Determination and Estimation of Generalized Entropy Rates for Markov Chains

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Shannon entropy rate of a stochastic process

• The entropy up to time n of a random sequence $\mathbf{X} = (X_n)_{n \in \mathbb{N}}$ with denumerable state space E is

$$-\sum_{i_1,...,i_n \in E} p_n(i_1^n) \log p_n(i_1^n),$$

where $p_n(i_1^n) = \mathbb{P}[(X_1, \dots, X_n) = (i_1, \dots, i_n)]$ is the likelihood of the sequence.

• The **entropy rate** of **X** is defined by

$$-\frac{1}{n} \sum_{i_1,\dots,i_n \in E} p_n(i_1^n) \log p_n(i_1^n) \longrightarrow \mathbb{H}(\mathbf{X}), \quad n \to +\infty,$$

when this quantity is finite.

• Asymptotic Equirepartition Property :

$$-\frac{1}{n}\log p_n(X_1^n) \longrightarrow \mathbb{H}(\mathbf{X}), \quad n \to +\infty,$$

weak if the convergence is in probability, strong if it holds almost surely.

Generalized entropy functionals

The (h, ϕ) -entropy of any measure ν on E is defined by

$$\mathbb{S}_{h(y),\phi(x)}(\nu) = h \left[\sum_{i \in E} \phi(\nu(i)) \right]$$

if $\sum_{i \in E} \phi(\nu(i))$ is finite, and as $+\infty$ either.

The functions $h: \mathbb{R} \to \mathbb{R}$ and $\phi: [0,1] \to \mathbb{R}_+$ are twice continuously differentiable functions, with either ϕ concave and h increasing or ϕ convex and h decreasing.

Some (h, ϕ) -entropies:

h(y)	$\phi(x)$	(h, ϕ) – entropies
y	$-x \log x$	Shannon (1948)
$(1-s)^{-1}\log y$	x^s	Renyi (1961)
$\left \left[t(t-r) \right]^{-1} \log y \right $	$\int x^{r/t}$	Varma (1966)
$\mid y \mid$	$(1-2^{1-s})^{-1}(x-x^s)$	Havrda and Charvat (1967)
$(t-1)^{-1}(y^t-1)$	$x^{1/t}$	Arimoto (1971)
$(r-1)^{-1}[y^{(r-1)/(s-1)}-1]$	x^s	Sharma and Mittal 1 (1975)
$(r-1)^{-1}[\exp(r-1)y-1]$	$-x \log x$	Sharma and Mittal 2 (1975)
$\mid y \mid$	$-x^s \log x$	Taneja (1975)
$\mid y \mid$	$(t-r)^{-1}(x^r-x^t)$	Sharma and Taneja (1975)
$(r-1)^{-1}(1-y)$	x^r	Tsallis (1988)

• The (h, ϕ) -entropy rate of a random sequence $\mathbf{X} = (X_n)_{n \in \mathbb{N}}$ with state space $E \subset \mathbb{N}$ is defined by

$$\frac{1}{n}\mathbb{S}_{h(y),\phi(x)}(p_n) \longrightarrow \mathbb{H}_{h,\phi}(\mathbf{X}), \quad n \to +\infty.$$

where $p_n(i_0^n) = \mathbb{P}(X_0 = i_0, \dots, X_{n-1} = i_{n-1})$ is the distribution of (X_0, \dots, X_{n-1}) .

Quasi-power property The process X satisfies the quasi-power property with parameters $[\sigma_0, \lambda, c, \rho]$ if:

- 1. $\sup_{i_0^n \in E^{n+1}} p_n(i_0^n) \longrightarrow 0 \text{ when } n \to \infty.$
- 2. $\exists \sigma_0 \in]-\infty, 1]$, such that $\forall s > \sigma_0$ and $\forall n \in \mathbb{N}$, the series

$$\Lambda_n(s) = \sum_{i_0^n \in E^{n+1}} p_n(i_0^n)^s$$

is convergent and satisfies

$$\Lambda_n(s) = c(s) \cdot \lambda(s)^n + R_n(s),$$

with $|R_n(s)| = O(\rho(s)^n \lambda(s)^n)$, where: c and λ are strictly positive analytic functions for $s > \sigma_0$; λ is strictly decreasing with $\lambda(1) = c(1) = 1$, R_n is also analytic, $\rho(s) < 1$.

Remarks:

The quasi-power property says that $\Lambda_n(s)$ behaves like the n-th power of some analytic function.

In dynamical systems theory, $\Lambda_n(s)$ is called the Dirichlet series of fundamental measures of depth n+1.

Classical entropy rates of a random sequence

satisfying the quasi-power property.

Entropy	Parameters Parameters	Entropy rate
Shannon		$-\lambda'(1)$
Rényi	s=1	$-\lambda'(1)$
	$s \neq 1$	$\frac{1}{1-s}\log\lambda(s)$ $-\frac{1}{m^2}\lambda'(1)$ $\frac{1}{t(t-r)}\log\lambda(r/t)$
Varma	r = t	$-\frac{1}{m^2}\lambda'(1)$
	$r \neq t$	$\frac{1}{t(t-r)}\log\lambda(r/t)$
Havrda-Charvat	s > 1	0
	s = 1	$\frac{-1}{\log 2}\lambda'(1)$
	s < 1	$+\infty$
Arimoto	t > 1	$+\infty$
	t = 1	$-\lambda'(1)$
	t < 1	0
Sharma-Mittal 1	r < 1	$+\infty$
	r > 1	0
	s = r = 1	$-\lambda'(1)$
	$r = 1 \neq s$	$\frac{1}{1-s}\log\lambda(s)$
Sharma-Mittal 2		$(1-s)^{-1}[\exp(-(s-1)\lambda'(1))-1]$
Taneja	r < 1	$+\infty$
	r = 1	$-\lambda'(1)$
	r > 1	0
Sharma-Taneja	r < 1 or s < 1	$+\infty$
	r > 1 and $s > 1$	0
	r = 1 and s > 1	0
	r = 1 and $s = 1$	$-\lambda'(1)$
	r > 1 and $s = 1$	0
Tsallis	r < 1	+∞
	r=1	$-\lambda'(1)$
	r > 1	0

For an i.i.d. sequence with common distribution ν Since $p_n(i_0, i_1, \dots, i_n) = \nu(i_0)\nu(i_1)\dots\nu(i_n)$, the Dirichlet series $\Lambda_n(s)$ can simply be written

$$\Lambda_n(s) = \left[\sum_{i \in E} \nu(i)^s\right]^{n+1}.$$

Hence, **X** satisfies the quasi-power property for s > 0 with functions λ , c and ρ defined by

$$\lambda(s) = \sum_{i \in E} \nu(i)^s$$
, $c(s) = 1$ and $\rho(s) = 0$.

For a finite chain

 $\Lambda_n(s) = \mathbf{1} \cdot P_s^n \cdot \nu_s$, where $P_s = (p(i,j)^s)_{i,j \in E}$, with ν the initial distribution of the chain, and $\nu_s = (\nu(i)^s)_{i \in E}$.

The following relation defines the functions λ , c and ρ of the quasi-power property:

$$P_s^n \cdot \mathbf{v} = \lambda(s)^n \cdot \langle \mathbf{v}, \mathbf{r}_s \rangle \mathbf{l}_s + R^n(s) \cdot \mathbf{v},$$

where $\lambda(s)$ is the unique dominant eigenvalue of P_s with maximum modulus, with associated left and right eigenvectors \mathbf{l}_s and \mathbf{r}_s .

For a denumerable chain

Theorem Ciuperca, Girardin, Lhote (2010)

Let $\mathbf{X} = (X_n)$ be an ergodic Markov chain with transition matrix P and initial distribution ν . Suppose that:

A.
$$\sup_{(i,j)\in E^2} P(i,j) < 1$$

B. $\exists \sigma_0 < 1 \text{ such that } \forall s > \sigma_0$,

$$\sup_{i \in E} \sum_{j \in E} P(i, j)^s < +\infty \quad \text{and} \quad \sum_{i \in E} \nu(i)^s < +\infty,$$

C. $\forall \epsilon > 0$ and $\forall s > \sigma_0$, $\exists A \subset E$ with $|A| < +\infty$ such that

$$\sup_{i \in E} \sum_{j \in E \setminus A} P(i, j)^s < \varepsilon.$$

Then **X** satisfies the quasi-power property.

Proof of the theorem

Lemma If Assumptions A, B, C hold true,

then $P_s: (\ell^1, ||.||_1) \to (\ell^1, ||.||_1)$ is a compact operator, $\forall s > \sigma_0$,

where
$$\ell^1 = \{ u = (u_i)_{i \in E} : ||u||_1 = \sum_{i \in E} |u_i| < \infty \}.$$

We deduce from the lemma that the spectrum of P_s is a sequence that converges to zero. Hence, P_s has a finite number of eigenvalues with maximum modulus and there exists a spectral gap separating these dominant eigenvalues from the remainder of the spectrum.

Further, since **X** is ergodic, P_s has a unique dominant eigenvalue $\lambda(s)$ which, moreover, is positive. Hence,

$$P_s^n u = \lambda(s)^n Q_s u + R_s^n u, \qquad u \in \ell^1,$$

where Q_s is the projector over the dominant eigenspace and R_s is the projector over the remainder of the spectrum. The spectral radius of R_s can be written $\rho(s) \cdot \lambda(s)$ with $\rho(s) < 1$.

Finally,

$$\Lambda_n(s) = \lambda(s)^n ||Q_s \nu_s||_1 (1 + O(\rho(s)^n \lambda(s)^n)),$$

which means that X satisfies the quasi-power property.

The analyticity of the involved functions is due jointly to the analyticity of $s \to P_s$ and to perturbation arguments.

Theorem Let **X** be a random sequence satisfying the quasi-power property with parameters $[\sigma_0, \lambda, c, \rho]$. Suppose that

$$\phi(x) \underset{x \to 0}{\sim} c_1 \cdot x^s \cdot (\log x)^k \tag{P}$$

with $s > \sigma_0$, $c_1 \in \mathbb{R}_+^*$ and $k \in \mathbb{N}^*$. Then the entropy rate $\mathbb{H}_{h,\phi}(\mathbf{X})$ is given by the following table.

Value of s	Condition on h	Entropy rate
	$h(x) \underset{x \to +\infty}{\sim} c_2 \cdot x^{1/k}$	$c_2 \cdot c_1^{1/k} \cdot \lambda'(1)$
s = 1	$h(x) = o(x^{1/k})$	0
	$x^{1/k} = o(h(x))$	$+\infty$
s > 1	$h(x) \underset{x \to 0^+}{\sim} c_2 \cdot \log x$	$c_2 \cdot \log \lambda(s)$
	$h(x) = o(\log x)$	0
	$\log x = o(h(x))$	$+\infty$
$\sigma_0 < s < 1$	$h(x) \underset{x \to +\infty}{\sim} c_2 \cdot \log x$	$c_2 \cdot \log \lambda(s)$
	$h(x) = o(\log x)$	0
	$\log x = o(h(x))$	$+\infty$

Proof $\sup_{i_0^n \in E^{n+1}} \nu_n(i_0^n) \to 0$ and (P) together induce that $\forall \epsilon > 0, \exists n_0 \in \mathbb{N}/ n \ge n_0$ and $i_0^n \in E^{n+1}$,

$$(1 - \epsilon)c_1 \nu_n(i_0^n)^s \log^k \nu_n(i_0^n) \le \phi(\nu_n(i_0^n))$$

$$\le (1 + \epsilon)c_1 \nu_n(i_0^n)^s \log^k \nu_n(i_0^n),$$

from which it follows that

$$(1 - \epsilon)c_1 \Lambda_n^{(k)}(s) \le \sum_{i_0^n \in E^{n+1}} \phi(\nu_n(i_0^n)) \le (1 + \epsilon)c_1 \Lambda_n^{(k)}(s).$$

Due to the analyticity of all involved functions,

$$\Lambda_n^{(k)}(s) = c(s) \cdot \lambda'(s)^k \cdot n^k \cdot \lambda(s)^{n-k} \cdot [1 + O(1/n)].$$

which yields

$$\sum_{i_0^n \in E^{n+1}} \phi(\nu_n(i_0^n)) \sim c_1 \cdot c(s) \cdot \lambda'(s)^k \cdot n^k \cdot \lambda(s)^{n-k}.$$

Since ϕ is nonnegative, this sum converges polynomially to infinity. This leads to the next equivalences:

$$h(\Sigma_n) \sim c_2 \cdot |c_1|^{1/k} \cdot |\lambda'(1)| \cdot n$$
 if $h(x) \sim c_2 \cdot x^{1/k}$,
 $h(\Sigma_n) \sim o(n)$ if $h(x) = o(x^{1/k})$,
 $h(\Sigma_n) \sim s_n \cdot n$ with $s_n \to \infty$ if $x^{1/k} = o(h(x))$.

Since by definition, the (h, ϕ) -entropy rate is the limit of $h(\Sigma_n)/n$ when n tends to infinity, the results follow immediately for s = 1.

The other cases can be studied similarly. \Box

Entropy	Parameters	Entropy rate
Shannon		$-\lambda'(1)$
Rényi	s = 1	$-\lambda'(1)$
	$s \neq 1$	$\frac{1}{1-s}\log\lambda(s)$
Varma	r = t	$-\frac{1}{m^2}\lambda'(1)$ $\frac{1}{t(t-r)}\log\lambda(r/t)$
	$r \neq t$	$\frac{1}{t(t-r)}\log\lambda(r/t)$
Havrda-Charvat	s > 1	0
	s = 1	$\frac{-1}{\log 2}\lambda'(1)$
	s < 1	$+\infty$
Arimoto	t > 1	$+\infty$
	t = 1	$-\lambda'(1)$
	t < 1	0
Sharma-Mittal 1	r < 1	$+\infty$
	r > 1	0
	s = r = 1	$-\lambda'(1)$
	$r = 1 \neq s$	$\frac{1}{1-s}\log\lambda(s)$
Sharma-Mittal 2		$(1-s)^{-1}[\exp(-(s-1)\lambda'(1))-1]$
Taneja	r < 1	$+\infty$
	r = 1	$-\lambda'(1)$
	r > 1	0
Sharma-Taneja	r < 1 or s < 1	$+\infty$
	r > 1 and $s > 1$	0
	r = 1 and s > 1	0
	r = 1 and s = 1	$-\lambda'(1)$
	r > 1 and $s = 1$	0
Tsallis	r < 1	+∞
	r=1	$-\lambda'(1)$
	r > 1	0

Values of classical entropy rates of a random sequence satisfying the quasipower property with parameters $[\lambda, c, \rho, \sigma_0]$. For an ergodic **Markov chain X** = $(X_n)_{n \in \mathbb{N}}$ with state space E with s states, transition matrix P = (P(i, j)), where $P(i, j) = \mathbb{P}(X_{n+1} = j/X_n = i)$, and stationary distribution π such that $\pi P = \pi$, and entropy

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

Proposition Anderson and Goodman (1957) The empirical estimators

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

are strongly convergent and asymptotically normal:

$$\sqrt{n}\left(\widehat{P}_n(i,j) - P(i,j)\right) \xrightarrow{\mathcal{L}} \mathcal{N}_{s^2}(0,\Gamma^2)$$

where $\Gamma_{ij}^2 = \delta_{ik} [\delta_{jl} P(i,j) - P(i,j) P(i,l)] / \pi(i)$.

• We define the plug-in estimator

$$\widehat{\mathbb{H}}_n = h(\widehat{P}_n)$$

of the entropy rate.

Theorem Ciuperca and Girardin (2007)

If the transition probabilities are not uniform, the plugin estimator $\widehat{\mathbb{H}}_n = h(\widehat{P}_n)$ of $\mathbb{H}(\mathbf{X})$ is **strongly convergent** and **asymptotically normal**.

Precisely,

$$\sqrt{n}[\widehat{h}_n - \mathbb{H}(\mathbf{X})] \xrightarrow{\mathcal{L}} \mathcal{N}(0, (\partial_i^j h) \Gamma(\partial_i^j h)'),$$

where $\partial_u^v h$ is the differential with order v with respect to variable u of h.

Proof

Continuous mapping theorem and delta method

For a two-state chain

The transition matrix of the chain is

$$P = \left(\begin{array}{cc} 1 - p & p \\ q & 1 - q \end{array}\right).$$

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

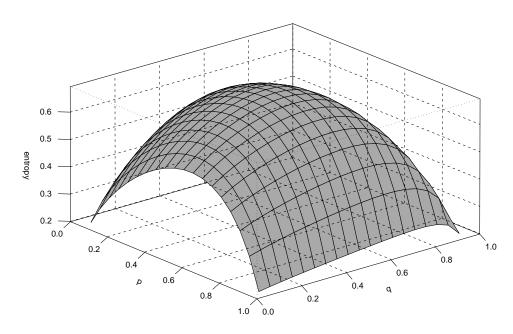
$$\pi(0) = \frac{q}{p+q}$$
 and $\pi(1) = \frac{p}{p+q}$.

The entropy rate is

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

$$= \frac{q}{p+q} [-p\log p - (1-p)\log(1-p)] + \frac{p}{p+q} [-q\log q - (1-q)\log(1-q)].$$

Entropy of a 2-state Markov chain



Theorem Girardin and Sesboue (2009)

$$\widehat{h}_n = h(\widehat{p}_n, \widehat{q}_n) \xrightarrow{a.s.} \mathbb{H}(\mathbf{X}).$$

If the chain is not uniform,

$$\sqrt{n}[\widehat{h}_n - \mathbb{H}(\mathbf{X})] \xrightarrow{\mathcal{L}} \mathcal{N}(0, \sigma^2)$$

where
$$\sigma^2 = \Gamma(0,0)^2 [\partial_1^1 h(p,q)]^2 + \Gamma(1,1)^2 [\partial_2^1 h(p,q)]^2$$

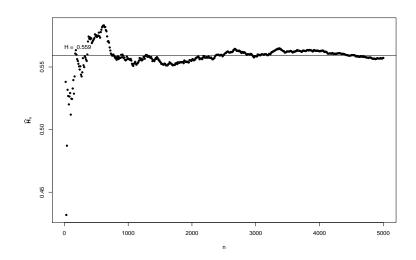
$$= pq(1-p) \left[\frac{S_q - S_p}{p+q} - \log \frac{p}{1-p} \right]$$

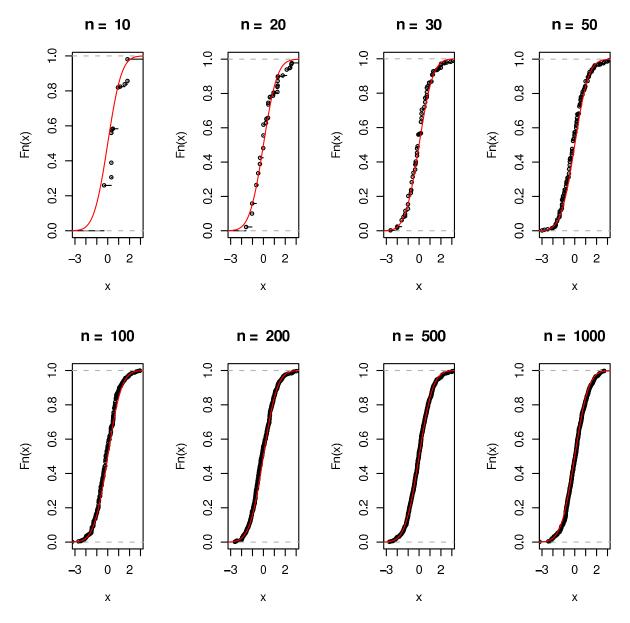
$$+ pq(1-q) \left[\frac{S_p - S_q}{p+q} - \log \frac{q}{1-q} \right]$$

For illustration, we have simulated a chain for p = 0.2 and q = 0.3, for which $\mathbb{H}(\mathbf{X}) = 0,559$.

The first figure shows the punctual convergence of h_n to $\mathbb{H}(\mathbf{X})$ for n = 10 to 5000 by steps of 10.

(computation of \hat{h}_n for $10 \le n \le 5000$ after simulation of one trajectory with length 5000)





This figure compares the empirical distribution function of $\sqrt{n}[\hat{h}_n - \mathbb{H}(\mathbf{X})]/\hat{\sigma}_n$ to that of the standard normal distribution for different values of $10 \le n \le 1000$.

(for T = 500 trajectories simulated for each n)

Theorem Girardin and Sesboue (2009)

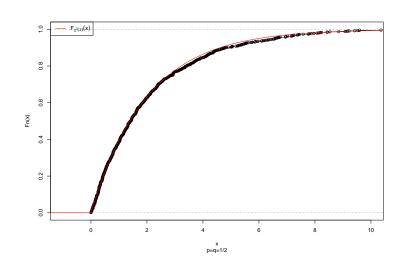
For a uniform chain, p = q = 1/2, \hat{h}_n is strongly convergent and $2n[\mathbb{H}(\mathbf{X}) - \hat{h}_n] \xrightarrow{\mathcal{L}} \chi^2(2)$.

Proof. $\widehat{h}_n - \mathbb{H}(\mathbf{X}) =$

$$\begin{split} &= [\partial_1^1 h(p,q)] [\widehat{P}(0,1)-p] + [\partial_2^1 h(p,q)] [\widehat{P}(1,0)-q] \\ &+ \frac{1}{2} [\partial_1^2 h(p,q)] [\widehat{P}(0,1)-p]^2 + \frac{1}{2} [\partial_2^2 h(p,q)] [\widehat{P}(1,0)-q]^2 \\ &+ o([\widehat{P}(0,1)-p]^2) + o([\widehat{P}(1,0)-q]^2) \\ &= \frac{1}{2\Gamma(0,0)^2} [\widehat{P}(0,1)-p]^2 + \frac{1}{2\Gamma(1,1)^2} [\widehat{P}(1,0)-q]^2 \\ &+ o([\widehat{P}(0,1)-p]^2) + o([\widehat{P}(1,0)-q]^2). \end{split}$$

and the result follows, since $\frac{\sqrt{n}[\widehat{P}(0,1)-p]}{\Gamma(0,0)}$ and $\frac{\sqrt{n}[\widehat{P}(1,0)-q]}{\Gamma(1,1)}$ are asymptotically standard normal.

The last figure compares the distribution function of $2n[\hat{h}_n - \mathbb{H}(\mathbf{X})]$ to that of the $\chi^2(2)$ -distribution for n = 1000. (T = 1000 simulated trajectories for n)



Estimation of generalized entropy rates

All the entropy rates are finite and non-zero only at a threshold where they are equal to the Rényi entropy rate up to a multiplicative factor. Therefore, we only estimate Shannon and Rényi entropy rates, that is

$$h(\theta) = -\lambda'(1; \theta_0),$$

and $h_s(\theta) = (1 - s)^{-1} \log \lambda(s; \theta_0).$

The transition probabilities of the ergodic chain \mathbf{X} with denumerable state space are supposed to depend on $\theta \in \Theta^r$, with true value θ^0 .

Proposition Billingsley (1962) Suppose that:

- **A.** $\forall x, \{y : P(x, y; \theta) > 0\}$ does not depend on θ .
- **B.** $\forall (x,y), P_u(x,y;\theta), P_{uv}(x,y;\theta) \text{ and } P_{uvw}(x,y;\theta)$ are in $\mathcal{C}^1(\Theta)$.
- C. $\forall \theta \in \Theta, \exists N$, neighborhood such that $\forall u, v, P_u(x, y; \theta)$ and $P_{uv}(x, y; \theta)$ are uniformly bounded in $L^1(\mu(dy))$ on N and

$$\mathbb{E}_{\theta}[\sup_{\theta' \in N} | P_u(x, y; \theta') |^2] < +\infty.$$

- **D.** $\exists \delta > 0$ such that $\mathbb{E}_{\theta}[|P_u(x, y; \theta)|^{2+\delta}]$ is finite $\forall u = 1, \ldots, r$.
 - E. The Fisher information matrix

$$\sigma(\theta) = (\mathbb{E}_{\theta}[P_u(x, y; \theta) P_v(x, y; \theta)])$$
 is non singular.

Then a strongly consistent maximum likelihood estimator $\widehat{\theta}_n$ of θ exists. Moreover, $\sqrt{n}(\widehat{\theta}_u - \theta_u)$ is asymptotically normal, with covariance matrix $\sigma^{-1}(\theta^0)$.

It is natural to consider the plug-in estimators:

$$h(\hat{\theta}_n) = -\lambda'(1; \theta_n)$$

and $h_s(\hat{\theta}_n) = (1-s)^{-1} \log \lambda(s; \hat{\theta}_n)$

of Shannon entropy rate and of Rényi entropy rate.

Theorem If Billingsley's assumptions are satisfied and if **X** satisfies the quasi-power property, then $h(\hat{\theta}_n)$ and $h_s(\hat{\theta}_n)$ are strongly consistent and asymptotically normal: $\sqrt{n}[h(\hat{\theta}_n) - h(\theta)] \to \mathcal{N}(0, \Sigma_1)$, where

$$\Sigma_{1} = \left\{ \frac{\partial}{\partial \theta} [-\lambda'(1;\theta)] \right\}^{t} \sigma^{-1}(\theta) \frac{\partial}{\partial \theta} [-\lambda'(1;(\theta))]$$

and $\sqrt{n}[h_s(\hat{\theta}_n) - \mathbf{H}_s(\theta^0)] \to \mathcal{N}(0, \Sigma_s)$, where

$$\Sigma_s = \frac{1}{(1-s)^2} \left\{ \frac{\partial}{\partial \theta} \lambda(s; \theta) \right\}^t \sigma^{-1}(\theta) \frac{\partial}{\partial \theta} \lambda(s; (\theta)).$$

Proof Due to operators properties, the eigenvalue $\lambda(s)$ and its derivative $\lambda'(1)$ are continuous with respect to the perturbated operator P_s . For a parametric chain depending on θ , Assumption B induces that P_s is a continuously differentiable function of θ . Therefore both $\lambda(s;\theta)$ and $\lambda'(s;\theta)$ are continuous with respect to θ . The results follow from the continuous mapping theorem and the delta method.

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