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On constrained simulation and optimization by Metropolis chains

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Abstract

Given an everywhere positive probability measure π on a finite state space E and the associated energy function H, this note gives convergence results for time-inhomogeneous Metropolis chains which are used to simulate π or minimize H under some constraints.

Keywords : Constrained simulation; constrained optimization; Metropolis algorithm

1 Introduction and notations

Let π be an everywhere positive probability measure on a finite state space E given by $\pi(x) = Z^{-1}\exp[-H(x)]$ where $H : E \to \mathbb{R}$ is the associated *energy* function. Assume that we are interested in some subset $E_c \subset E$ defined by a constrained equation $E_c := \{J = 0\}$ where the function of constraints $J : E \to \mathbb{R}^+$ is otherwise positive. Let π_c be the restriction of π on E_c : $\pi_c(x) = 1_{E_c}(x)Z_c^{-1}\exp[-H(x)]$ (throughout the note, the letter Z is used to denote generic normalizing factors). We consider the following two problems:

1. Problem **[S]**: simulate the distribution π_c.
2. Problem **[M]**: minimize H over E_c.

To solve these problems, Markov chains endowed with a time-inhomogeneous Metropolis dynamic is a natural idea. Let (β_k), (λ_k) be two positive non decreasing sequences and q a *symmetric* and *irreducible* Markov transition kernel on E and set

$$H_k(x) := \beta_k[H(x) + \lambda_k J(x)]\ , k \geq 1\ . \tag{1}$$

The transition probability kernel at time k of such an inhomogeneous Markov chain $(X_k)_{k\geq 0}$ is given by the following Metropolis rule (we write a^+ for $\max(a, 0)$):

$$P_k(x,y) = \begin{cases} q(x,y)e^{-[H_k(y)-H_k(x)]^+}, & y \neq x, \\ 1 - \sum_{z\neq x} P_k(x,z), & y = x. \end{cases} \tag{2}$$

It is easy to check that for each k, P_k is irreducible and reversible with respect to the probability measure (hereafter p.m.)

$$\pi_k(x) = Z_k^{-1}\exp[-H_k(x)]\ ,$$

and consequently, π_k is the unique invariant probability measure (i.p.m) of P_k. Let us set

$$H_0 \quad := \quad \min\{H(x) : x \in E_c\}, \quad E_0 := \{x \in E_c\ :\ H(x) = H_0\},$$

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which are respectively the constrained minimum value and the set of constrained minimum points of H. We also denote by π_0 the uniform distribution on E_0. It is straightforward to find that

$$\begin{aligned} \text{with } \beta_k \equiv 1, \lambda_k \uparrow \infty, \qquad \lim_{k\to\infty} \pi_k(x) &= \pi_c(x), \qquad x \in E, & (3)\\ \text{with } \beta_k \uparrow \infty, \lambda_k \uparrow \infty, \qquad \lim_{k\to\infty} \pi_k(x) &= \pi_0(x), \qquad x \in E. & (4) \end{aligned}$$

Let us set $P^{(m,k)} = P_{m+1} \cdots P_k$, the transition probabilities from time m to k ($k > m$). The aim of this note is to establish conditions on the control sequences (β_k) and (λ_k) which guarantee that the chain (X_k) is strongly ergodic in the following sense ((Isaacson and Madsen, 1976)): there is some p.m. π_∞ on E such that

$$\text{for all } m \geq 1, \quad \lim_{k\to\infty} \sup_\mu ||\mu P^{(m,k)} - \pi_\infty|| = 0 \ . \tag{5}$$

Here $||\cdot||$ is the total variation distance and the supremum is taken over all p.m.'s on E. The target measure π_∞ will be π_c or π_0 according to the considered problem. In other words, under ergodicity, the inhomogeneous Markov chain (X_k) endowed with the dynamic defined in (1)-(2)-(3) will simulate the constrained distribution π_c, while with the dynamic defined in (1)-(2)-(4), the chain provides a minimizing sequence of H over E_c.

The class of Metropolis chains has become a widely used tool for simulation or optimization problems. We refer to (Metropolis et al., 1953; Kirkpatrick et al., 1983; Hasting, 1970) for original accounts, and to (Aarts and Korst, 1989; Azencott, 1992; Tierney, 1994; Geman, 1990; Guyon, 1995) for recent and synthetic reviews on the subject. Nevertheless, most of these references concern the *unconstrained* case, except (Aarts and Korst, 1989) and (Geman, 1990). Actually (Aarts and Korst, 1989) has examined several combinatorial optimization problems with constraints, but without giving any theoretical results on the convergence of the underlying Markov chains in this constrained case. The only convergence results we are aware of are found in (Geman, 1990) (see also (Geman and Geman, 1987)) where the authors proposed a solution to the problems **[S]** and **[M]** by using the Gibbs sampler when the state space is a product space, i.e. $E = \Pi_{s\in S} F_s$ for some finite space of sites S and individual state spaces (F_s). However, Gibbs sampling is no more suited to general state space E considered here and instead, we need Metropolis-type dynamics. This note, inspired by (Geman, 1990), is intended to establish convergence results for constrained Metropolis chains on a general (though finite) state space.

We will denote by $|F|$ the cardinal number of any finite set F. For illustration purpose, let us consider the graph coloring problem. Given an undirected graph $\mathcal{G} = (V, \mathcal{E})$ with vertex set V and edge set $\mathcal{E}$, the problem is to find a *minimal coloring* such that (1) no neighboring vertices have a same coloring and (2) the total number of used colors is minimal. A standard coding of this problem is to consider the set E of all possible colorings, i.e. partitions $x = (V_1, \ldots, V_K)$ of V where V_i stands for the set of vertices colored with color i (K is some known upper bound for number of colors). Let $J(x)$ be the number of pairs of neighboring vertices colored with a same color in x, that is

$$J(x) = J(V_1, \ldots, V_K) = \text{card}\,\{\{u, v\} : \{u, v\} \in \mathcal{E} \text{ and for some } i,\ u \in V_i \text{ and } v \in V_i\} \ .$$

Therefore (see e.g. (Aarts and Korst, 1989), p. 82-86 for additional details), it is possible to find a weight sequence $w_1 > \ldots > w_K > 0$ such that the problem is equivalent to

$$\text{Minimize } H(x) = -\sum_{i=1}^{K} w_i |V_i| \ , \quad \text{subject to the constraint } J(x) = 0 \ .$$

The results we will derive can be applied to this problem where it is worth noting that the state space E is not a product space.

2 Main steps

Our approach as that of (Geman, 1990) is based on Dobrushin's ergodicity coefficients (Dobrushin, 1956). More precisely, the ergodicity coefficient of a Markov kernel Q is defined as

$$a(Q) := \min_{x,x' \in E} \sum_{y \in E} Q(x,y) \wedge Q(x',y). \tag{6}$$

By taking into account the convergences (3)-(4), a well-known result (see e.g. (Isaacson and Madsen, 1976)) implies that the ergodicity (5) is ensured if the following two conditions are satisfied:

(C1) $\sum_{k \geq 1} ||\pi_{k+1} - \pi_k|| < \infty$;

(C2) for some positive integer p, $\sum_{k=1}^{\infty} a(P_{kp+1} \cdots P_{(k+1)p}) = \infty$.

Furthermore, if we subtract H_0 from the energy function H, neither the P_k's nor the π_k's are changed. Therefore we will hereafter assume $H_0 = 0$ without loss of generality.

To solve the problem **[S]**, the sequence (β_k) is kept constant: $\beta_k \equiv 1$ while (λ_k) will be a sequence of positive numbers increasing to infinity. On the other hand, to solve the problem **[M]**, both the sequences are required to increase to infinity (see Eqs. (3)-(4)). We examine in more details the conditions **(C1)-(C2)** for these two problems.

3 Condition (C1) on invariant probability measures (π_k)

We first give a lemma which is an easy adaptation from Corollary 3.1 of (Geman, 1990). Since the proof is short, we provide it for the convenience of the readers.

Lemma 1 ((Geman, 1990)) *The condition (C1) is fulfilled if the following conditions are themselves fulfilled :*

(a) *For all $x \in E$, there is an integer k_0 such that for all $k \geq k_0$, $H_k(x) \leq H_{k+1}(x)$.*

(b) *There is some $x_0 \in E$ for which $\sup_{k \geq 1} H_k(x_0) < \infty$.*

Proof. Since

$$\sum_{k\geq 1}||\pi_{k+1}-\pi_k|| = \sum_{k\geq 1}\sum_{x\in E}|\pi_{k+1}(x)-\pi_k(x)|\,,$$

it is enough to establish that for all x, $\sum_{k\geq 1}|\pi_{k+1}(x)-\pi_k(x)|<\infty$. Let $x\in E$ be fixed and $u_k=\exp[-H_k(x)]$. We have

$$\begin{aligned}|\pi_{k+1}(x)-\pi_k(x)| &= (Z_kZ_{k+1})^{-1}\,|u_{k+1}Z_k-u_kZ_{k+1}| \\ &\leq (Z_kZ_{k+1})^{-1}\{u_{k+1}\,|Z_{k+1}-Z_k|+Z_{k+1}\,|u_{k+1}-u_k|\} \\ &\leq (\inf_k Z_k)^{-2}\{[\sup_k u_k]\,|Z_{k+1}-Z_k|+[\sup_k Z_k]\,|u_{k+1}-u_k|\}\end{aligned}$$

By **(a)**, $\sup_k u_k<\infty$ and as E is finite, $\sup_k Z_k<\infty$. Furthermore by **(b)**, $\inf_k Z_k\geq \exp\{-\sup_k H_k(x_0)\}>0$. The conclusion follows by taking into account that the sequences (Z_k) and (u_k) are positive and decreasing for large k. ■

By using this lemma, we now prove that

Proposition 1 *Condition (C1) is fulfilled for both problems [S] and [M] without any additional assumption.*

Proof. **The simulation problem [S].** Recall that $\beta_k\equiv 1,\lambda_k\uparrow\infty$ for this problem so that $H_k(x)=H(x)+\lambda_kJ(x)$. Since $J(x)\geq 0$, **(a)** clearly holds. On the other hand, **(b)** is satisfied with any $x_0\in E_c$ for which $J(x_0)=0$ and $H_k(x_0)\equiv H(x_0)$.

The optimization problem [M]. Here we have $H_k(x)=\beta_k[H(x)+\lambda_kJ(x)]$ with $\beta_k\uparrow\infty$ and $\lambda_k\uparrow\infty$.

- Condition **(a)** : for $x\in E_c$, $J(x)=0$ and $H(x)\geq H_0=0$, hence $H_k(x)$ is non decreasing. For $x\notin E_c$ but $H(x)\geq 0$, the same holds. It remains to consider the x's such that $x\notin E_c$ and $H(x)<0$. We have

  $$H_{k+1}(x)-H_k(x)=(\beta_{k+1}-\beta_k)\,[H(x)+\lambda_{k+1}J(x)]+\beta_k\,(\lambda_{k+1}-\lambda_k)\,J(x)\,.$$

  This difference is positive for large k, since $J(x)>0$, $\beta_{k+1}>\beta_k$ and $\lambda_k\uparrow\infty$.

- Condition **(b)** is satisfied for any $x_0\in E_0$ for which $H(x_0)=J(x_0)=0$. ■.

4 Condition (C2) on the ergodicity coefficients

We write $Q>0$ for a Markov kernel Q on E satisfying $Q(x,y)>0,\ \forall(x,y)$. Let be:

$$\begin{aligned}\delta_H &:= \max\left\{[H(y)-H(x)]^+ :\quad x,y\in E,\quad q(x,y)>0\right\},\\ \delta_J &:= \max\left\{[J(y)-J(x)]^+ :\quad x,y\in E,\quad q(x,y)>0\right\},\\ \gamma &:= \min\left\{q(x,y) :\quad x,y\in E,\quad q(x,y)>0\right\},\\ \partial x &:= \left\{y\in E\ :\quad q(x,y)>0\right\}.\end{aligned}$$

We first prove two auxiliary lemmas.

Lemma 2 *Consider the Metropolis algorithm with transition probabilities* (P_k) *defined in (2) For both the problems* ***[S]*** *and* ***[M]****, there are two positive integers* p*,* k_0 *such that*

$$\textit{for all} \quad k \geq k_0, \quad P^{(k,k+p)} > 0 \; . \tag{7}$$

Proof. *Case 1.* If the kernel q is aperiodic, q is positive recurrent since E is finite. Therefore there is an integer $p > 0$ such that $q^p > 0$. Since for all x, y and j,

$$P_j(x,y) \geq q(x,y)\; e^{-[H_j(y)-H_j(x)]^+} \geq q(x,y)\; e^{-\beta_j(\delta_H+\lambda_j\delta_J)} \;,$$

we get for all k,

$$P^{(k,k+p)}(x,y) \geq q^p(x,y)\; e^{-(\beta_{k+1}+\cdots+\beta_{k+p})(\delta_H+\lambda_{k+p}\delta_J)} > 0.$$

Case 2. Otherwise, let q be a periodic kernel with period d. Since q is irreducible, there is a partition $E = E_1 + \cdots + E_d$ such that the iterated kernel q^d is positive recurrent on each subclass E_j. We can then find a s_0 such that for all $s \geq s_0$, $q^{sd}(x,y) > 0$ if (and only if) x, y are two points in a same subclass.

On the other hand, let us take a point $a \in E_c$ for which there is a $b \in \partial a$ but not in E_c. This is always possible since q is irreducible and $E_c \neq E$. Therefore, $H_k(a) = \beta_k H(a) < \beta_k[H(b) + \lambda_k J(b)]$ for large enough k for both problems. Hence there is a k_0 such that $P_k(a,a) > 0$ for all $k \geq k_0$. It follows that for $p = 2s_0 d + d - 1$ and $k \geq k_0$, we have $P^{(k,k+p)}(x,y) > 0$, for all x, y. ■

In the sequel, we will write p for the smallest integer satisfying (7).

Lemma 3 *With the same assumptions made in Lemma 2, there is an integer* k_1 *such that for all* $k \geq k_1$*, we have*

$$a\left(P^{(k,k+p)}\right) \geq \gamma^p |E|\; e^{-p\beta_{k+p}\left(\delta_H+\lambda_{k+p}\delta_J\right)}. \tag{8}$$

Proof. By Lemma 2, for $k \geq k_0$ and $(a,b) \in E^2$, there is a path $a = a_0 \to a_1 \to \cdots \to a_p = b$ for which $P_{k+p-j}(a_j, a_{j+1}) > 0,\ 0 \leq j < p$. It is thus enough to prove that for large enough k

$$P_k(x,y) > 0 \quad \text{implies that} \quad P_k(x,y) \geq \gamma\; e^{-\beta_k(\delta_H+\lambda_k\delta_J)} \;, \tag{9}$$

since in this case, we actually have $P^{(k,k+p)}(a,b) \geq \gamma^p\; e^{-p\beta_{k+p}\left(\delta_H+\lambda_{k+p}\delta_J\right)}$, and the required result (8) follows.

Let us prove (9). For $x \neq y$ or $x = y$ with $q(x,x) > 0$, we have for all k,

$$P_k(x,y) \geq q(x,y) e^{-[H_k(y)-H_k(x)]^+} \geq \gamma\; e^{-\beta_k(\delta_H+\lambda_k\delta_J)}.$$

A more intricate case concerns those transition probabilities $P_k(x,x)$ for which $q(x,x) = 0$. Let us recall that

$$0 < P_k(x,x) = \sum_{z \neq x} q(x,z)\; \left(1 - e^{-[H_k(z)-H_k(x)]^+}\right).$$

There is then some $z_0 \in \partial x$ s.t. $H_k(z_0) - H_k(x) = \beta_k\left\{H(z_0) - H(x) + \lambda_k[J(z_0) - J(x)]\right\} > 0$. On the other hand, if (x', z') are some neighboring points belonging to the set

$$G := \{(x',z') \;:\; z' \in \partial x',\ J(z') < J(x') \quad \text{or} \quad \{J(z') = J(x') \quad \text{and} \quad H(z') \leq H(x')\}\ \},$$

there is an integer $m(x', z')$ such that $H_k(z') \leq H_k(x')$ for all $k \geq m(x', z')$. Let be $m^* := \max_{(x',z') \in G} m(x', z')$. For z_0 defined above and $k \geq m^*$, since $H_k(z_0) - H_k(x) > 0$, $(x, z_0) \notin G$ and hence one of the following holds

$$(i).\ J(z_0) > J(x), \quad \text{or} \quad (ii).\ J(z_0) = J(x) \quad \text{with} \quad H(z_0) > H(x).$$

In the first case, we get $H_k(z_0) - H_k(x) \to \infty$ and

$$P_k(x, x) \geq q(x, z_0)[1 - e^{-[H_k(z_0) - H_k(x)]}] \to q(x, z_0).$$

And in the second case, we have $H_k(z_0) - H_k(x) \geq \beta_1[H(z_0) - H(x)]$ and

$$P_k(x, x) \geq q(x, z_0)[1 - e^{-[H_k(z_0) - H_k(x)]}] \geq q(x, z_0)[1 - e^{-\beta_1[H(z_0) - H(x)]}].$$

Since these lower bounds are positive and independent of k, and $\gamma\ e^{-\beta_k(\delta_H + \lambda_k \delta_J)} \to 0$, there is an integer $n(x) \geq m^*$ such that for all $k \geq n(x)$,

$$P_k(x, x) \geq \gamma\ e^{-\beta_k(\delta_H + \lambda_k \delta_J)}\ .$$

Taking $k_1 = k_0 \vee \max_x n(x)$ proves the inequality (9). ■

An immediate consequence of the last lemma is that the condition (**C2**) is fulfilled if

$$\sum_{k=1}^{\infty} e^{-p\beta_{(k+1)p}[\delta_H + \lambda_{(k+1)p}\delta_J]} = \infty. \tag{10}$$

5 Main results

Summarizing the results established in the previous sections gives the following main results of this note.

Theorem 1 *Consider the Metropolis algorithm with (P_k) defined in (1)-(2)-(3) with $\beta_k \equiv 1$ and $\lambda_k \uparrow \infty$. Let p be the smallest integer satisfying (7). The underlying inhomogeneous Markov chain $(X_k)_{k \geq 0}$ is strongly ergodic with limit p.m. π_c if the control sequence (λ_k) fulfills the following condition :*

$$\sum_{k=1}^{\infty} e^{-p\lambda_{kp}\delta_J} = \infty. \tag{11}$$

Theorem 2 *Consider the Metropolis algorithm with (P_k) defined in (1)-(2)-(4) with $\beta_k \uparrow \infty$ and $\lambda_k \uparrow \infty$. Let p be the smallest integer satisfying (7). The underlying inhomogeneous Markov chain $(X_k)_{k \geq 0}$ is strongly ergodic with limit p.m. π_0 if the control sequences (β_k) and (λ_k) fulfill the condition (10).*

It is worth noting that the condition (11) is satisfied for a logarithmic sequence $\lambda_k = c\log(k + D)$ with some constants $D > 0$ and $0 < c \leq (p\delta_J)^{-1}$, while the condition (10) is fulfilled for sequences $\beta_k \uparrow \infty$, $\lambda_k \uparrow \infty$ satisfying $\beta_k\lambda_k = c\log(k + D)$ with some constants $D > 0$ and $0 < c < (p\delta_J)^{-1}$.

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