operator T .

1. INTRODUCTION

In many applications, for example volume computation [LS93, KLS97, LV06b] or integration of functions [LV06a, MN07, Rud09, Rud12], it is essential that one can approximately sample a distribution in a convex body. The dimension d might be very large. One approach that is feasible for a general class of problems is to run a Markov chain that has the desired distribution as its limit distribution. In the following let us explain why the positivity of the Markov operator is helpful to prove efficiency results for such sampling procedures.

We assume that we have a Markov chain in $K \subset \mathbb{R}^d$ which is reversible with respect to (w.r.t.) the distribution π . Let $P: L_2(\pi) \rightarrow L_2(\pi)$ be the corresponding Markov operator and let $L_2(\pi)$ be all (w.r.t. π) square integrable functions $f: K \rightarrow \mathbb{R}$. We assume that P is *ergodic*, which means that $Pf = f$ implies that f is constant. Then let $\text{gap}(P) = 1 - \beta$ be the *absolute spectral gap*, where β denotes the largest absolute value of the elements of the spectrum of P without 1. In formulas $\beta = \sup\{|\alpha| : \alpha \in \text{spec}(P) \setminus 1\}$, where $\text{spec}(P)$ denotes the spectrum of P . For example a lower bound for $\text{gap}(P)$ implies an upper bound of the total variation distance [LS93] and on the mean square error of Markov chain Monte Carlo algorithms for the approximation of expectations with respect to π , see e.g. [Rud12].

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Maybe the most successful technique to bound $\text{gap}(P)$ is the conductance technique [LS88, LS93]. But, unfortunately, bounds on the conductance allow only bounds on the second largest element of the spectrum of the Markov operator. This is known as Cheeger's inequality [LS88]. To handle variation distance and absolute spectral gap it is necessary to consider also the smallest element of the spectrum, which describes some kind of periodicity of the Markov chain. Usually, this problem is avoided by considering a *lazy version* of the Markov chain. That is, in each step, the Markov chain remains at the current state with probability $1/2$. Such a lazy version induces a Markov operator with non-negative spectrum, which implies that the smallest element of the spectrum does not matter. This strategy has almost no influence on the computational cost, since, compared to the overall cost of one step of the chain, one additional random number is mostly negligible. However, it is desirable to omit any slowdown whenever possible.

In the following we present a technique to prove that the spectrum of a Markov operator is positive, which is based on a simple and well known lemma from functional analysis. This technique was already successfully applied in a discrete setting to prove positivity (and comparison results) for the Swendsen-Wang process from statistical physics, see [Ull12a, Ull12b]. Here, we show that the hit-and-run algorithm, random scan Gibbs sampler, slice sampler and the Metropolis algorithm with positive proposal are positive. In particular, it implies that the independent Metropolis algorithm is positive. The result is new for the hit-and-run algorithm and the Metropolis algorithm with positive proposal, whereas for the random scan Gibbs sampler and the slice sampler it is known [LWK95, MT02].

2. THE PROCEDURE

We consider a time-homogeneous Markov chain $(X_i)_{i \in \mathbb{N}}$, where the X_i are random variables on a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$ that map into \mathbb{R}^d , equipped with the Borel σ -algebra \mathcal{B} , and satisfy the Markov property. Namely,

$$\mathbb{P}(X_n \in A_n \mid X_{n-1} \in A_{n-1}, \dots, X_0 \in A_0) = \mathbb{P}(X_n \in A_n \mid X_{n-1} \in A_{n-1})$$

for all $n \geq 1$ and any sequence of \mathcal{B} -measurable sets A_0, A_1, \dots with $\mathbb{P}(X_{n-1} \in A_{n-1}, \dots, X_0 \in A_0) > 0$. We assume that the Markov chain has a unique stationary distribution π and that it is reversible with respect to this measure. For a more comprehensive introduction to the theory of Markov chains we refer to [MT09, RR04].

To every Markov chain $(X_i)_{i \in \mathbb{N}}$ corresponds a *Markov kernel* $P: \mathbb{R}^d \times \mathcal{B} \rightarrow [0, 1]$ such that for each $x \in \mathbb{R}^d$, $P(x, \cdot)$ is a probability measure

on \mathcal{B} and, for each $A \in \mathcal{B}$, $P(\cdot, A)$ is \mathcal{B} -measurable. This Markov kernel is given by

$$P(x, A) = \mathbb{P}(X_{n+1} \in A \mid X_n = x), \quad x \in \mathbb{R}^d, A \in \mathcal{B}, n \in \mathbb{N}$$

and describes the probability that the Markov chain reaches the set A in one step from x . Using this Markov kernel we define the *Markov operator* P (for notational convenience we use the same letter as for the Markov kernel) by

$$Pf(x) = \int_{\mathbb{R}^d} f(y) P(x, dy), \quad x \in \mathbb{R}^d$$

for all functions $f \in L_2 = L_2(\pi)$, where L_2 is the Hilbert space of functions on $f: \mathbb{R}^d \rightarrow \mathbb{R}$ with inner product

$$\langle f, g \rangle = \int_{\mathbb{R}^d} f(x) g(x) d\pi(x).$$

By reversibility of the Markov chain we know that P is a self-adjoint operator on L_2 . A self-adjoint operator P is called *positive*, written $P \geq 0$, if

$$\langle Pf, f \rangle \geq 0, \quad \forall f \in L_2.$$

It is well known that positive operators have only non-negative spectrum, for further details see for example [Kre89].

Our aim is to show that several Markov chains that are used to sample from distributions in \mathbb{R}^d induce positive Markov operators. In this case, we say that the Markov chain is positive. We will basically utilize the following lemma.

Lemma 1. *Let H_1 and H_2 be Hilbert spaces and $M: H_1 \rightarrow H_2$ be a bounded, linear operator. Let M^* be the adjoint operator of M and let $T: H_2 \rightarrow H_2$ be a bounded, linear and positive operator. Then $MTM^*: H_1 \rightarrow H_1$ is also positive.*

Proof. We denote the inner product of H_i by $\langle \cdot, \cdot \rangle_i$ for $i = 1, 2$. By the definition of the adjoint operator and positivity of T ,

$$\langle MTM^*f, f \rangle_1 = \langle TM^*f, M^*f \rangle_2 \geq 0.$$

This proves the statement. \square

Suppose we have an operator $P: H_1 \rightarrow H_1$ on a Hilbert space with the property that it can be written as $P = MTM^*$, where $T: H_2 \rightarrow H_2$, $M: H_1 \rightarrow H_2$ and M^* is the adjoint of M for some (other) Hilbert space H_2 . If we can show, additionally, that T is a positive operator, we obtain by the lemma above that P is also positive. Thus, the proof of positivity of the Markov chains under consideration is done by a construction of a suitable second Hilbert space such that the corresponding Markov operator can be written in the above mentioned form.

3. APPLICATIONS

Throughout this section we consider Markov chains in a bounded subset K of \mathbb{R}^d with non-empty interior. Additionally, we denote by B_d the d -dimensional unit ball and by S^{d-1} its boundary. Let $\rho: K \rightarrow [0, \infty)$ be a (not necessarily normalized) density, i.e. a non-negative Lebesgue-integrable function. We define the measure with density ρ by

$$\pi(A) = \frac{\int_A \rho(x) \, dx}{\int_K \rho(x) \, dx}$$

for all measurable sets $A \subset K$. For example, if $\rho(x) = \mathbf{1}_K(x)$ then π is simply the uniform distribution on K . In what follows we present some Markov chains that can be used sample approximately from π , that is, π is their stationary distribution. We will see that each of them is positive, independent from the choice of the density ρ .

We will define only the Markov operators for the corresponding Markov chains, since the corresponding Markov kernel can be obtained by applying the operators to indicator functions.

3.1. Hit-and-run. The hit-and-run algorithm consists of two steps: Starting from $x \in K$, choose a random direction $\theta \in S^{d-1}$ and then choose the next state of the Markov chain with respect to the density ρ restricted to the chord determined by x and θ .

For $x \in K$ and $\theta \in S^{d-1}$ we denote by $L(x, \theta)$ the *chord* in K through x and $x + \theta$, i.e.

$$L(x, \theta) = \{x + s\theta \in K \mid s \in \mathbb{R}\}.$$

Additionally we write κ_d for the volume of the $(d-1)$ -dimensional unit sphere and

$$(1) \quad \ell(x, \theta) = \int_{L(x, \theta)} \rho(y) \, dy$$

for the total weight of the chord $L(x, \theta)$. The Markov operator H that corresponds to the hit-and-run chain is defined by

$$Hf(x) = \frac{1}{\kappa_d} \int_{S^{d-1}} \frac{1}{\ell(x, \theta)} \int_{L(x, \theta)} f(y) \rho(y) \, dy \, d\theta$$

for all $f \in L_2(\pi)$. To rewrite H in the desired form let μ be the product measure of π and the uniform distribution on S^{d-1} and $L_2(\mu)$ be the Hilbert space of functions $g: K \times S^{d-1} \rightarrow \mathbb{R}$ with inner-product

$$\langle g_1, g_2 \rangle_\mu = \frac{1}{\kappa_d} \int_K \int_{S^{d-1}} g_1(x, \theta) g_2(x, \theta) \, d\theta \, d\pi(x)$$

for $g_1, g_2 \in L_2(\mu)$. We define the operators $M: L_2(\mu) \rightarrow L_2(\pi)$ and $T: L_2(\mu) \rightarrow L_2(\mu)$ by

$$Mg(x) = \frac{1}{\kappa_d} \int_{S^{d-1}} g(x, \theta) d\theta$$

and

$$Tg(x, \theta) = \frac{1}{\ell(x, \theta)} \int_{L(x, \theta)} g(y, \theta) \rho(y) dy.$$

Recall that the adjoint operator of M is the unique operator M^* that satisfies $\langle f, Mg \rangle = \langle M^* f, g \rangle_\mu$ for all $f \in L_2(\pi)$, $g \in L_2(\mu)$, see [Kre89, Thm. 3.9-2]. Since

$$\langle f, Mg \rangle = \frac{1}{\kappa_d} \int_K \int_{S^{d-1}} f(x) g(x, \theta) d\theta d\pi(x),$$

we obtain that, for all $\theta \in S^{d-1}$ and $x \in K$,

$$M^* f(x, \theta) = f(x).$$

This implies

$$MTM^* f(x) = \frac{1}{\kappa_d} \int_{S^{d-1}} \frac{1}{\ell(x, \theta)} \int_{L(x, \theta)} f(y) \rho(y) dy d\theta = Hf(x)$$

and thus, that M and T are the desired “building blocks” for Lemma 1. First of all, note that by Fubini’s Theorem the operator T is self-adjoint in $L_2(\mu)$. It remains to show that T is positive. We know that $L(x, \theta) = L(y, \theta)$ for all $y \in L(x, \theta)$. It follows that

$$\begin{aligned} T^2 g(x, \theta) &= \frac{1}{\ell(x, \theta)} \int_{L(x, \theta)} Tg(y, \theta) \rho(y) dy \\ &= \frac{1}{\ell(x, \theta)} \int_{L(x, \theta)} \frac{1}{\ell(y, \theta)} \int_{L(y, \theta)} g(z, \theta) \rho(z) dz \rho(y) dy \\ &= \frac{1}{\ell(x, \theta)^2} \int_{L(x, \theta)} g(z, \theta) \rho(z) dz \int_{L(x, \theta)} \rho(y) dy \\ &= Tg(x, \theta). \end{aligned}$$

Thus, T is a self-adjoint and idempotent operator on $L_2(\mu)$, which implies that T is a projection and, in particular, that it is positive, see e.g. [Kre89, Thm. 9.5-2]. Finally, Lemma 1 shows that H is positive.

3.2. Gibbs sampler. The Gibbs sampler, or specifically the random scan Gibbs sampler, is conceptually very similar to the hit-and-run algorithm. In each step, we choose a direction and sample with respect to ρ restricted to the chord in this direction. But, in contrast to the hit-and-run, we choose the direction from the d possible directions of the coordinate axes.

Let $e_1 = (1, 0, \dots, 0), \dots, e_d = (0, \dots, 0, 1)$ be the Euclidean standard basis in \mathbb{R}^d and $\ell(\cdot, \cdot)$ be from (1). The Markov operator G of the Gibbs sampler is given by

$$Gf(x) = \frac{1}{d} \sum_{j=1}^d \frac{1}{\ell(x, e_j)} \int_{L(x, e_j)} f(y) \rho(y) \, dy,$$

for all $f \in L_2(\pi)$. We follow almost the same lines as for the hit-and-run chain. Let m be the product measure of π and the uniform distribution on $[d] = \{1, \dots, d\}$. By $L_2(m)$ we denote the Hilbert space of functions $g: K \times [d] \rightarrow \mathbb{R}$ equipped with the inner product

$$\langle g_1, g_2 \rangle_m = \frac{1}{d} \sum_{j=1}^d \int_K g_1(x, j) g_2(x, j) \, d\pi(x)$$

for $g_1, g_2 \in L_2(m)$. We define the operators $M: L_2(m) \rightarrow L_2(\pi)$ and $T: L_2(m) \rightarrow L_2(m)$ by

$$Mg(x) = \frac{1}{d} \sum_{j=1}^d g(x, j)$$

and

$$Tg(x, j) = \frac{1}{\ell(x, e_j)} \int_{L(x, e_j)} g(y, j) \rho(y) \, dy.$$

By the same calculations as in Subsection 3.1 we obtain for all $f \in L_2(\pi)$, $x \in K$ and $j \in [d]$, that $M^*f(x, j) = f(x)$ and that $G = MTM^*$. It is easily seen that T is self-adjoint and idempotent. Hence, T is a projection and thus, positive, which proves the assertion by Lemma 1.

3.3. Slice sampler. For any $t \geq 0$ assume that R_t is the transition kernel of a Markov chain on the level set $K(t)$ of ρ , i.e.

$$K(t) = \{x \in K \mid \rho(x) \geq t\}.$$

Further let R_t be reversible with respect to U_t , the uniform distribution on $K(t)$, i.e.

$$U_t(A) = \frac{\text{vol}_d(A \cap K(t))}{\text{vol}_d(K(t))}, \quad A \subset K,$$

where vol_d denotes the d -dimensional Lebesgue measure. The slice sampler, starting from a state x works as follows: First choose a level t uniformly distributed in $[0, \rho(x)]$ and then sample the next state with respect to $R_t(x, \cdot)$ in the level set $K(t)$. If $R_t(x, \cdot) = U_t(\cdot)$ then the slice sampler is called simple slice sampler [MT02]. The corresponding Markov operator is defined by

$$Rf(x) = \frac{1}{\rho(x)} \int_0^{\rho(x)} R_t f(y) \, dt = \frac{1}{\rho(x)} \int_0^{\rho(x)} \int_{K(t)} f(y) R_t(x, dy) \, dt,$$

for all $f \in L_2(\pi)$. For any $t \geq 0$ we assume that R_t is a positive operator on $L_2(U_t)$, which is the set of all square integrable real functions with respect U_t on $K(t)$, i.e.

$$\langle R_t f, f \rangle_{U_t} = \int_{K(t)} R_t f(x) f(x) U_t(dx) \geq 0.$$

To show that R is positive, let

$$K_\rho = \{(x, t) \mid x \in K, t \in [0, \rho(x)]\} \subset \mathbb{R}^{d+1}$$

and let μ be the uniform distribution in K_ρ . Let $L_2(\mu)$ be the Hilbert space of functions $g: K_\rho \rightarrow \mathbb{R}$ with inner product

$$\langle g_1, g_2 \rangle_\mu = \int_{K_\rho} g_1(x, t) g_2(x, t) d\mu(x, t)$$

for $g_1, g_2 \in L_2(\mu)$. We define the operators $M: L_2(\mu) \rightarrow L_2(\pi)$ and $T: L_2(\mu) \rightarrow L_2(\mu)$ by

$$Mg(x) = \frac{1}{\rho(x)} \int_0^{\rho(x)} g(x, t) dt.$$

and

$$Tg(x, t) = \int_{K(t)} g(y, t) R_t(x, dy)$$

for $g \in L_2(\mu)$. The adjoint operator $M^*: L_2(\pi) \rightarrow L_2(\mu)$ is $M^*f(x, t) = f(x)$. The operator T is self-adjoint, since R_t is reversible with respect to U_t . For the positivity define $g_t(x) = g(x, t)$, $(x, t) \in K_\rho$. We have

$$\langle Tf, f \rangle_\mu = \int_0^\infty \langle R_t g_t, g_t \rangle_{U_t} \frac{\text{vol}_d(K(t))}{\text{vol}_{d+1}(K_\rho)} dt,$$

which implies positivity of T by the positivity of R_t . By the fact that $R = MTM^*$ and by Lemma 1 it is proven that R is positive.

3.4. Metropolis algorithm. Assume we have a positive proposal kernel B which is reversible with respect to U_0 , the uniform distribution in K . Then the Markov operator of the Metropolis algorithm is given by

$$Mf(x) = \int_K f(y) \alpha(x, y) B(x, dy) + \left(1 - \int_K \alpha(x, y) B(x, dy)\right) f(x)$$

where $\alpha(x, y) = 1 \wedge \frac{\rho(y)}{\rho(x)}$ and $f \in L_2(\pi)$. We interpret the Metropolis algorithm as a slice sampler. For $t \geq 0$, $x \in K(t)$ and $A \subset K$ define

$$R_t(x, A) = B(x, A \cap K(t)) + (1 - B(x, K(t))) \mathbf{1}_A(x).$$

Recall that

$$Rf(x) = \frac{1}{\rho(x)} \int_0^{\rho(x)} \int_{K(t)} f(y) R_t(x, dy) dt,$$

is the Markov operator of the slice sampler and that U_t is the uniform distribution in $K(t)$.

- Lemma 2.** (1) *If B is reversible with respect to U_0 , then R_t is reversible with respect to U_t for any $t \geq 0$.*
(2) *If B is positive on $L_2(U_0)$, then R_t is positive on $L_2(U_t)$ for any $t \geq 0$.*
(3) *The general slice sampler and the Metropolis algorithm coincide, i.e. $Rf = Mf$ for $f \in L_2(\pi)$.*

Proof. We have for any $f, g \in L_2(U_t)$ that

$$\begin{aligned} \langle R_t f, g \rangle_{U_t} &= \int_{K(t)} \int_{K(t)} f(y) g(x) \mathbf{1}_{K(t)}(y) B(x, dy) U_t(dx) \\ &\quad + \int_{K(t)} (1 - B(x, K(t))) f(x) g(x) U_t(dx) \\ &= \langle B(\mathbf{1}_{K(t)} f), \mathbf{1}_{K(t)} g \rangle_{U_0} \frac{\text{vol}_d(K)}{\text{vol}_d(K(t))} \\ &\quad + \int_{K(t)} (1 - B(x, K(t))) f(x) g(x) U_t(dx). \end{aligned}$$

By using the self-adjointness of B on $L_2(U_0)$ we obtain that R_t is self-adjoint on $L_2(U_t)$ for any $t \geq 0$, which proves (1). Assertion (2) follows by similar arguments. One obtains

$$\begin{aligned} \langle R_t f, f \rangle_{U_t} &= \langle B(\mathbf{1}_{K(t)} f), \mathbf{1}_{K(t)} f \rangle_{U_0} \frac{\text{vol}_d(K)}{\text{vol}_d(K(t))} \\ &\quad + \int_{K(t)} (1 - B(x, K(t))) f(x)^2 U_t(dx), \end{aligned}$$

which, by using the positivity of B , proves the positivity of R_t . Note that the Markov operator of the slice sampler can be written as

$$\begin{aligned} Rf(x) &= \frac{1}{\rho(x)} \int_0^{\rho(x)} \int_{K(t)} f(y) B(x, dy) dt \\ &\quad + \frac{f(x)}{\rho(x)} \int_0^{\rho(x)} \mathbf{1}_{K(t)}(x) (1 - B(x, K(t))) dt \\ &= \frac{1}{\rho(x)} \int_K \int_0^\infty \mathbf{1}_{K(t)}(x) \mathbf{1}_{K(t)}(y) dt f(y) B(x, dy) \\ &\quad + f(x) \left(1 - \frac{1}{\rho(x)} \int_K \int_0^\infty \mathbf{1}_{K(t)}(x) \mathbf{1}_{K(t)}(y) dt B(x, dy) \right). \end{aligned}$$

Then (3) follows by

$$\frac{1}{\rho(x)} \int_0^\infty \mathbf{1}_{K(t)}(x) \mathbf{1}_{K(t)}(y) dt = \alpha(x, y).$$

□

Note that, by the previous lemma all assumptions of Subsection 3.3 are satisfied if we additionally assume that B is positive. Hence, the Metropolis algorithm defines a positive Markov operator if the proposal is positive.

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