Markov Chain Order Estimation and $\chi^2 - divergence$ measure

A.R. Baigorri*
Mathematics Department
UnB

C.R. Gonçalves †
Mathematics Department
UnB

P.A.A. Resende ‡
Mathematics Department
UnB

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Abstract

We use the $\chi^2 - divergence$ as a measure of diversity between probability densities and review the basic properties of the estimator $\Delta_2(.\|.)$. We define a few objects which capture relevant information from the sample of a Markov Chain to be used in the definition of a couple of estimators i.e. the *Local Dependency Level* and *Global Dependency Level* for a Makov chain sample. After exploring their properties we propose a new estimator for the Markov chain order. Finally we show a few tables containing numerical simulation results, comparing the perfomance of the new estimator with the well known and already established AIC, BIC and EDC estimators.

*baig@unb.br
†The author was partially supported by PROCAD/CAPES, CASADINHO/CAPES and PRONEX/FAPDF — catia@mat.unb.br
‡pa@mat.unb.br

1 Introduction

A Markov Chain is a discrete stochastic process $\mathbb{X} = \{X_n\}_{n\geq 0}$ with state space E, cardinality $|E| < \infty$ for which there is a $k \geq 1$ such that for $n \geq k,\ (x_1, ..., x_n) \in E^n$

$$P(\mathbf{X}_1 = x_1, .., \mathbf{X}_n = x_n) = P(\mathbf{X}_1 = x_1, .., \mathbf{X}_k = x_k)\Pi_{i=k+1}^{n} Q(x_i|x_{i-k}, ..., x_{i-1})$$

for suitable transition probabilities $Q(.|.)$. The class of processes that holds the above condition for a given $k \geq 1$ will be denoted by $\mathcal{M}_k$, and $\mathcal{M}_0$ will denote the class of i.i.d. processes. The order of a process in $\cup_{i=0}^{\infty} \mathcal{M}_i$ is the smallest integer κ such that $\mathbb{X} = \{X_n\}_{n\geq 0} \in \mathcal{M}_\kappa$.

Along the last few decades there has been a great number of research on the estimation of the order of a Markov Chains, starting with M.S. Bartlett [6], P.G. Hoel [16], I.J. Good [15], T.W. Anderson & L.A. Goodman [4], P. Billingsley [7], [8] among others, and more recently, H. Tong [24], G. Schwarz [22], R.W. Katz [17], I. Csiszar and P. Shields [11], L.C. Zhao et all [25] had contributed with new Markov chain order estimators.

Since 1973, H. Akaike [1] entropic information criterion, known as AIC, has had a fundamental impact in statistical model evaluation problems. The AIC has been applied by Tong, for example, to the problem of estimating the order of autoregressive processes, autoregressive integrated moving average processes, and Markov chains. The Akaike-Tong (AIC) estimator was derived as an asymptotic approximate estimate of the Kullback-Leibler information discrepancy and provides a useful tool for evaluating models estimated by the maximum likelihood method. Later on, Katz derived the asymptotic distribution of the estimator and showed its inconsistency, proving that there is a positive probability of overestimating the true order no matter how large the sample size. Nevertheless, AIC is the most used and succesfull Markov chain order estimator used at the present time, mainly because it is more efficient than BIC for small sample.

The main consistent estimator alternative, the BIC estimator, does not perform too well for relatively small samples, as it was pointed out by Katz [17] and Csiszar & Shields [11]. It is natural to admit that the expansion of the Markov Chain complexity (size of the state space and order) has significant influence on the sample size required for the identification of the unknown order, even though, most of the time it is difficult to obtain sufficiently large samples.

In this notes we'll use a different entropic object called $\chi^2 - divergence$, and study its behaviour when applied to samples from random variables with multinomial empirical distributions

$$\mathcal{X} = \{X_i\}_{1 \leq i \leq r}$$

derived from a Markov Chain sample. Finally, we shall propose a new strongly consistent Markov Chain order estimator more efficacious than the already established AIC and BIC, which it shall be exhibited through the outcomes of several numerical simulations.

In Section 2 we succinctly review the concept of $f-divergence$ and its properties. In Section 3, the χ^2-divergence estimator is defined reviewing some results concerning its convergence, as well as we briefly elaborate about the Law of Iterated Logarithm (LIL) for our particular situation. In Section 4 the Makov chain sample is brought to attention, some notation introduced and the estimators *Local Dependency Level* and *Global Dependency Level*, which are the groundsill of the consistent Markov chain order estimator, subsequently defined. Finally, in Section 4 we describe the procedures used and the results obtained in an exploratory numerical simulations.

2 Entropy and f-divergences

2.1 Definitions and Notations

An $f-divergence$ is a function that measures the discrepancy between two probability distributions P and Q. The divergence is intuitively an average of the function f of the odds ratio given by P and Q.

These divergences were introduced and studied independently by Csiszar, Csiszar&Shields and Ali&Silvey among others ([10], [12], [3]) and sometimes are referred as *Ali-Silvey distances.*

Definition 2.1. *Let P and Q be discrete probability densities with support $S(P) = S(Q) = E = \{1, ...m\}$. For $f(t)$ convex function defined for $t > 0, f(1) = 0$, the $f-divergence$ for the distributions P and Q is*

$$D_f(P \| Q) = \sum_{a \in A} Q(a) f\left(\frac{P(a)}{Q(a)}\right).$$

Here we take $0f(\frac{0}{0}) = 0$, $f(0) = \lim_{t\to 0} f(t)$, $0f(\frac{a}{0}) = \lim_{t\to 0} tf(\frac{a}{t}) = a \lim_{u\to\infty} \frac{f(u)}{u}$. ♦

For example:

$$f(t) = t\log(t) \Rightarrow D_f(P\|Q) = D(P\|Q) = \sum_{a\in A} P(a)\log\left(\frac{P(a)}{Q(a)}\right),$$

$$f(t) = (1-t^2) \Rightarrow D_f(P\|Q) = \sum_{a\in A} \frac{(P(a)-Q(a))^2}{Q(a)},$$

which are called *relative entropy* and $\chi^2 - divergence$, respectively. From now on the $\chi^2 - divergence$ shall be denote by $D_2(P\|Q)$.
Observe that the triangular inequality is not satisfied in general, so that $D_2(P\|Q)$ defines no distance in the strict sense.

A basic theorem about *f-divergences* is the following approximation by the $D_2(P\|Q)$.

Theorem 2.1. *(Csiszar & Shields [12]) If f is twice differentiable at t=1 and $f^{''}(1) > 0$ then for any Q with support $S(Q) = A$ and P **close** to Q*

$$D_f(P\|Q) \sim \frac{f^{''}(1)}{2} D_2(P\|Q).$$

Formally, $D_f(P\|Q)/D_2(P\|Q) \to f^{''}(1)/2$ as $P \xrightarrow{D} Q$ ♦

The χ^2-square divergence $D_2(P\|Q)$ test is well known statistical test procedure close related to the chi-square distribution. See [19] for thorough and detailed references.

3 Derived Markov Chains

Let $\mathbf{X}_1^n = (X_1, ..., X_n)$ be a sample from a multiple stationary Markov chain $\mathbb{X} = \{X_n\}_{n\geq 1}$ of unknown order κ. Assume that $\mathbb{X}$ take values on a finite state space $E = \{1, 2, ..., m\}$ with transition probabilities given by

$$p(x_{\kappa+1}|x_1^\kappa) = P(X_{n+1} = x_{n+1}|X_{n-\kappa+1}^n = x_1^\kappa) > 0 \tag{1}$$

where $x_1^\kappa = x_1^j\, x_{j+1}^\kappa = (x_1, ..., x_\kappa) \in E^\kappa$.

Following Doob [13], from the process $\mathbb{X}$ we can derive a first order MC, $\mathbb{Y}^{(\kappa)} = \{Y_n^{(\kappa)}\}_{n\geq 0}$ by setting $Y_n^{(\kappa)} = (X_n, ..., X_{n+\kappa-1})$ so that for $v = (i_1, ...i_\kappa)$ and $w = (i^{'}_1, ..., i^{'}_\kappa)$

$$P(Y_{n+1}^{(\kappa)} = w|Y_n^{(\kappa)} = v) = \tilde{p}_{vw} = \begin{cases} p(i^{'}_\kappa|i_1....i_\kappa), \; i^{'}_j = i_{j+1}, \;\; j = 1, ..., (\kappa-1) \\ 0, \;\; otherwise. \end{cases}$$

Clearly $\mathbb{Y}^{(\kappa)}$ is a first order and homogeneous MC that from now on shall be called the derived process, which by (1) is irreducible and positive recurrent MC having unique stationary distribution, say Π_κ. It is well known, see [[13]-Chap. 5.3], that the derived Markov Chains $\mathbb{Y}^{(l)}, \; l \geq \kappa$ is irreducible and aperiodic, consequently ergodic.

There exists an equilibrium (stationary) distribution $\Pi_\kappa(.)$ satisfying for any initial distribution ν on E^κ

$$\lim_{n\to\infty} |P_\nu(Y_n^{(\kappa)} = x_1^\kappa) - \Pi_\kappa(x_1^\kappa)| = 0,$$

and

$$\Pi_\kappa(x_1^\kappa) = \sum_{z_1^\kappa} \Pi_\kappa(z_1^\kappa)\, p(x_\kappa|z_1^\kappa) = \sum_x \Pi_\kappa(x\, x_1^{\kappa-1})\, p(x_\kappa|x\, x_1^{\kappa-1}).$$

Likewise, for $\mathbb{Y}^{(l)}, \; l > \kappa$

$$\Pi_l(x_1^l) = \Pi_\kappa(x_1^\kappa)\, p(x_{\kappa+1}|x_1^\kappa)...p(x_l|x_{l-\kappa}^{l-1}) = \sum_x \Pi_l(x\, x_1^{l-1})\, p(x_l|x\, x_{l-\kappa}^{l-1}). \quad (2)$$

which shows that Π_l defined above, is a stationary distribution for $\mathbb{Y}^{(l)}$. For the sake of notation's simplicity we'll use, from now on

$$\boxed{\Pi(a_1^l) = \Pi_l(a_1^l), \quad l \geq \kappa.} \quad (3)$$

Now, let us return to $\mathbf{X}_1^n = (X_1, X_2, ..., X_n)$ and define

$$N(x_1^l|\mathbf{X}_1^n) = \sum_{j=1}^{n-l+1} 1(X_j = x_1, ..., X_{j+l-1} = x_l) \quad (4)$$

i.e. the number of ocurrences of x_1^l in X_1^n. If $l = 0$ we take $N(\,.\,|\mathbf{X}_1^n) = n$. The sums are taken over positive terms $N(x_1^{l+1}|\mathbf{X}_1^n) > 0$, or else, we convention $0/0$ or $0.\infty$ as 0.

Now we define the empirical random variables $\mathbf{X}_{i\,\alpha}$, for $i \in E$ and $\alpha \in E^\eta$.

Definition 3.1. *For $\alpha = (a_1, ..., a_\eta) = a_1^\eta \in E^\eta$ and $i \in E$, let $X_{i\,\alpha}$ be the random variable taking values in E, extracted from the MC sample $\boldsymbol{X}_1^n$, defined as*

$$P(X_{i\,\alpha} = l) = \frac{N(i\,a_1^\eta\,l\,|\,\boldsymbol{X}_1^n)}{N(i\,a_1^\eta\,|\,\boldsymbol{X}_1^n)},\ l \in E. \tag{5}$$

with
$\boldsymbol{X}_{i\,\alpha} = \left(X_{i\,\alpha}^{(1)}, ..., X_{i\,\alpha}^{(n_{i\alpha})}\right)$ *its sample of size $n_{i\,\alpha}$.*

Observe that for $i, j \in E$

$$\mathbf{O}_n^\alpha(i,j) = N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)$$

where $\mathbf{O}_n^\alpha$ is the empirical random variables that describe the $X_{i\,\alpha}$, $1 \leq i \leq m$ observed frequencies. Likewise, we define the expected frequencies

$$\mathbf{E}_n^\alpha(i,j) = \frac{\sum_l O_n^\alpha(i,l) \sum_l O_n^\alpha(l,j)}{\sum_{kl} O_n^\alpha(k,l)}$$

and the respective probability functions

$$\boldsymbol{P}_{\mathbf{O}_n^\alpha}(i,j) = \frac{\mathbf{O}_n^\alpha(i,j)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)},\ \ i,j \in E$$

$$\boldsymbol{P}_{\mathbf{E}_n^\alpha}(i,j) = \frac{\mathbf{E}_n^\alpha(i,j)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)},\ \ i,j \in E.$$

Finally the χ^2-square divergence

$$\begin{aligned} \hat{\varDelta}_2(\boldsymbol{P}_{\mathbf{O}_n^\alpha} \| \boldsymbol{P}_{\mathbf{E}_n^\alpha}) &= n \sum_{i=1}^{r} \sum_{j=1}^{m} \frac{(\boldsymbol{P}_{\mathbf{O}_n^\alpha}(i,j) - \boldsymbol{P}_{\mathbf{E}_n^\alpha}(i,j))^2}{\boldsymbol{P}_{\mathbf{E}_n^\alpha}(i,j)} \\ &= n\ \varDelta_2(\boldsymbol{P}_{\mathbf{O}_n^\alpha} \,\|\, \boldsymbol{P}_{\mathbf{E}_n^\alpha}). \end{aligned} \tag{6}$$

Now we derive a version of the Law of Iterated Logarithm, significant for the establisment of subsequent results about the convergence of $\hat{\Delta}_2(\boldsymbol{P}_{\mathbf{O}_n^\alpha}\|\boldsymbol{P}_{\mathbf{E}_n^\alpha})$.

Lemma 3.1. *[18](Theorems 17.0.1 & 17.2.2) Let $\mathbb{X}=\{X_n\}_{n>0}$ be a ergodic Markov chain with finite state space E and stationary distribution Π, $g:\ E\longrightarrow\mathbb{R}$, $S_n(g)=\sum_{j=1}^n g(X_j)$ and*

$$\sigma_g^2=E_\pi\left(g^2(X_1)\right)+2\sum_{j=2}^{n}E_\pi\left(g(X_1)g(X_j)\right)$$

then:

(a) If $\sigma_g^2=0$, then a.s. $\lim_{n\to\infty}\frac{1}{\sqrt{n}}[S_n(g)-E_\pi(S_n(g))]=0$.
(b) If $\sigma_g^2>0$, then a.s.

$$\limsup_{n\to\infty}\frac{S_n(g)-E_\pi(S_n(g))}{\sqrt{2\,\sigma_g^2\,n\,log(log(n))}}=1$$

and

$$\liminf_{n\to\infty}\frac{S_n(g)-E_\pi(S_n(g))}{\sqrt{2\,\sigma_g^2\,n\,log(log(n))}}=-1,$$

(E_Π : expectation with initial distribution Π; a.s. : almost surely). ♦

Lemma 3.2. *[14](Lemma 2) If $\mathbb{Y}^{(\kappa)}$ is ergodic then for $\eta\geq\kappa-1$, $\alpha=a_1^\eta$ and $i\,\alpha\,j=(i,a_1,...,a_\eta,j)=i\,a_1^\eta\,j\in E^{\eta+2}$ we have a.s.*

$$\limsup_{n\to\infty}\frac{\left(N(i\,a_1^\eta\,j\mid\boldsymbol{X}_1^n)-N(i\,a_i^\eta\mid\boldsymbol{X}_1^n)\,p(j|i\,a_1^\eta)\right)^2}{n\log(\log(n))}=2\,\Pi(i\,a_1^\eta\,j)(1-p(j|i\,a_1^\eta)).\quad ♦$$

Theorem 3.3. *Let us refer to (6) for the definition of $\hat{\Delta}_2(P_{\boldsymbol{O}_n^\alpha}\|P_{\boldsymbol{E}_n^\alpha})$, as well as the beginning of the present section for complementary definitions and references related to the following result:*

If $\kappa \leq \eta$, there exist $\mathcal{L} < \infty$ so that for every $\alpha = i_1^\eta \in E^\eta$

$$\boxed{P\left(\limsup_{n\to\infty}\left[\frac{\hat{\Delta}_2(P_{\boldsymbol{O}_n^\alpha}\|P_{\boldsymbol{E}_n^\alpha})}{2\,\log(\log(n))}\right] \leq \mathcal{L}\right) = 1.} \tag{7}$$

If $\eta = \kappa - 1$, there exist a_1^η & $i, j, k \neq i$ such that, $p(j\,|\,i\,a_1^\eta) \neq p(j\,|\,k\,a_1^\eta)$, consequently

$$\boxed{P\left(\limsup_{n\to\infty}\left[\frac{\hat{\Delta}_2(P_{\boldsymbol{O}_n^\alpha}\|P_{\boldsymbol{E}_n^\alpha})}{2\,log(log(n))}\right] = \infty\right) = 1.} \quad \blacklozenge \tag{8}$$

***Proof*:** The following proof shall be divided in the next two cases.

Case I: $0 \leq \kappa \leq \eta$.

From ([25], *Lemma 3.1*) and by Definition **??** we can calculate

$$\mathbf{O}_n^\alpha(i,j) - \mathbf{E}_n^\alpha(i,j) = N(i\,a_1^\eta\,j\,|\,\mathbf{X}_1^n) - \frac{N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)N(a_1^\eta\,j\,|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}$$

or, in the limit

$$\lim_{n\to\infty}\Big(\mathbf{O}_n^\alpha(i,j) - \mathbf{E}_n^\alpha(i,j)\Big)^2 = \lim_{n\to\infty}\Big(N(i\,a_1^\eta\,j\,|\,\mathbf{X}_1^n) - N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)\,p(j\big|i\,a_1^\eta)\Big)^2$$

$$\begin{aligned}
&\limsup_{n\to\infty}\frac{\Big(\mathbf{O}_n^\alpha(i,j) - \mathbf{E}_n^\alpha(i,j)\Big)^2}{n\,\log(log(n))\,\mathbf{P}_{\mathbf{E}_n^\alpha}(i,j)} = \\
= &\limsup_{n\to\infty}\left[\frac{\Big(N(i\,a_1^\eta\,j\,|\,\mathbf{X}_1^n) - N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)\,p(j\big|i\,a_1^\eta)\Big)^2}{n\,\log(log(n))}\frac{1}{\mathbf{P}_{\mathbf{E}_n^\alpha}(i,j)}\right].
\end{aligned}$$

Similarly

$$\lim_{n\to\infty} \mathbf{P}_{\mathbf{E}_n^\alpha}(i,j) = \lim_{n\to\infty} \frac{\mathbf{E}_n^\alpha(i,j)}{N(a_1^\eta|\,\mathbf{X}_1^n)} = \lim_{n\to\infty} \Big(\frac{N(i\,a_1^\eta|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\frac{N(a_1^\eta\,j\,|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\Big) =$$
$$= \lim_{n\to\infty} \Big(\frac{N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)}{n}\frac{n}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\frac{N(a_1^\eta\,j\,|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\Big) = \Pi(i\,a_1^\eta)\frac{1}{\Pi(a_1^\eta)}\,p(j\,|\,a_1^\eta) =$$
$$= \theta(i,j) > 0.$$

By (1) and Lemma 3.2 we have that $\min_{i,j}\theta(i,j) > 0$ with

$$\mathcal{L} = \min_{i,j}\theta(i,j)\sum_{i=1}^{m}\sum_{j=1}^{m}\Pi(i\,a_1^\eta\,j)(1-p(j\big|i\,a_1^\eta)) \le 1$$

$$P\left(\limsup_{n\to\infty}\frac{\hat{\Delta}_2(P_{\mathbf{O}_n^\alpha}\|P_{\mathbf{E}_n^\alpha})}{2\,\log(log(n))} \le \mathcal{L}\right) = 1.$$

Case II: $\eta = \kappa - 1$.
In accordance with the following

$$\lim_{n\to\infty}\frac{N(a_1^\eta\,|\,\mathbf{X}_1^n)}{n} = \lim_{n\to\infty}\sum_{a\in E}\frac{N(a\,a_1^\eta\,|\,\mathbf{X}_1^n)}{n} = \sum_{a\in E}\Pi(a\,a_1^\eta) \quad a.s.$$
$$\lim_{n\to\infty}\frac{N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)}{n} = \Pi(i\,a_1^\eta) \quad a.s.$$

we can obtain, as in previous case

$$\lim_{n\to\infty} \mathbf{P}_{\mathbf{E}_n^\alpha}(i,j) = \lim_{n\to\infty} \frac{\mathbf{E}_n^\alpha(i,j)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)} = \lim_{n\to\infty} \Big(\frac{N(i\,a_1^\eta\,|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\frac{N(a_1^\eta\,j\,|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\Big) =$$
$$= \frac{\Pi(i\,a_1^\eta)}{\sum_{a\in E}\Pi(a\,a_1^\eta)}\frac{\Pi(a_1^\eta\,j)}{\sum_{a\in E}\Pi(a\,a_1^\eta)} \neq 0,$$

and

$$\lim_{n\to\infty} \mathbf{P}_{\mathbf{O}_n^\alpha}(i,j) = \lim_{n\to\infty} \frac{\mathbf{O}_n^\alpha(i,j)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)} = \lim_{n\to\infty} \Big(\frac{N(i\,a_1^\eta\,j\,|\,\mathbf{X}_1^n)}{N(a_1^\eta\,|\,\mathbf{X}_1^n)}\Big) =$$
$$= \frac{\Pi(i\,a_1^\eta)\,p(j\,|\,i\,a_1^\eta)}{\sum_{a\in E}\Pi(a\,a_1^\eta)} \neq 0.$$

Clearly, if $\eta = \kappa - 1$, there exist $\alpha = a_1^\eta$ & $i, j \in E$ so that

$$\lim_{n\to\infty} (\mathbf{P}_{\mathbf{O}_n^\alpha}(i,j) - \mathbf{P}_{\mathbf{E}_n^\alpha}(i,j)) \neq 0$$

since, otherwise, it should imply that

$$p(j \,|\, i\, a_1^\eta) = \frac{\Pi(a_1^\eta\, j)}{\sum_{a\in E} \Pi(a\, a_1^\eta)}$$

i.e. $p(j \,|\, i\, a_1^\eta)$ does not depend on $i \in E$, contradicting the assumption that the order $\kappa > \eta$.

$$P\left(\hat{\Delta}_2(P_{\mathbf{O}_n^\alpha} \| P_{\mathbf{E}_n^\alpha}) = n\, O(1)\right) = 1$$

and (8) is proved. ✓

3.1 Local and Global Dependency Level

Herein we define the Local Dependency Level and the Global Dependency Level.

Definition 3.2. *Let $\boldsymbol{X}_n = \{X_i\}_{i=1}^n$ be a sample of a Markov chain $\mathbb{X}$ of order $\kappa \geq 0$ and $\hat{\Delta}_2(P_{\boldsymbol{O}_n^\alpha} \| P_{\boldsymbol{E}_n^\alpha})$ with $\alpha = a_1^\eta$, $\eta \geq 0$ as previously defined. Let us assume that V is a χ^2 random variable with $(m-1)^2$ degrees of freedom where $\mathcal{P}$ is the continuous strictly decreasing function $\mathcal{P} : \mathbb{R}^+ \longrightarrow [0,1]$*

$$\mathcal{P}(x) = P(V \geq x), \quad x \in \mathbb{R}^+.$$

We define the Local Dependency Level $\widehat{LDL}_n(a_1^\eta)$, for $\alpha = a_1^\eta$ as

$$\boxed{\widehat{LDL}_n(a_1^\eta) = \frac{\hat{\Delta}_2(P_{\boldsymbol{O}_n^\alpha} \| P_{\boldsymbol{E}_n^\alpha})}{2\,\log(\log(n))},}$$

and the Global Dependency Level $\widehat{GDL}_n(\eta)$ as

$$\boxed{\widehat{GDL}_n(\eta) = \mathcal{P}\left(\sum_{a_1^\eta \in E^\eta} \left(\frac{N(a_1^\eta \,|\, \boldsymbol{X}_1^n)}{n}\right) \widehat{LDL}_n(a_1^\eta)\right).} \quad \blacklozenge$$

Observe that, if the hypothesis $\mathbf{H}_0^\alpha$ is true, then $\forall a_1^\eta,\ \eta \geq \kappa,$

$$P\left(\liminf_{n\to\infty}\left(\widehat{GDL}_n(\eta)\right) \geq \mathcal{P}(\mathcal{L})\right) = 1 \tag{9}$$

and for $\eta = \kappa - 1$

$$P\left(\lim_{n\to\infty}\left(\widehat{GDL}_n(\eta)\right) = \mathcal{P}(\infty) = 0\right) = 1. \tag{10}$$

By (9) and (10) it is clear that, for n sufficiently large,

$$P\left(\widehat{GDL}_n(\eta) \approx 0\right) = 1, \quad \eta = \kappa - 1,$$

and

$$P\left(\widehat{GDL}_n(\eta) \approx \mathcal{P}(\mathcal{L})\right) = 1, \quad \eta \geq \kappa.$$

and consequently, for a multiple stationary Markov chain $\mathbb{X}_{n\geq 1}$ of order κ

$$\begin{aligned} \kappa &= 0 \ \Leftrightarrow \ \lim_{n\to\infty}\widehat{GDL}_n(\eta) = \mathcal{P}(\mathcal{L}),\ \eta = 0, 1, .., B\,, \\ \kappa &= \max_{0\leq\eta\leq B}\left\{\ \eta\ :\ \lim_{n\to\infty}\widehat{GDL}_n(\eta) = 0\ \right\} + 1. \end{aligned}$$

Finally, let us define the Markov chain order estimator based on the information contained in the vector GDL_n.

Definition 3.3. *Given a fixed number* $0 < B \in \mathbb{N}$, *let us define the set* $\mathcal{S} = \{0, 1\}^{B+1}$ *and the application* $T : \mathcal{S} \to \mathbb{N}$

$$\begin{aligned} T(s) &= -1 \ \Leftrightarrow \ s_i = 1,\ \ i = 0, 1, .., B \\ T(s) &= \max_{0\leq i\leq B}\left\{i\ :\ s_i = 0,\ s_{i+1} = \mathcal{P}(\mathcal{L})\right\},\ \ s = (s_0, s_1, ..., s_B). \quad \blacklozenge \end{aligned}$$

Definition 3.4. *Let $\boldsymbol{X}_n = \{X_i\}_{i=1}^n$ be a sample for the Markov chain $\mathbb{X}$ of order κ, $0 \le \kappa < B \in \mathbb{N}$ and $\{\widehat{GDL}_n(i)\}_{i=1}^B$ as above. We define the order's estimator $\widehat{\kappa}_{GDL}(\boldsymbol{X}_n)$ as*

$$\widehat{\kappa}_{GDL}(\boldsymbol{X}_n) = T(\sigma_n) + 1$$

with $\sigma_n \in \mathcal{S}$ so that $\forall\, s \in \mathcal{S}$

$$\sum_{i=0}^{B} \left(\widehat{GDL}_n(i) - \sigma_n(i)\right)^2 \le \sum_{i=0}^{B} (\widehat{GDL}_n(i) - s(i))^2. \quad \blacklozenge$$

By (9),(10) and (3.1) it is clear that, for n large enough, $\{GDL_n(i)\}_{i=1}^B$ satisfies the hypothesis of therefore, the order estimator converges almost surely to its value, i.e.,

$$\boxed{P\left(\lim_{n\to\infty} \widehat{\kappa}_{GDL}(\mathbf{X}_n) = \kappa\right) = 1, \quad \kappa = 0, 1, 2, .., B.} \tag{11}$$

4 Numerical Simulations

In what follows we shall compare the non-asymptotic performance, mainly for small samples, of some of the most used Markov chains order estimators. Recalling the previous notations $\alpha = (a_1, ..., a_{k+1}) = a_1^{k+1}$, $N(i\, a_1^{k+1} \,|\, \mathbf{X}_1^n)$ as in (4) and denoting

$$\hat{L}(\eta) = \mathit{\Pi}_{a_1^{\eta+1}} \left[\frac{N(i\, a_1^{\eta+1} \,|\, \mathbf{X}_1^n)}{N(i\, a_1^{\eta} \,|\, \mathbf{X}_1^n)}\right]^{N(i\, a_1^{\eta+1} \,|\, \mathbf{X}_1^n)}$$

the estimators of the Markov chain order κ, are defined, under the hypothesis:

$$\boxed{\textit{There exist a known } B \textit{ so that } 0 \le \kappa \le B}$$

as

$$\widehat{\kappa}_{AIC} = \operatorname{argmin}\{AIC(\eta)\,;\, \eta = 0, 1, ..., B\},$$
$$\widehat{\kappa}_{BIC} = \operatorname{argmin}\{BIC(\eta)\,;\, \eta = 0, 1, ..., B\},$$
$$\widehat{\kappa}_{EDC} = \operatorname{argmin}\{EDC(\eta)\,;\, \eta = 0, 1, ..., B\},$$

where

$$AIC(\eta) = -2\log \hat{L}(\eta) \quad + \quad |E|^{\eta+1}\, 2\,(|E|-1),$$
$$BIC(\eta) = -2\log \hat{L}(\eta) \quad + \quad |E|^{\eta+1}\, 2\,(|E|-1)\left(\frac{\log(n)}{2}\right),$$
$$EDC(\eta) = -2\log \hat{L}(\eta) \quad + \quad |E|^{\eta+1}\, 2\,(|E|-1)\left(\frac{\log\log(n)}{2(|E|-1)}\right),$$
$$AIC(\eta) \ \leq \ EDC(\eta) \ \leq \ BIC(\eta).$$

Clearly, for a given η, the order estimator $GDL(\eta)$, as well as $AIC(\eta)$ [24], $BIC(\eta)$ [22] and $EDC(\eta)$ [25, 14] contain much of the information concerning the sample's relative dependency, nevertheless numerical simulations as well as theoretical considerations anticipates a great deal of variability for small samples.

The following numerical simulation, based on an algorithm due to Raftery[21], starts on with the generation of a Markov chain transition matrix, $\mathbf{Q} = (q_{i_1 i_2 \ldots i_\kappa; i_{\kappa+1}})$ with entries

$$q_{i_1 i_2 \ldots i_\kappa; i_{\kappa+1}} = \sum_{t=1}^{\kappa} \lambda_{i_t} R(i_{\kappa+1}, i_t), \ 1 \leq i_t, i_{\kappa+1} \leq m. \tag{12}$$

where the matrix

$$R(i,j), \ 0 \leq i, j \leq m, \quad \sum_{i=1}^{m} R(i,j) = 1, \ 1 \leq j \leq m$$

and the positive numbers

$$\{\lambda_i\}_{i=1}^{\kappa}, \ \sum_{i=1}^{\kappa} \lambda_i = 1$$

are arbitrarily chosen in advance.

Once the matrix $\mathbf{Q} = (q_{i_1 i_2 \ldots i_\kappa; i_{\kappa+1}})$ is obtained, two hundreds replications of the Markov chain sample of size n, space state E and transition matrix $\mathbf{Q}$ are generated to compare $GDL(\eta)$ performance against the standards, well known and already established order estimators just mentioned above.

Katz(1981) [17] obtained the asymptotic distribution of $\widehat{\kappa}_{AIC}$ and proved its inconsistency showing the existence of a positive probability to overestimate the order. See also Shibata(1976) [23].

On the contrary Schwarz (1978) [22] and Zhao(2001) [25] proved strong consistency for the estimators $\widehat{\kappa}_{BIC}$ and $\widehat{\kappa}_{EDC}$, respectively.

It is quite intuitive that the random information regarding the order of a Markov chain, is spread over an exponentially growing set of empirical distributions Θ with $|\Theta| = m^{B+1}$, where **B** is the maximum integer η, as in $\alpha = (i_1 i_2 ... i_\eta)$. It seems reasonable to think that a small *viable* sample, i.e. samples able to retrieve enough information to estimate the chain order, should have size $n \approx O(m^{B+1})$. Keeping in mind that for the present numerical simulation, the maximum length to be used is $B = 5$, from now on the sample sizes for $|E| = 3$ and $|E| = 4$ should be $n \approx 1.500$ and $n \approx 5.000$, respectively.

Finally, after applying all estimators to each one of the replicated samples, the final results are registered in the form of tables.

Case I: Markov Chain Examples with $\kappa = 0$, $|E| = 3$.

Firstly, we choose the matrix $\{Q_1, Q_2, Q_3\}$ to produce samples with sizes $500 \leq n \leq 2.000$, originated from Markov chains of order $\kappa = 0$ with quite different probability distributions.

$$Q_1 = \begin{bmatrix} 0.33 & 0.335 & 0.335 \\ 0.33 & 0.335 & 0.335 \\ 0.33 & 0.335 & 0.335 \end{bmatrix}, \; Q_2 = \begin{bmatrix} 0.05 & 0.475 & 0.475 \\ 0.05 & 0.475 & 0.475 \\ 0.05 & 0.475 & 0.475 \end{bmatrix}, \; Q_3 = \begin{bmatrix} 0.05 & 0.05 & 0.90 \\ 0.05 & 0.05 & 0.90 \\ 0.05 & 0.05 & 0.90 \end{bmatrix}.$$

$\lvert E\rvert = 3$ $\leftrightarrow$ $\kappa = 0$ $\leftrightarrow$ $\lambda_i = 1/3,\ i = 1,2,3.$												
	Q_1				Q_1				Q_1			
	$n = 500$				$n = 1.000$				$n = 1.500$			
k	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*
0	75.5%	100%	100%	99%	80%	100%	100%	99.5%	71.5%	100%	100%	99%
1	24.5%			1%	18%			0.5%	22.5%			1%
2					2%				6%			
3												
4												

$\|E\| = 3$ $\leftrightarrow$ $\kappa = 0$ $\leftrightarrow$ $\lambda_i = 1/3,\ i = 1,2,3.$												
	Q_2				Q_2				Q_2			
	$n = 1.000$				$n = 1.500$				$n = 500$			
k	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*
0	63.5%	100%	100%	99%	63%	100%	100%	99%	59%	100%	100%	99%
1	29%			1%	34.5%			1%	37%			1%
2	7.5%				2.5%				4%			
3												
4												

$\|E\| = 3$ $\leftrightarrow$ $\kappa = 0$ $\leftrightarrow$ $\lambda_i = 1/3,\ i = 1,2,3.$												
	Q_3				Q_3				Q_3			
	$n = 1.000$				$n = 1.500$				$n = 2.000$			
k	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*
0	43%	100%	100%	98%	47%	100%	99.5%	96%	46%	100%	100%	97%
1	53%			2%	51.5%		0.5%	4%	50.5%			2%
2	4%				1.5%				3.5%			1%
3												
4												

Notice that for a fixed sample size $n = \{500, 1.000, 1.500, 2.000\}$, the order estimator $\widehat{\kappa}_{AIC}$ steadily overestimate the real order $\kappa = 0$ with the excessiveness depending on the probability distribution of the Markov chain. Differently, the order estimators $\widehat{\kappa}_{BIC}$, $\widehat{\kappa}_{EDC}$ and $\widehat{\kappa}_{GDL}$ show consistent performance, mainly obtaining the right order, free from the influence of the sample size and the generating matrix. Regarding $\widehat{\kappa}_{BIC}$ and $\widehat{\kappa}_{EDC}$ improved effect, most likely depends on their correcting factor, $\frac{\log(n)}{2}$ and $\left(\frac{\log\log(n)}{2(|E|-1)}\right)$ which tend to decrease the estimated order.

Case II: Markov Chain Examples with $\kappa = 3, |E| = 3$ and $\kappa = \{2, 3, 0\}, |E| = 4$

Secondly, we choose the matrix $\{Q_4, Q_5\}$ to produce samples with sizes $n \in \{500, 1.000, 1.500, 2.000\}$, originated from Markov chains for $|E| = 3$ of order $\kappa = 3$.

$$Q_4 = \begin{bmatrix} 0.05 & 0.05 & 0.90 \\ 0.05 & 0.90 & 0.05 \\ 0.90 & 0.05 & 0.05 \end{bmatrix}, \qquad Q_5 = \begin{bmatrix} 0.475 & 0.475 & 0.05 \\ 0.475 & 0.05 & 0.475 \\ 0.05 & 0.475 & 0.475 \end{bmatrix}.$$

$\lvert E\rvert = 3 \quad \leftrightarrow \quad \kappa = 3 \quad \leftrightarrow \quad \lambda_i = 1/3,\ i = 1,2,3.$												
	Q_4				Q_4				Q_4			
	$n = 1.000$				$n = 1.500$				$n = 2.000$			
k	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*
0												
1												
2		99.5%	88.5%	41%		76.5%	16.5%	5%		17%	0.5%	1%
3	100%	0.5%	11.5%	59%	100%	23.5%	83.5%	95%	100%	83%	99.5%	99%
4												

$\lvert E\rvert = 3 \quad \leftrightarrow \quad \kappa = 3 \quad \leftrightarrow \quad \lambda_i = 1/3,\ i = 1,2,3.$												
	Q_5				Q_5				Q_5			
	$n = 1.000$				$n = 1.500$				$n = 2.500$			
k	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*
0		0.5%										
1		92.5%	69.5%	6.5%		54.5%	19.5%	1%				
2	16.5%	7%	30.5%	92%	2%	45.5%	80.5%	80.5%		100%	98.5%	8.5%
3	83.5%			1.5%	98%			18.5%	100%		1.5%	91.5%
4												

For $|E| = 3$, $\kappa = 3$ the estimator $\widehat{\kappa}_{AIC}$ overestimate the order in a lesser extent than the previous case, while $\widehat{\kappa}_{BIC}$ and $\widehat{\kappa}_{EDC}$ overweighted by the respective constants $\frac{\log(n)}{2}$ and $\left(\frac{\log\log(n)}{2(|E|-1)}\right)$, underestimate the order more than it was supposed to be. Concerning $\widehat{\kappa}_{GDL}$, it rapidly converges to the right order depending on the sample size n.

For $|E| = 4$ the greater complexity of a Markov chain of order $\kappa = 3$ impose the use of larger sample size for estimators to acomplish some reliability. Finally, we choose the matrix $\{Q_6, Q_7\}$ to produce samples with size $n = 5.000$, originated from Markov chains of order $\kappa \in \{2, 3, 0\}$ like in the previous cases.

$$Q_6 = \begin{bmatrix} 0.05 & 0.05 & 0.05 & 0.85 \\ 0.05 & 0.05 & 0.85 & 0.05 \\ 0.05 & 0.85 & 0.05 & 0.05 \\ 0.85 & 0.05 & 0.05 & 0.05 \end{bmatrix}, \qquad Q_7 = \begin{bmatrix} 0.05 & 0.05 & 0.05 & 0.85 \\ 0.05 & 0.05 & 0.05 & 0.85 \\ 0.05 & 0.05 & 0.05 & 0.85 \\ 0.05 & 0.05 & 0.05 & 0.85 \end{bmatrix}.$$

$\lvert E\rvert = 4 \quad \leftrightarrow \quad n = 5.000$												
	$Q_6 \Leftrightarrow \lambda_i = 1/2,\ i = 1,2.$				$Q_6 \Leftrightarrow \lambda_i = 1/3,\ i = 1,2,3.$				$Q_7 \Leftrightarrow \lambda_i = 1/3,\ i = 1,2,3.$			
	$\kappa = 2$				$\kappa = 3$				$\kappa = 0$			
k	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*	*Aic*	*Bic*	*Edc*	*Gdl*
0									85%	100%	100%	100%
1									15%			
2	100%	100%	100%	100%		99%		4%				
3					100%	1%	100%	96%				
4												
5												
6												

For the order for $|E| = 4$, $\kappa = 0$, apparently $\widehat{\kappa}_{AIC}$ keeps overestimating the order in some degree, while $\widehat{\kappa}_{BIC}$ as in example $\kappa = 3$ severely underestimate the order, presumably due to the excessive weight of the correcting factors $\frac{\log(n)}{2}$. On the contrary $\widehat{\kappa}_{EDC}$ and $\widehat{\kappa}_{GDL}$ behaves quite well in same setting.

5 Conclusion

The pioneer research started with the contributions of Bartlett[6], Hoel[16], Good [15], Anderson & Goodman [4], Billingsley([7], [8]) among others, where they developed tests of hypothesis for the estimation of the order of a given Markov chain.

Later on these procedures were adapted and improved with the used of *Penalty Functions* (Tong[24], Katz[17]) together with other tools created in the realm of Models Selection (Akaike[1], Schwarz[22]). Since then, there have been a considerable number of subsequent contributions on this subject, several of them consisting in the enhancement of the already existing techniques (Csiszar[11], Zhao et all[25]).

In this notes we propose a new Markov chain order estimator based on a different idea which makes it behave in a quite different form. This estimator is strongly consistent and more efficient than AIC (inconsistent), outperforming the well established and consistent BIC and EDC, mainly on relatively small samples.

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