

Estimation of the Entropy Rate of Ergodic Markov Chains

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Abstract. In this paper an approximation for entropy rate of an ergodic Markov chain via sample path simulation is calculated. Although there is an explicit form of the entropy rate here, the exact computational method is laborious to apply. It is demonstrated that the estimated entropy rate of Markov chain via sample path not only converges to the correct entropy rate but also does it exponentially fast.

Keywords. Entropy rate, ergodic Markov chain, exponential convergence, simulation.

MSC: 60J10, 94A17

1 Introduction

In probability theory, entropy is introduced by Shannon (1948). The entropy of a distribution P taking values from a finite set E is defined by him as

$$H(P) = - \sum_{i \in E} P_i \log P_i, \quad (1)$$

with the convention $0 \log 0 = 0$. This definition can be obviously extended to any other countable set. Consider a Markov chain with a state set X and a state transition probability matrix \mathbf{P} . The probability of a transition from the state $x \in X$ to the state $y \in X$ is denoted as

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P_{xy} . The Shannon entropy rate of the Markov chain is

$$H(\mathcal{X}) = \lim_{n \rightarrow \infty} \frac{H(X_1, X_2, \dots, X_n)}{n}, \quad (2)$$

where X_t is a random variable demonstrating the state at time t , and $H(X_1, X_2, \dots, X_n)$ is the joint entropy of (X_1, X_2, \dots, X_n) with the joint distribution $P(x_1, x_2, \dots, x_n)$ where

$$\begin{aligned} & H(X_1, X_2, \dots, X_n) \\ &= - \sum_{x_1 \in X} \sum_{x_2 \in X} \dots \sum_{x_n \in X} P(x_1, x_2, \dots, x_n) \log P(x_1, x_2, \dots, x_n) \quad (3) \\ &= -\mathbf{E}_{X_1, X_2, \dots, X_n} \log P(X_1, X_2, \dots, X_n). \end{aligned}$$

Shannon (1948) proved the convergence in probability of $-\frac{1}{n} \log P(x_1, x_2, \dots, x_n)$ to $H(\mathcal{X})$. The convergence in mean for any stationary ergodic process with a finite state space is illustrated by McMillan (1953). In sequence, the extension to a countable state set was made by Carleson (1958) for the convergence in mean and by Chung (1961) for the almost sure convergence.

Courbage and Saberi Fathi (2008) have computed the entropy functionals for non-stationary distributions of particles of Lorentz gas and hard disks.

Based on our best knowledge, the entropy rate of Markov chain with infinite state space has not been achieved yet. In this paper we have succeeded in obtaining entropy rate of Markov chain by conditioning on its probability transition matrix. The achieved entropy rate is very close to the real one. Our study concentrates on the estimation of the entropy rate of the Markov chain. This paper is organized as follows: section 2 includes some required preliminaries, and considers two assumptions. Section 3 is the most important section and the theorem is proved there. In section 4 the entropy rate of a birth and death chain as a Markov chain is included.

2 Preliminaries

In this paper an ergodic Markov chain with countable state set X is analyzed where the weakest ergodicity of condition for the finite Markov chains is:

Assumption 2.1. *There exists a positive number $\alpha < 1$ such that*

$$\sup_{x, x' \in X} \sum_{y \in X} |P_{xy} - P_{x'y}| \leq 2\alpha. \tag{4}$$

This assumption implies that there exists a unique stationary distribution ρ over X . Also, for a countable Markov chain to be an ergodic chain, we need another assumption :

Assumption 2.2. *For any $x \in X$*

$$|\{y | P_{xy} \neq 0\}| < \infty. \tag{5}$$

Suppose that a given Markov chain is not ergodic. For finite state set X , we can add an artificial state \hat{x} to X such that \hat{x} is reachable from any state x with a probability very close to zero. Hence, we can transform the given Markov chain into a new Markov chain, and an optimal solution for the new Markov chain can also approximate an optimal solution for the original Markov chain very closely.

For an ergodic stochastic process X , Cover (2006) proved that

$$H(\mathcal{X}) = \lim_{n \rightarrow \infty} H(X_n | X_{n-1}, \dots, X_1), \tag{6}$$

and for the homogeneous ergodic Markov chain one can show

$$H(\mathcal{X}) = H(X_2 | X_1), \tag{7}$$

so we can conclude easily

$$H(\mathcal{X}) = \sum_{x \in X} \rho(x) S(x), \tag{8}$$

where

$$S(x) = - \sum_{y \in X} P_{xy} \log P_{xy}, \tag{9}$$

and $\rho(x)$ is the unique stationary distribution of state $x \in X$.

To obtain $H(\mathcal{X})$ computing the stationary distribution ρ is essential. Unfortunately, obtaining exactly the stationary distribution ρ is difficult where X is large. In general, direct method extracted from the standard Gaussian elimination often suffers from fill-in phenomenon and iterative method from a slow convergence that one can see in Gambin and Pokarowski (2001). If the given Markov chain has geometric ergodicity (e.g., Assumption 2.1), the convergence rate to the stationary distribution from the iterative multiplication of P is fast or geometric

(refer to Meyn and Tweedie (1993)). With an approximation of the stationary distribution ρ , $H(\mathcal{X})$ by a simple summation can be estimated. A sample path simulation with relatively sparse \mathbf{P} is considered.

3 Main Result

Consider a set of $\{x_1, x_2, \dots, x_n\}$ as a sample path where $x_i \in X$ for any $1 \leq i \leq n$. Let

$$N_n(i) := \sum_{t=1}^n 1_{\{x_t=x_i\}}, \quad (10)$$

where $1_{\{x_t=x_i\}} = \begin{cases} 1 & x_t = x_i \\ 0 & x_t \neq x_i \end{cases}$. $\frac{1}{n}N_n(i)$ is an estimator for $\rho(i)$.

Define

$$\hat{H}_n(x) = \sum_{i \in X} \frac{N_n(i)}{n} S(i), \quad X_0 = x, \quad (11)$$

as an estimator for the entropy rate of Markov chain via sample path simulation.

Theorem 3.1. *Assume that Assumption 2.1 and Assumption 2.2 are held. Let $C = 2M/(1 - \alpha)$ where $M = \log \sup_{x \in X} |\{y | P_{xy} \neq 0\}|$. For a given $\epsilon > 0$ and for any fixed $x \in X$, if $N > 2C/\epsilon$, then there exists $\beta > 0$ such that*

$$Pr\{|\hat{H}_N(x) - H(\mathcal{X})| > \epsilon\} \leq \exp(-\beta N). \quad (12)$$

Proof. The proof of here is adapted from the proof of Theorem 2.1 in Chang (2004). Let $\rho^n(y|x)$ denote the probability that state y is reached from state x in n -steps and ρ be the unique stationary distribution of the Markov chain. Then

$$\begin{aligned} \left| \sum_{y \in X} S(y)(\rho^n(y|x) - \rho(y)) \right| &\leq \sum_{y \in X} |S(y)| |\rho^n(y|x) - \rho(y)| \\ &\leq M \cdot \left(\sum_{y \in X} |\rho^n(y|x) - \rho(y)| \right) \leq 2M\alpha^n, \end{aligned} \quad (13)$$

where the last inequality follows from Lemma 3.3 in Hernandez-Lerma (1989).

Let

$$\xi(x) := \sum_{n=0}^{\infty} \sum_{y \in X} S(y)(\rho^n(y|x) - \rho(y)). \tag{14}$$

The property of $\sum_{y \in X} \rho(y)S(y) = H(\mathcal{X})$, ξ satisfies that

$$\xi(y) + H(\mathcal{X}) = S(y) + \sum_{z \in X} P_{yz}\xi(z). \tag{15}$$

Define $M_n := \xi(X_n) - E[\xi(X_n)|X_0, \dots, X_{n-1}]$ with $X_0 = x$. From (15)

$$\xi(X_n) + H(\mathcal{X}) = S(X_n) + E[\xi(X_{n+1})|X_n, \dots, X_0]. \tag{16}$$

By some algebraic manipulation on (15), we have

$$\begin{aligned} \sum_{n=1}^N M_n + \xi(X_0) - \xi(X_N) &= \sum_{n=1}^N S(X_n) - NH(\mathcal{X}) \\ &= \sum_{i=1}^{\infty} N_N(i)S(i) - NH(\mathcal{X}) \\ &= N(\widehat{H}_N(x) - H(\mathcal{X})) \quad X_0 = x. \end{aligned} \tag{17}$$

It follows by

$$\begin{aligned} &E[\exp(N(\widehat{H}_N(x) - H(\mathcal{X})))] \\ &\leq \exp(2\|\xi\|)E[\exp(\sum_{n=1}^{N-1} M_n)]E[\exp(M_N)|X_0, \dots, X_{N-1}] \\ &\leq \exp(2\|\xi\|)E[\exp(\sum_{n=1}^{N-1} M_n)] \exp(\Phi(2\|\xi\|)\sigma^2), \end{aligned} \tag{18}$$

where $\sigma^2 \geq E[M_N^2|X_0, \dots, X_{N-1}]$ and $\Phi(a) = (e^a - a - 1)/a^2$ if $a \neq 0$ and 0.5 otherwise. In Appendix A, the last inequality is proved.

By recursive applications we have

$$E[\exp(N(\widehat{H}_N(x) - H(\mathcal{X})))] \leq \exp(2\|\xi\| + N\Phi(2\|\xi\|)\sigma^2), \tag{19}$$

and by Markov's inequality

$$\begin{aligned} &Pr\{\exp(N(\widehat{H}_N(x) - H(\mathcal{X}))) \geq \exp(N\epsilon)\} \\ &\leq \exp(2\|\xi\| + N\Phi(2\|\xi\|)\sigma^2) / \exp(N\epsilon), \end{aligned} \tag{20}$$

so

$$\begin{aligned} Pr\{\widehat{H}_N(x) - H(\mathcal{X}) \geq \epsilon\} &\leq \exp(2\|\xi\| + N\Phi(2\|\xi\|)\sigma^2 - N\epsilon) \\ &= \exp(2\|\xi\| - N\epsilon + N\sigma^2 \frac{e^{2\|\xi\|} - 2\|\xi\| - 1}{4\|\xi\|^2}). \end{aligned} \quad (21)$$

Let $\sigma^2 = 4\|\xi\|^2$

$$\begin{aligned} Pr\{\widehat{H}_N(x) - H(\mathcal{X}) \geq \epsilon\} &\leq \exp(2\|\xi\| - N\epsilon + N(e^{2\|\xi\|} - 2\|\xi\| - 1)) \\ &= \exp(-N(\frac{-2\|\xi\|}{N} - e^{2\|\xi\|} + 2\|\xi\| + 1 + \epsilon)) \\ &= \exp(-\beta N), \end{aligned} \quad (22)$$

where $\beta = \frac{-2\|\xi\|}{N} - e^{2\|\xi\|} + 2\|\xi\| + 1 + \epsilon > 0$ if $N > 2C/\epsilon$. Note that $\|\xi\| \leq C = \frac{2M}{1-\alpha}$.

For the proof of other tail, let

$$\xi(x) := \sum_{n=0}^{\infty} \sum_{y \in X} S(y)(\rho(y) - \rho^n(y|x)). \quad (23)$$

then we have

$$\sum_{n=1}^N M_n + \xi(X_0) - \xi(X_N) = N(H(\mathcal{X}) - \widehat{H}_N(x)) \quad X_0 = x. \quad (24)$$

Now with the similar reasoning, $Pr\{H(\mathcal{X}) - \widehat{H}_N(x) > \epsilon\} \leq \exp(-\beta N)$ can be proved

4 Numerical example

Consider a birth and death chain with one reflecting barrier over $X = \{0, 1, 2, \dots\}$ with following parameters

$$P_{x \ x+1} = \frac{x+2}{(x+3)^2}, \quad P_{x \ x-1} = \frac{1}{x+1}, \quad P_{x \ x} = 1 - p_x - q_x, \quad (25)$$

where $x \geq 1$ and $p_0 = 1$. We get $p_x := P_{x \ x+1}$, $q_x := P_{x \ x-1}$ and $r_x := P_{x \ x}$. In this paper a Markov chain that satisfies Assumption

2.1 and Assumption 2.2 is required. This birth and death chain satisfies Assumption 2.2 with $M = 3$. We use Lemma 4.1 from Bermaud (1998) to satisfy Assumption 2.1.

Lemma 4.1. *A birth and death chain with parameters p_x, q_x and r_x , has unique stationary distribution if and only if*

$$\sum_{i=2}^{\infty} \frac{p_1 \dots p_{i-1}}{q_1 q_2 \dots q_i} < \infty. \tag{26}$$

One can obtain the unique stationary distribution of this chain from

$$\begin{cases} \rho(1) = \rho(0) \frac{1}{q_1} \\ \rho(i) = \rho(0) \frac{p_1 \dots p_{i-1}}{q_1 q_2 \dots q_i} \quad i \geq 2 \\ \sum_{i=0}^{\infty} \rho(i) = 1 \end{cases} \tag{27}$$

Also consider a birth and death chain with two reflecting barriers over $X = \{0, 1, 2, \dots, k\}$ with following parameters p_x, q_x and r_x (25), where $x \in \{1, 2, \dots, k - 1\}$ and $p_0 = q_k = 1$.

This chain satisfies Assumption 2.1 and Assumption 2.2. The unique stationary distribution of this chain was obtained from

$$\begin{cases} \rho(1) = \rho(0) \frac{1}{q_1} \\ \rho(i) = \rho(0) \frac{p_1 \dots p_{i-1}}{q_1 q_2 \dots q_i} \quad 2 \leq i \leq k \\ \sum_{i=0}^k \rho(i) = 1 \end{cases} \tag{28}$$

So we can compute the entropy rate of these chains directly. The entropy rate of the birth and death chain with one reflecting barrier chain is

$$H := H(\mathcal{X}) = - \sum_{i=0}^{\infty} \rho(i) S(i).$$

Calculating the above series follows

$$- \sum_{i=0}^{\infty} \rho(i) S(i) = 0.6924620 + \varepsilon, \quad \text{for } \varepsilon \leq 10^{-6}, \tag{29}$$

More details are mentioned in Appendix B. Note that in this section we obtain results 7-decimally and due to the noncontrollable calculations,

there are some errors. Now we try to estimate $H(\mathcal{X})$ with samples in table 1 and table 2.

Table 1: \hat{H}_N for $|X| = 10$

| $ X $ | 10 | | | |
|---------------|-----------|-----------|-----------|-----------|
| H | 0.7813217 | | | |
| N | 10^4 | 10^5 | 10^6 | 10^7 |
| \hat{H}_N | 0.7859416 | 0.7836277 | 0.7815468 | 0.7814328 |
| | 0.7749093 | 0.7815980 | 0.7805482 | 0.7814196 |
| | 0.7838243 | 0.7815555 | 0.7811086 | 0.7810723 |
| | 0.7798157 | 0.7806728 | 0.7807021 | 0.7812658 |
| | 0.7855056 | 0.7839759 | 0.7808171 | 0.7814986 |
| | 0.7822891 | 0.7813946 | 0.7817993 | 0.7814496 |
| | 0.7828118 | 0.7800310 | 0.7812329 | 0.7814329 |
| | 0.7781985 | 0.7828447 | 0.7803726 | 0.7811364 |
| | 0.7798441 | 0.7813342 | 0.7813246 | 0.7812238 |
| | 0.7852608 | 0.7803726 | 0.7810109 | 0.7813408 |
| \hat{H}_N^* | 0.7818401 | 0.7817407 | 0.7810463 | 0.7813273 |

Table 2: \hat{H}_N for $|X| = 100$ and $|X| = 1000$

| $ X $ | 100 | | | 1000 | | |
|---------------|-----------|-----------|-----------|-----------|-----------|-----------|
| H | 0.7165776 | | | 0.6939823 | | |
| N | 10^5 | 10^6 | 10^7 | 10^5 | 10^6 | 10^7 |
| \hat{H}_N | 0.7272087 | 0.7327888 | 0.7167925 | 0.7129858 | 0.7030381 | 0.6962057 |
| | 0.7175089 | 0.6909413 | 0.7155904 | 0.7026311 | 0.6959066 | 0.6885889 |
| | 0.7335587 | 0.7302528 | 0.7187245 | 0.7288800 | 0.7038811 | 0.7076252 |
| | 0.7423985 | 0.7281338 | 0.7071163 | 0.7083498 | 0.6970961 | 0.6931346 |
| | 0.7338309 | 0.7006550 | 0.7181671 | 0.7285714 | 0.6843995 | 0.7049802 |
| | 0.7450219 | 0.7249378 | 0.7028489 | 0.6910547 | 0.7054787 | 0.6903988 |
| | 0.7117454 | 0.6802888 | 0.7150568 | 0.7058754 | 0.6901041 | 0.6841475 |
| | 0.7289969 | 0.6977386 | 0.7234855 | 0.7154222 | 0.7059025 | 0.6783689 |
| | 0.7256536 | 0.7426642 | 0.7138050 | 0.6864514 | 0.6946754 | 0.7035494 |
| | 0.7283608 | 0.7246335 | 0.7136284 | 0.7058230 | 0.6891336 | 0.6951037 |
| \hat{H}_N^* | 0.7294284 | 0.7153035 | 0.7145215 | 0.7086045 | 0.6949616 | 0.6942103 |

Where $|X|$ is the size of the state set X , and N is the size of sample path. For any pair of $(|X|, N)$, ten sample paths were generated, and the mean of the estimate of the entropy rate of them was used. The tables show that $\hat{H}_N^*(x)$ converges to $H(\mathcal{X})$ when N increases asymptotically. Also when $|X|$ increases, the entropy rate of the birth and death chain with two reflecting barriers converges to the entropy rate of the birth and death chain with one reflecting barrier.

Conclusions

In this paper the entropy rate of a Markov chain with the countable state set is reviewed. First, an estimator for the stationary distribution of Markov chain via sample-path is obtained and then the entropy rate of the Markov chain is estimated. We illustrated that the estimated entropy rate of the Markov chain asymptotically converges to the true entropy rate exponentially fast with regard to the size of the sample-path.

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Appendix

Appendix A. THE PROOF OF INEQUALITY (18)

$$\begin{aligned}
 & E[\exp(N(\widehat{H}_N(x) - H(\mathcal{X})))] \\
 & \leq \exp(2\|\xi\|)E[\exp(\sum_{n=1}^N M_n)] \\
 & \leq \exp(2\|\xi\|)E[\exp(\sum_{n=1}^{N-1} M_n)]E[\exp(M_N)|X_0, \dots, X_{N-1}].
 \end{aligned} \tag{30}$$

Note that $\Phi(a) \geq 0$ for all $a \in \mathbf{R}$ and $\Phi(a)$ is nondecreasing.

$$\begin{aligned}
 & E[\exp(M_N)|X_0, \dots, X_{N-1}] \\
 & = \exp(\log(E[e^{M_N}|X_0, \dots, X_{N-1}])) \\
 & = \exp(\log(E[e^{M_N} - 1 - M_N + 1 + M_N|X_0, \dots, X_{N-1}])) \\
 & = \exp(\log(E[e^{M_N} - 1 - M_N|X_0, \dots, X_{N-1}] + 1)),
 \end{aligned} \tag{31}$$

where the last equality is concluded from $E[M_N|X_0, \dots, X_{N-1}] = 0$.
Now we have

$$\begin{aligned}
 & e^{(\log(E[e^{M_N - 1 - M_N | X_0, \dots, X_{N-1}}] + 1))} \\
 &= \exp(\log(E[\Phi(M_N)M_N^2 | X_0, \dots, X_{N-1}] + 1)) \tag{32} \\
 &\leq \exp(E[\Phi(M_N)M_N^2 | X_0, \dots, X_{N-1}]),
 \end{aligned}$$

by using $\log(a + 1) \leq a$ for $a \geq 0$. Now by monotonicity of Φ and $|M_N| \leq 2\|\xi\|$, we have

$$\begin{aligned}
 & \exp(E[\Phi(M_N)M_N^2 | X_0, \dots, X_{N-1}]) \\
 &\leq \exp(\Phi(2\|\xi\|)E[M_N^2 | X_0, \dots, X_{N-1}]) \tag{33} \\
 &\leq \exp(\Phi(2\|\xi\|)\sigma^2),
 \end{aligned}$$

where $\sigma^2 \geq E[M_N^2 | X_0, \dots, X_{N-1}]$.

Appendix B. THE ESTIMATION OF SERIES IN (29)

For estimating of the series in (29), we calculate it for finite cases. Let

$$H_n(\mathcal{X}) = - \sum_{i=0}^{n-1} \rho(i)S(i).$$

The results of calculation are mentioned in the following table.

Table 3: $H_n(\mathcal{X})$ for $n = 10, 10^2, \dots, 10^7$ and 2.5×10^7

| n | $H_n(\mathcal{X})$ | n | $H_n(\mathcal{X})$ |
|--------|--------------------|-------------------|--------------------|
| 10 | 0.7813217 | 10^5 | 0.6924781 |
| 10^2 | 0.7165776 | 10^6 | 0.6924643 |
| 10^3 | 0.6939823 | 10^7 | 0.6924629 |
| 10^4 | 0.6926162 | 2.5×10^7 | 0.6924628 |

