LINEARLY CONSTRAINED IOSIFESCU-THEODORESCU ENTROPY MAXIMIZATION FOR HOMOGENEOUS STATIONARY MULTIPLE MARKOV CHAINS

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Using the maximum entropy principle and the geometric programming method we solve the problem of maximization of the Iosifescu-Theodorescu entropy for discrete time finite homogeneous stationary Markov chains of order r with linear constraints on r-step transition probabilities.

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1. PROBLEM STATEMENT

Let $\{X(t),\ t \in \mathbb{N}\}$ be a homogeneous stationary Markov chain of order r ($r \in \mathbb{N}^*$) with the finite state space $I = \{1, \dots, n\}$ ($n \in \mathbb{N}^*$). We denote by $\mathrm{P}^{(r)} = \big(P^{(r)}_{i_1,\dots,i_r,j}\big)_{(i_1,\dots,i_r,j)\in I^{r+1}}$ the r-step transition probabilities, i.e.,

$$P^{(r)}_{i_1,\dots,i_r,j} = P(X(t+r) = j | X(t) = i_1, \dots, X(t+r-1) = i_r), \quad \forall t \in \mathbb{N},$$

for any $i_1, \dots, i_r, j \in I$. Also, we denote by $\pi^{(r)} = \big(\pi^{(r)}_{i_1,\dots,i_r}\big)_{(i_1,\dots,i_r)\in I^r}$ the joint probability of the states at r consecutive times, i.e.,

$$\pi^{(r)}_{i_1,\dots,i_r} = P(X(t) = i_1, \dots, X(t+r-1) = i_r), \quad \forall t \in \mathbb{N},$$

for any $i_1, \dots, i_r \in I$. Clearly, the following relations hold

$$\pi^{(r)}_{i_1,\dots,i_r} \geq 0, \quad \forall i_1, \dots, i_r \in I, \tag{1}$$

$$\sum_{i_1,\dots,i_r \in I} \pi^{(r)}_{i_1,\dots,i_r} = 1, \tag{2}$$

$$\sum_{i_1,\dots,i_k \in I} \pi^{(r)}_{i_1,\dots,i_k,i_{k+1},\dots,i_r} = \sum_{i_1,\dots,i_k \in I} \pi^{(r)}_{i_{k+1},\dots,i_r,i_1,\dots,i_k}, \quad \forall k \in \{1, \dots, r-1\}, \tag{3}$$

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$$P^{(r)}_{i_1,\ldots,i_r,j} \geq 0, \quad \forall i_1,\ldots,i_r,j \in I,$$

$$\sum_{j\in I} P^{(r)}_{i_1,\ldots,i_r,j} = 1, \quad \forall i_1,\ldots,i_r \in I, \tag{4}$$

$$\sum_{i_1,\ldots,i_r\in I} \pi^{(r)}_{i_1,\ldots,i_r} P^{(r)}_{i_1,\ldots,i_r,j} = \sum_{i_1,\ldots,i_{r-1}\in I} \pi^{(r)}_{i_1,\ldots,i_{r-1},j}, \quad \forall j \in I. \tag{5}$$

For $r \geq 2$, at any time $t \in \mathbb{N}$, the state probability distribution $\pi^{(1)} = \big(\pi^{(1)}_j\big)_{j\in I}$ is given by

$$\pi^{(1)}_j = P(X(t)=j) = \sum_{i_1,\ldots,i_{r-1}\in I} \pi^{(r)}_{i_1,\ldots,i_{r-1},j}, \quad \forall j \in I,$$

and the (1-step) transition probabilities $\big(P^{(1)}_{ij}\big)_{i,j\in I}$ are given by

$$P^{(1)}_{ij} = P(X(t+1)=j|X(t)=i) = \frac{\sum\limits_{i_1,\ldots,i_{r-2}\in I} \pi^{(r)}_{i_1,\ldots,i_{r-2},i,j}}{\sum\limits_{i_1,\ldots,i_{r-1}\in I} \pi^{(r)}_{i_1,\ldots,i_{r-1},i}}, \quad \forall i,j \in I.$$

Hence the chain $\{X(t),\ t \in \mathbb{N}\}$ is completely characterized by the distribution $\pi^{(r)}$ and the transition probabilities $\mathrm{P}^{(r)}$.

Definition 1.1 (see [9]). Let $\{X(t),\ t \in \mathbb{N}\}$ be a homogeneous stationary Markov chain of order r as above. The *Iosifescu-Theodorescu entropy* (*IT-entropy*) of this chain is defined as

$$H^{(r)}\big(\mathrm{P}^{(r)}\big) = -\sum_{i_1,\ldots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\ldots,i_r} P^{(r)}_{i_1,\ldots,i_r,j} \ln P^{(r)}_{i_1,\ldots,i_r,j}.$$

For notational convenience, $0 \ln 0 = 0$.

Remark 1.1. The IT-entropy measures the amount of remained uncertainty of the chain at any arbitrary time after the knowledge of its behavior at r latest times or, equivalently, at all previous times.

The reconstruction of such multiple Markov chain, when only a partial information is given, arises in many practical applications from various fields as economics, psychology, biology (see, e.g., Iosifescu [7], Iosifescu and Grigorescu [8]). The r-step transition probabilities are to be found only from the knowledge of the stationary distribution $\pi^{(r)}$ and, possibly, of some additional constraints, usually expressed by mean values. The maximum entropy principle, introduced by Jaynes [10, 11], states that one should choose the r-step transition probabilities that are consistent with the given constraints but maximize the IT-entropy of the chain.

In this paper we study the useful case of linear equality constraints. Thus, we consider the following optimization problem

$$(P): \quad \left| \begin{array}{l} \max H^{(r)}(\mathrm{P}^{(r)}) = -\sum\limits_{i_1,\dots,i_r\in I}\sum\limits_{j\in I}\pi^{(r)}_{i_1,\dots,i_r}P^{(r)}_{i_1,\dots,i_r,j}\ln P^{(r)}_{i_1,\dots,i_r,j} \text{ s.t.} \\ \mathrm{AP}^{(r)} = \mathrm{b}, \\ \mathrm{P}^{(r)} \geq 0, \end{array} \right.$$

where $\mathrm{P}^{(r)} = \big(P^{(r)}_{i_1,\dots,i_r,j}\big)_{(i_1,\dots,i_r,j)\in I^{r+1}} \in \mathbb{R}^{n^{r+1}}$ (so it is an n^{r+1}-dimensional column vector), $\pi^{(r)} = \big(\pi^{(r)}_{i_1,\dots,i_r}\big)_{(i_1,\dots,i_r)\in I^r} \in \mathbb{R}^{n^r}$ is a given stationary distribution which verifies (1), (2) and (3), $\mathrm{A} = (a_{k;i_1,\dots,i_r,j})_{k\in\{1,\dots,m\},\,(i_1,\dots,i_r,j)\in I^{r+1}} \in \mathbb{R}^{m\times n^{r+1}}$ is a known matrix and $\mathrm{b} = (b_1,\dots,b_m)^\top \in \mathbb{R}^m$ is a known vector ($m \in \mathbb{N}^*$).

We assume that

$$\pi^{(r)} > 0. \tag{6}$$

Also, we assume that the equalities (4) and (5) hold for any feasible solution $\mathrm{P}^{(r)}$ of problem (P).

Remark 1.2. This assumption is not restrictive since every of equations (4) and (5) is a linear constraint of type $\mathrm{AP}^{(r)} = b$.

Remark 1.3. The problem (P) is an linearly constrained programming problem with a concave objective function.

Next, we use the geometric entropic programming method, introduced by Erlander [1], to solve problem (P). We would like to point out that the maximum entropy principle and the geometric entropic programming method were used by Gerchak [3], Gzyl and Velásquez [5], Preda and Bălcău [15] for maxentropic reconstruction of simple Markov chains.

2. THE GEOMETRIC DUAL PROBLEM

To construct a geometric dual problem for problem (P), we use the following result concerning the IT-entropy.

LEMMA 2.1. *Let* $\mathrm{P}^{(r)}$ *be a feasible solution of problem* (P)*. Then, for any vector* $y = (y_{i_1,\dots,i_r,j})_{(i_1,\dots,i_r,j)\in I^{r+1}} \in \mathbb{R}^{n^{r+1}}$ *the next inequality holds*

$$\begin{aligned} H^{(r)}(\mathrm{P}^{(r)}) \leq \ln \sum_{i_1,\dots,i_r\in I}\sum_{j\in I} e^{y_{i_1,\dots,i_r,j}} - H(\pi^{(r)}) - \\ - \sum_{i_1,\dots,i_r\in I}\sum_{j\in I}\pi^{(r)}_{i_1,\dots,i_r}P^{(r)}_{i_1,\dots,i_r,j}y_{i_1,\dots,i_r,j}, \end{aligned} \tag{7}$$

where

$$H\big(\pi^{(r)}\big) = -\sum_{i_1,\dots,i_r\in I} \pi^{(r)}_{i_1,\dots,i_r} \ln \pi^{(r)}_{i_1,\dots,i_r}$$

is the Shannon entropy of distribution $\pi^{(r)}$. *Moreover, the inequality becomes an equality if and only if*

$$P^{(r)}_{i_1,\dots,i_r,j} = \frac{e^{y_{i_1,\dots,i_r,j}}}{\pi^{(r)}_{i_1,\dots,i_r} \sum\limits_{s_1,\dots,s_r\in I} \sum\limits_{t\in I} e^{y_{s_1,\dots,s_r,t}}}, \quad \forall i_1,\dots,i_r,j\in I. \tag{8}$$

Proof. *Case* 1. Assume that $P^{(r)}_{i_1,\dots,i_r,j} > 0$, $\forall i_1,\dots,i_r,j\in I$. It follows from (4) and (2) that

$$\sum_{i_1,\dots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} = \sum_{i_1,\dots,i_r\in I} \pi^{(r)}_{i_1,\dots,i_r} = 1. \tag{9}$$

Applying the Jensen's inequality for the strictly concave function $\ln x$ we obtain that

$$\ln \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} \frac{e^{y_{i_1,\dots,i_r,j}}}{\pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j}} \geq$$
$$\geq \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} \ln \frac{e^{y_{i_1,\dots,i_r,j}}}{\pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j}},$$

and the equality holds if and only if

$$\frac{e^{y_{i_1,\dots,i_r,j}}}{\pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j}} = C, \quad \forall i_1,\dots,i_r,j\in I,$$

where C is a real constant, $C>0$. Using (4) we derive that

$$\ln \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} e^{y_{i_1,\dots,i_r,j}} \geq \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} y_{i_1,\dots,i_r,j} -$$
$$- \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} \ln P^{(r)}_{i_1,\dots,i_r,j} - \sum_{i_1,\dots,i_r\in I} \pi^{(r)}_{i_1,\dots,i_r} \ln \pi^{(r)}_{i_1,\dots,i_r},$$

and hence we obtain the inequality (7). The equality holds if and only if there exists a non-negative constant C such that

$$P^{(r)}_{i_1,\dots,i_r,j} = \frac{e^{y_{i_1,\dots,i_r,j}}}{C\pi^{(r)}_{i_1,\dots,i_r}}, \quad \forall i_1,\dots,i_r,j\in I.$$

Using (9) we deduce that

$$C = \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} e^{y_{i_1,\dots,i_r,j}},$$

and hence we obtain the equality (8).

Case 2. Let now $P^{(r)}_{i_1,\dots,i_r,j} \geq 0,\ \forall i_1,\dots,i_r,j \in I$. We set

$$J = \{(i_1,\dots,i_r,j) \in I^{r+1} \mid P^{(r)}_{i_1,\dots,i_r,j} > 0\}.$$

It follows from (9) that

$$\sum_{(i_1,\dots,i_r,j)\in J} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} = 1.$$

According to Case 1 we have

$$\ln \sum_{(i_1,\dots,i_r,j)\in J} e^{y_{i_1,\dots,i_r,j}} \geq \sum_{(i_1,\dots,i_r,j)\in J} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} y_{i_1,\dots,i_r,j} - \\ - \sum_{(i_1,\dots,i_r,j)\in J} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} \ln\left(\pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j}\right).$$

But, using the definition of the set J and the monotonicity of the logarithm function, we have

$$\ln \sum_{(i_1,\dots,i_r,j)\in J} e^{y_{i_1,\dots,i_r,j}} \leq \ln \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} e^{y_{i_1,\dots,i_r,j}},$$

$$\sum_{(i_1,\dots,i_r,j)\in J} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} y_{i_1,\dots,i_r,j} = \sum_{i_1,\dots,i_r\in I} \sum_{j\in I} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} y_{i_1,\dots,i_r,j},$$

$$\sum_{(i_1,\dots,i_r,j)\in J} \pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j} \ln\left(\pi^{(r)}_{i_1,\dots,i_r} P^{(r)}_{i_1,\dots,i_r,j}\right) = -H^{(r)}(\mathrm{P}^{(r)}) - H(\pi^{(r)}),$$

and hence we obtain the inequality (7). The equality holds if and only $J = I^{r+1}$ and

$$P^{(r)}_{i_1,\dots,i_r,j} = \frac{e^{y_{i_1,\dots,i_r,j}}}{\pi^{(r)}_{i_1,\dots,i_r} \sum\limits_{(s_1,\dots,s_r,t)\in J} e^{y_{s_1,\dots,s_r,t}}}, \quad \forall (i_1,\dots,i_r,j) \in J,$$

which is equivalent to (8). $\square$

Based on Lemma 2.1, we can define the geometric dual problem of problem (P), namely,

$$(D): \quad \left| \begin{array}{l} \min d(\mathrm{z}) = \ln \sum\limits_{i_1,\dots,i_r\in I} \sum\limits_{j\in I} e^{-\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}}{\pi^{(r)}_{i_1,\dots,i_r}}} + \mathrm{b}^{\top}\mathrm{z} - H(\pi^{(r)}) \text{ s.t.} \\ \mathrm{z} \in \mathbb{R}^m, \end{array} \right.$$

where $\mathrm{z} = (z_1,\dots,z_m)^{\top} \in \mathbb{R}^m$ and, for any $i_1,\dots,i_r,j \in I$, $\mathrm{A}_{i_1,\dots,i_r,j} = (a_{k;i_1,\dots,i_r,j})_{k\in\{1,\dots,m\}}$ denotes the $(i_1,\dots,i_r,j)$-th column of matrix A.

Remark 2.1. The dual problem (D) is an unconstrained convex programming problem having a continuously differentiable objective function. Thus, compared to the primal problem (P), the dual problem (D) is more attractive from the computational point of view.

We can now prove the weak duality between problems (P) and (D).

THEOREM 2.1 (Weak duality). *If* $\mathrm{P}^{(r)}$ *and* z *are feasible solutions of problems* (P) *and* (D)*, respectively, then*

$$H^{(r)}(\mathrm{P}^{(r)}) \leq d(\mathrm{z}).$$

Proof. From $\mathrm{AP}^{(r)} = \mathrm{b}$ it follows that $\left(\mathrm{AP}^{(r)}\right)^\top \mathrm{z} = \mathrm{b}^\top \mathrm{z}$. Therefore, according to (7) we have

$$H^{(r)}(\mathrm{P}^{(r)}) \leq \ln \sum_{i_1,\ldots,i_r \in I} \sum_{j \in I} e^{y_{i_1,\ldots,i_r,j}} - \sum_{i_1,\ldots,i_r \in I} \sum_{j \in I} \pi^{(r)}_{i_1,\ldots,i_r} P^{(r)}_{i_1,\ldots,i_r,j} y_{i_1,\ldots,i_r,j} - \\ - H(\pi^{(r)}) + \mathrm{b}^\top \mathrm{z} - \sum_{k=1}^{m} \sum_{i_1,\ldots,i_r \in I} \sum_{j \in I} a_{k;i_1,\ldots,i_r,j} P^{(r)}_{i_1,\ldots,i_r,j} z_k,$$

for any $\mathrm{y} = (y_{i_1,\ldots,i_r,j})_{(i_1,\ldots,i_r,j) \in I^{r+1}} \in \mathbb{R}^{n^{r+1}}$. By rearranging the terms we obtain

$$H^{(r)}(\mathrm{P}^{(r)}) \leq \ln \sum_{i_1,\ldots,i_r \in I} \sum_{j \in I} e^{y_{i_1,\ldots,i_r,j}} + \mathrm{b}^\top \mathrm{z} - H(\pi^{(r)}) - \\ - \sum_{i_1,\ldots,i_r \in I} \sum_{j \in I} \left(\mathrm{A}_{i_1,\ldots,i_r,j}{}^\top \mathrm{z} + \pi^{(r)}_{i_1,\ldots,i_r} y_{i_1,\ldots,i_r,j} \right) P^{(r)}_{i_1,\ldots,i_r,j}.$$

Taking

$$y_{i_1,\ldots,i_r,j} = -\frac{\mathrm{A}_{i_1,\ldots,i_r,j}{}^\top \mathrm{z}}{\pi^{(r)}_{i_1,\ldots,i_r}}, \quad \forall i_1, \ldots, i_r, j \in I$$

it follows that $H^{(r)}(\mathrm{P}^{(r)}) \leq d(\mathrm{z})$. $\square$

3. STRONG DUALITY

In this section we establish the strong duality between problems (P) and (D). The next theorem is the main result of this paper.

THEOREM 3.1 (Strong duality). *If* z^* *is an optimal solution of the dual problem* (D)*, then* $\mathrm{P}^{*(r)}$ *given by*

$$P^{*(r)}_{i_1,\dots,i_r,j} = \frac{e^{-\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{i_1,\dots,i_r}}}}{\pi^{(r)}_{i_1,\dots,i_r}\sum\limits_{s_1,\dots,s_r\in I}\sum\limits_{t\in I} e^{-\frac{\mathrm{A}_{s_1,\dots,s_r,t}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{s_1,\dots,s_r}}}}, \quad \forall i_1,\dots,i_r,j\in I$$

is an optimal solution of the primal problem (P) *and the duality gap vanishes, i.e.,* $H^{(r)}(\mathrm{P}^{*(r)}) = d(\mathrm{z}^*)$.

Proof. Since the point z^* minimizes $d(\mathrm{z})$ over $\mathbb{R}^m$ it follows that the first partial derivatives of $d(\mathrm{z})$ must be zero at this point, i.e.,

$$0 = \frac{\partial d}{\partial z_k}(\mathrm{z}^*) = -\frac{\sum\limits_{i_1,\dots,i_r\in I}\sum\limits_{j\in I}\frac{a_{k;i_1,\dots,i_r,j}}{\pi^{(r)}_{i_1,\dots,i_r}} e^{-\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{i_1,\dots,i_r}}}}{\sum\limits_{i_1,\dots,i_r\in I}\sum\limits_{j\in I} e^{-\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{i_1,\dots,i_r}}}} + b_k =$$

$$= -\sum_{i_1,\dots,i_r\in I}\sum_{j\in I} a_{k;i_1,\dots,i_r,j} P^{*(r)}_{i_1,\dots,i_r,j} + b_k, \quad \forall k\in\{1,\dots,m\},$$

which means that $\mathrm{AP}^{*(r)} = \mathrm{b}$. Obviously, $\mathrm{P}^{*(r)} \geq 0$, and hence $\mathrm{P}^{*(r)}$ is a feasible solution for problem (P). Applying the equality part of Lemma 2.1 for

$$\mathrm{P}^{(r)} = \mathrm{P}^{*(r)} \quad \text{and} \quad y_{i_1,\dots,i_r,j} = -\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{i_1,\dots,i_r}}, \quad \forall i_1,\dots,i_r,j\in I,$$

we obtain that

$$H^{(r)}(\mathrm{P}^{*(r)}) - \ln\sum_{i_1,\dots,i_r\in I}\sum_{j\in I} e^{-\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{i_1,\dots,i_r}}} + H(\pi^{(r)}) =$$

$$= -\sum_{i_1,\dots,i_r\in I}\sum_{j\in I}\pi^{(r)}_{i_1,\dots,i_r} P^{*(r)}_{i_1,\dots,i_r,j}\left(-\frac{\mathrm{A}_{i_1,\dots,i_r,j}{}^{\top}\mathrm{z}^*}{\pi^{(r)}_{i_1,\dots,i_r}}\right) =$$

$$= \sum_{k=1}^{m}\left(\sum_{i_1,\dots,i_r\in I}\sum_{j\in I} a_{k;i_1,\dots,i_r,j} P^{*(r)}_{i_1,\dots,i_r,j}\right) z^*_k = \sum_{k=1}^{m} b_k z^*_k,$$

and hence $H^{(r)}(\mathrm{P}^{*(r)}) = d(\mathrm{z}^*)$.

Finally, according to Theorem 2.1 it follows that

$$H^{(r)}(\mathrm{P}^{*(r)}) = d(\mathrm{z}^*) \geq H^{(r)}(\mathrm{P}^{(r)}),$$

for any feasible solution $\mathrm{P}^{(r)}$ of problem (P), so $\mathrm{P}^{*(r)}$ is an optimal solution for this problem. □

Remark 3.1. In the particular case when problem (P) has not additional constraints, i.e., this problem has only the obligatory constraints (4) and (5), we can solve the corresponding dual problem (D) and, by using Theorem 3.1, we obtain that problem (P) has an unique optimal solution $\mathrm{P}^{*(r)}$ given by

$$P^{*(r)}_{i_1,\dots,i_r,j} = \pi^{(1)}_j, \quad \forall i_1,\dots,i_r,j \in I,$$

and its optimal value is

$$H^{(r)}(\mathrm{P}^{*(r)}) = H(\pi^{(1)}).$$

We mention that this result can also be obtained by using the properties of the conditional entropy (see Preda and Bălcău [16]).

Remark 3.2. By taking $r = 1$ we regain the result of Gerchak [3] concerning the maximum entropy of simple Markov chain.

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