Asymptotic study of an estimator of the entropy rate of a two-state Markov chain for one long trajectory

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Abstract. The entropy rate of an ergodic homogeneous Markov chain taking only two values is an explicit function of its transition probabilities. We study a plug-in estimator of this entropy rate obtained from the observation of one trajectory with long length. Its exact asymptotic distribution is given. The case of uniform transition probabilities is especially considered. A detailed numerical study using simulation results is provided.

Keywords: empirical estimation, entropy rate, homogeneous two-state Markov Chain, plug-in estimator
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INTRODUCTION

Markov chains and entropy have been linked since the introduction of entropy in probability theory in [12]. Shannon defined the entropy rate of an ergodic homogeneous Markov chain with a finite (or countable) state space E as the sum of the entropies of the transition distributions $(P(i,j))_{j\in E}$ weighted by the probability of occurrence of each state i according to the stationary distribution π of the chain, namely

$$\mathbb{H}(\mathbf{X}) = -\sum_{i\in E}\pi(i)\sum_{j\in E}P(i,j)\log P(i,j), \tag{1}$$

with the convention $0\log 0 = 0$. He proved the convergence in probability of $\frac{1}{n}\log\mathbb{P}(X_1 = i_1,\ldots,X_n = i_n)$ to $\mathbb{H}(\mathbf{X})$. Convergence in mean was proven in [9] and almost sure convergence in [4]. See [8] and the references therein for details and extensions to many other classes of stochastic processes.

The Shannon-entropy of distributions is widely used in all applications involving random variables. Similarly, having an explicit form for the entropy rate of a Markov chain allows one to consider maximum entropy methods. Through its links to Kolmogorov-Sinai complexity, the entropy rate of an information source measures its degree of algorithmic complexity. The entropy rate is also involved in coding and in compression algorithms. See [6] and also [5] and the references therein.

When only observations of the process are available, estimation of the entropy rate is required for using entropy in the above applications. Very few results exist in this aim for Markov chains. Bhat [1] introduced estimation for explicit functions of the transition matrix which may be used for the entropy rate. Misevichyus [10] considered a plug-in estimator of the entropy rate for stationary ergodic Markov chains with finite state spaces. Mukhamedkhanova [11] stated different asymptotic properties of the plug-in estimator for a two-state stationary ergodic chain, in the so-called series schemes: the number of observed states is supposed to vary with the length of the observed trajectory. In [5], the plug-in estimator using maximum likelihood estimators of the transition probabilities and an empirical estimator of the stationary distribution of the chain was proven to be consistent for any countable ergodic Markov chain, not necessarily stationary. For a finite state space and non uniform transition distributions, asymptotic normality holds, but an explicit expression for the asymptotic variance cannot be given in general.

We specialize in the following in two-state Markov chains. Markov chains and more generally stochastic processes taking values in a two state space are well-known to constitute a useful tool in modelling many real situations; they appear in numerous applied fields including telecommunications networks, reliability, survival analysis, etc.

We consider a plug-in estimator of the entropy rate obtained from maximum likelihood estimators of the transition probabilities. We prove its strong consistency. Then, we determine its exact asymptotic distribution with the speed of convergence: a normal distribution for non uniform transition probabilities with speed $\sqrt{n}$, and a $\chi^2(2)$ distribution for uniform transition probabilities with speed $2n$. We present a detailed numerical study of these properties.

DEFINITIONS

We will consider an ergodic (that is, irreducible, positive recurrent and aperiodic) homogeneous Markov chain $\mathbf{X} = (X_n)$ with a two-state space, say $E = \{0,1\}$. Its transition matrix is $P = (P(i,j))_{i,j\in E}$ with transition probabilities $P(i,j) = \mathbb{P}(X_n = j|X_{n-1} = i)$, for $n \geq 1$, and its stationary distribution is $\pi = (\pi(i))_{i\in E}$, satisfying $\sum_{i\in E}\pi(i)P(i,j) = \pi(j)$, for $j \in E$. The chain is stationary if π is the initial distribution of the chain, that is, $\mathbb{P}(X_0 = i) = \pi(i)$, and then $\mathbb{P}(X_n = i) = \pi(i)$ for all n.

Let us set $P(0,1) = p$ and $P(1,0) = q$. The transition matrix of the chain is

$$P = \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix}.$$

The stationary distribution satisfies $\pi P = \pi$, so that

$$\pi(0) = \frac{q}{p+q} \quad \text{and} \quad \pi(1) = \frac{p}{p+q}.$$

For a two-state chain, the entropy rate of the chain given by (1) can be written as an explicit function $h(p,q)$, namely

$$\mathbb{H}(\mathbf{X}) = h(p,q) = \pi(0)S_p + \pi(1)S_q = \frac{q}{p+q}S_p + \frac{p}{p+q}S_q,$$

where

$$S_p = -p\log p - (1-p)\log(1-p) \quad \text{and} \quad S_q = -q\log q - (1-q)\log(1-q).$$

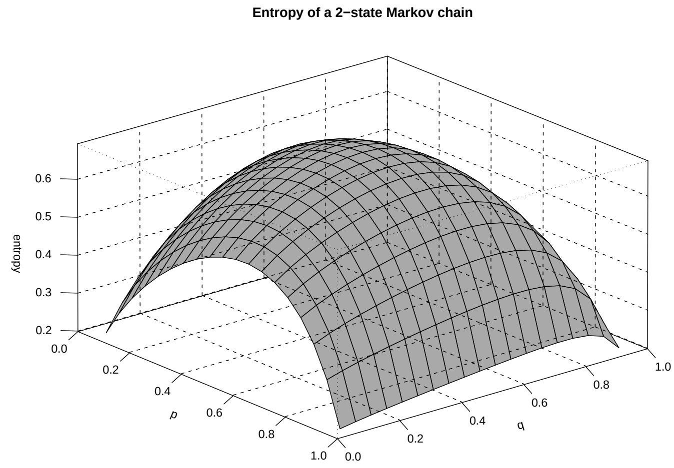


FIGURE 1. The entropy rate of a two-state Markov chain

The graph of this function is shown in Figure 1. The dissymmetry between the cases $p = q = 0$ and $p = 1 = 1 - q$ appears clearly.

PROPERTIES OF THE ESTIMATOR

Suppose we are given one observation of the chain, say $(X_0, \ldots, X_n)$. Let us consider the following empirical estimators of the transition probabilities $P(i, j)$,

$$\widehat{P}_n(i,j) = \frac{\sum_{m=1}^{n} \mathbb{1}_{\{X_{m-1}=i, X_m=j\}}}{\sum_{m=1}^{n} \mathbb{1}_{\{X_m=i\}}}, \quad i, j \in E,$$

with $\widehat{P}_n(i,j) = 0$ when $\sum_{m=1}^{n} \mathbb{1}_{\{X_m=i\}} = 0$. It is well-known that for a finite number of states, they are maximum likelihood estimators.

Replacing the probabilities by their estimators, we get the plug-in estimator of the entropy rate of the chain, that is

$$\widehat{h}_n = h(\widehat{P}_n(0,1), \widehat{P}_n(1,0)). \tag{2}$$

For a general countable state space E, the stationary probabilities cannot be expressed as explicit functions of the transition probabilities, and hence have to be estimated separately, for example by their empirical estimators $\widehat{\pi}_n(i) = \frac{1}{n} \sum_{m=1}^{n} \mathbb{1}_{\{X_m=i\}}$ for $i \in E$. A plug-in estimator $\widehat{\mathbb{H}}_n$ of the entropy rate is then obtained by replacing in (1) the transition probabilities $P(i,j)$ by $\widehat{P}_n(i,j)$ and the stationary probabilities $\pi(i)$ by $\widehat{\pi}_n(i)$, for $i, j \in E$. In [5], $\widehat{\mathbb{H}}_n$ is proven to be strongly consistent.

For a two-state Markov chain, since the entropy rate is an explicit function of the transition probabilities, the plug-in estimator $\widehat{h}_n$ is easily shown to be consistent.

Proposition 1 *Let* $\mathbf{X}$ *be an ergodic homogeneous two-state Markov chain. The plug-in estimator* $\widehat{h}_n$ *of the entropy rate* $\mathbb{H}(\mathbf{X})$ *given in* (2) *is strongly consistent.*

Proof As proven in [3], the estimators $\widehat{P}_n(i,j)$ are strongly consistent for $i,j \in E$. Moreover, the function h is clearly a continuous function. Therefore, the strong consistency of $\widehat{h}_n$ is a straightforward consequence of the continuous mapping theorem (see, e.g., [2]). □

Misevichyus [10] considers the estimator $\widehat{\mathbb{H}}_n$ of the entropy rate for any finite state space, but his proof of the asymptotic normality is incomplete. In [5], $\widehat{\mathbb{H}}_n$ is proven to be asymptotically normal when the transition probabilities are not uniform. Due to the numerous correlations between the involved variables, the computation of the asymptotic variance is not carried through in general. For a two-state Markov chain, the exact asymptotic distribution of $\widehat{h}_n$ can be obtained.

Proposition 2 *Let* $\mathbf{X}$ *be an ergodic homogeneous two-state Markov chain with non uniform transition probabilities. Then* $\sqrt{n}[\widehat{h}_n - \mathbb{H}(\mathbf{X})]$ *converges in distribution when* n *tends to infinity to a normal distribution with mean zero and variance*

$$\sigma^2 = \gamma_0^2[\partial_1^1 h(p,q)]^2 + \gamma_1^2[\partial_2^1 h(p,q)]^2,$$

where

$$\partial_1^1 h(p,q) = \frac{q}{(p+q)^2}[S_q - S_p] - \frac{q}{p+q}\log\frac{p}{1-p}$$

and

$$\partial_2^1 h(p,q) = \frac{p}{(p+q)^2}[S_p - S_q] - \frac{p}{p+q}\log\frac{q}{1-q}.$$

Proof The column vector $\sqrt{n}(\widehat{P}_n(0,1) - p, \widehat{P}_n(1,0) - q)$ is proven in [3] to converge in distribution when n tends to infinity to a centered Gaussian vector with covariance matrix

$$\Gamma = \begin{pmatrix} \gamma_0^2 & 0 \\ 0 & \gamma_1^2 \end{pmatrix},$$

where

$$\gamma_0^2 = \frac{p(1-p)}{\pi(0)} = \frac{p(1-p)(p+q)}{q} \quad \text{and} \quad \gamma_1^2 = \frac{q(1-q)}{\pi(1)} = \frac{q(1-q)(p+q)}{p}.$$

By a direct application of the delta method (see, e.g., [2]), we know that $\sqrt{n}[\widehat{h}_n - \mathbb{H}(\mathbf{X})]$ is asymptotically normal, with mean zero and variance

$$\sigma^2 = \left(\partial_1^1 h(p,q), \partial_2^1 h(p,q)\right) \Gamma \left(\partial_1^1 h(p,q), \partial_2^1 h(p,q)\right)',$$

where $\partial_u^v h$ denotes the v-th order differential with respect to the u-th variable of the function h.

We compute

$$\partial_1^1 h(p,q) = -[\partial_1^1 \pi(0)]S_p - \pi(0)[\partial_1^1 S_p] - [\partial_1^1 \pi(1)]S_q,$$

with $\partial_1^1\pi(0) = \partial_1^1\pi(1) = q/(p+q)^2$. By computing symmetrical expressions for $\partial_2^1\pi(0)$ and $\partial_2^1\pi(1)$, and $\partial_2^2 h(p,q)$, we get the result. □

For non uniform transition probabilities, the asymptotic variance is naturally estimated by

$$\widehat{\sigma}_n^2 = \gamma_0^2[\partial_1^1 h(\widehat{P}_n(0,1), \widehat{P}_n(1,0))]^2 + \gamma_1^2[\partial_2^1 h(\widehat{P}_n(0,1), \widehat{P}_n(1,0))]^2.$$

Thanks to the strong consistency of the estimator of the transition probabilities, this estimator is strongly consistent too. Thus we get that

$$\frac{\sqrt{n}}{\widehat{\sigma}_n}[\widehat{h}_n - \mathbb{H}(\mathbf{X})]$$

is asymptotically standard normal.

If the transition probabilities are uniform, the entropy rate under the constraint $\pi P = \pi$ is maximum (see [7]), the gradient is degenerated and the delta method cannot be applied. To our knowledge, no result exist in the literature concerning the asymptotic distribution of the plug-in estimator of the entropy rate obtained from the observation of one long trajectory of the Markov chain. For a two-state chain, convergence to a $\chi^2(2)$-distribution holds, as stated in the following result.

Proposition 3 *Let* $\mathbf{X}$ *be an ergodic homogeneous two-state Markov chain with uniform transition probabilities. Then* $2n[\widehat{h}_n - \mathbb{H}(\mathbf{X})]$ *converges in distribution when* n *tends to infinity to a* $\chi^2(2)$*-distribution.*

Proof For any transition matrix, since $\widehat{P}(0,1)$ converges almost surely to p and $\widehat{P}(1,0)$ to q when n tends to infinity, the Taylor's expansion for $h(p,q)$ at (p,q) implies that

$$\begin{aligned}
\widehat{h}_n &= \mathbb{H}(\mathbf{X}) + [\partial_1^1 h(p,q)][\widehat{P}(0,1)-p] + [\partial_2^1 h(p,q)][\widehat{P}(1,0)-q] \\
&\quad + \frac{1}{2}[\partial_1^2 h(p,q)][\widehat{P}(0,1)-p]^2 + \frac{1}{2}[\partial_2^2 h(p,q)][\widehat{P}(1,0)-q]^2 \\
&\quad + [\widehat{P}(0,1)-p]^2 \varepsilon_i([\widehat{P}(0,1)-p]^2) + [\widehat{P}(1,0)-q]^2 \varepsilon_i([\widehat{P}(1,0)-q]^2),
\end{aligned}$$

where the remainder converges to zero almost surely when n tends to infinity. We compute

$$\begin{aligned}
\partial_1^2 h(p,q) &= \frac{p}{(p+q)^3}(S_p - S_q) + \frac{2q}{(p+q)^2}\log\frac{p}{1-p} - \frac{q}{(p+q)p(1-p)}, \\
\partial_2^2 h(p,q) &= \frac{q}{(p+q)^3}(S_q - S_p) + \frac{2p}{(p+q)^2}\log\frac{q}{1-q} - \frac{p}{(p+q)q(1-q)}.
\end{aligned}$$

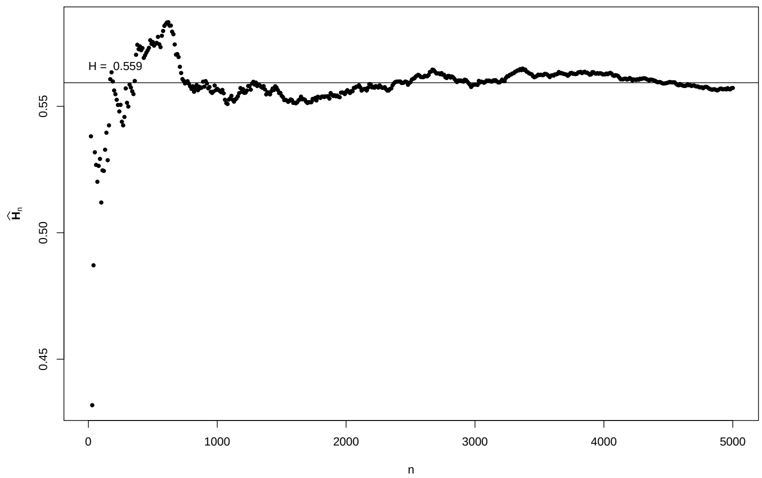


FIGURE 2. Punctual convergence of the plug-in estimator

For uniform transition probabilities, that is $p = q = 0.5$, and hence $\pi(0) = \pi(1) = 0.5$, the term of order one is null. Moreover, first $S_p = S_q = 0$ and $\log[q/(1-q)] = 0$, and second $q/(p+q)q(1-q) = 1/\gamma_0$ and $p/(p+q)q(1-q) = 1/\gamma_1$, thus

$$\begin{aligned}\widehat{h}_n &= \mathbb{H}(\mathbf{X}) - \frac{1}{2\gamma_0^2}[\widehat{P}(0,1)-p]^2 - \frac{1}{2\gamma_1^2}[\widehat{P}(1,0)-q]^2 \\ &\quad + [\widehat{P}(0,1)-p]^2\varepsilon_i([\widehat{P}(0,1)-p]^2) + [\widehat{P}(1,0)-q]^2\varepsilon_i([\widehat{P}(1,0)-q]^2).\end{aligned}$$

Since $\sqrt{n}[\widehat{P}(0,1)-p]/\gamma_0$ and $\sqrt{n}[\widehat{P}(01,0)-q]/\gamma_1$ are asymptotically standard normal and are independent, the conclusion follows. □

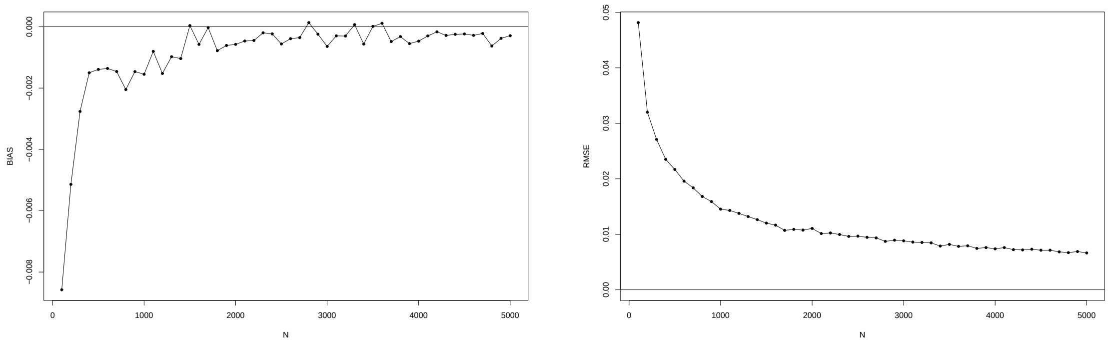
SIMULATION

For illustrating the above results for non uniform transition probabilities, we have chosen to consider a two-state Markov chain with transition probabilities $p = 0.2$ and $q = 0.3$.

Figure 2 shows the punctual convergence of the plug-in estimator for $n = 10$ to 5000 by steps of 10. We have first simulated a trajectory with length 5000 of the chain. Then we have computed $\widehat{h}_n$ for $10 \leq n \leq 5000$ from this trajectory.

Figure 3 shows the bias and the root mean squared error of the plug-in estimator for $100 \leq n \leq 5000$ by steps of 10, where $K = 1000$ trajectories have been simulated for each value of n. The bias and the root mean squared error (RMSE) of the estimator $\widehat{h}_n$ are computed by

$$\text{Bias} = \mathbb{H}(\mathbf{X}) - \frac{1}{K}\sum_{k=1}^{I}\widehat{h}_n^k \quad \text{and} \quad \text{RMSE} = \sqrt{\frac{1}{K-1}\sum_{k=1}^{K}\left[\widehat{h}_n^k - \frac{1}{K}\sum_{k=1}^{K}\widehat{h}_n^k\right]^2},$$



Bias RMSE

FIGURE 3. Bias and RMSE of the plug-in estimator $\widehat{h}_n$

where $\widehat{h}_n^k$ is the estimator of $\mathbb{H}(\mathbf{X})$ for the k-th trajectory.

Figure 4 shows the empirical distribution function of $\sqrt{n}[\widehat{h}_n - \mathbb{H}(\mathbf{X})]/\widehat{\sigma}_n$ compared to the standard normal distribution function for different values of n between 10 and 1000, for $K = 500$ simulated trajectories for each value of n.

For uniform transition probabilities, that is $p = q = 0.5$, Figure 5 shows the empirical distribution function of $2n[\widehat{h}_n - \mathbb{H}(\mathbf{X})]$ compared to the $\chi^2(2)$-distribution function, for $n = 1000$ and $K = 1000$ simulated trajectories.

These numerical results show the good behavior of the plug-in estimator, as well in the non uniform as in the uniform case.

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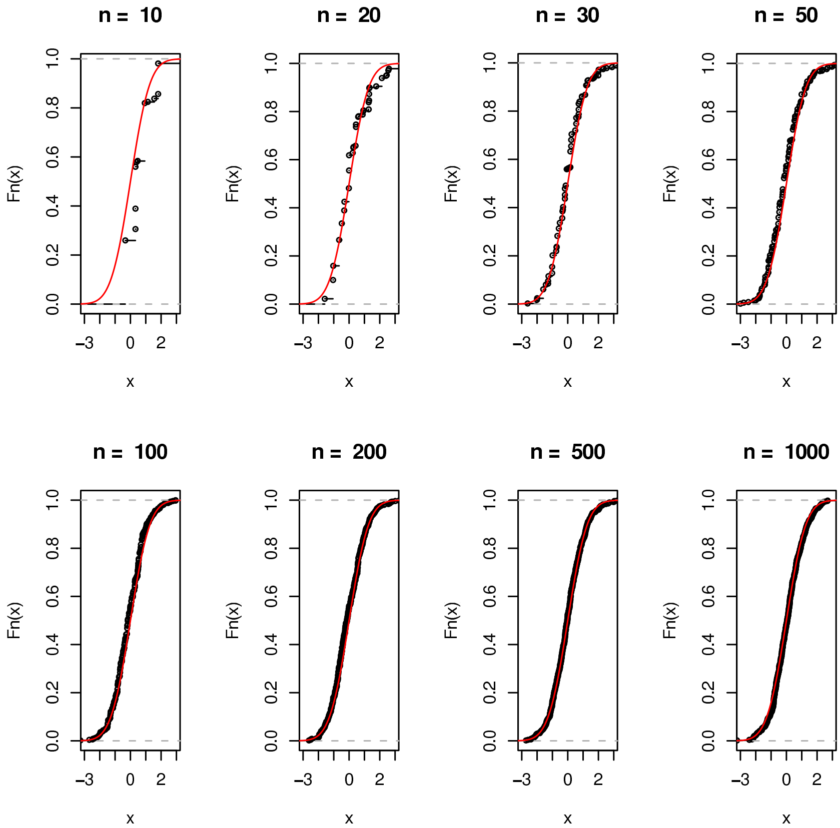

FIGURE 4. Non uniform transition probabilities: normal asymptotic distribution.

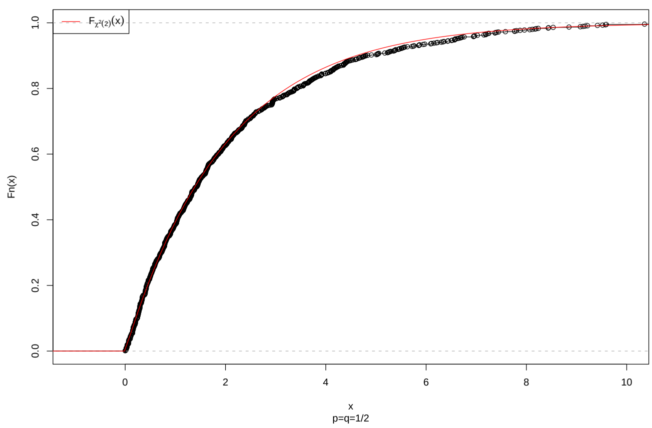

FIGURE 5. Uniform transition probabilities: χ^2 asymptotic distribution.

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