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## Statistical problems related to irrational rotations

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**Abstract** Let  $\xi_i := [i\alpha + \beta] - [(i-1)\alpha + \beta]$  ( $i = 1, 2, \dots, m$ ) be random variables as functions of  $\beta$  in the probability space  $[0, 1)$  with the Lebesgue measure, where  $\alpha \in [0, 1]$  is considered to be an unknown parameter which we want to estimate from the observation  $\xi := \xi_1, \xi_2, \dots, \xi_m$ . Let an observation  $\xi$  be given, which is a finite Sturmian sequence. We determine the likelihood function  $P_\alpha(\xi)$  as a function of parameter  $\alpha$ , and obtain the maximum likelihood estimator  $\hat{\alpha}(\xi)$  as the relative frequency of 1s in a minimal cycle of  $\xi$ , where a factor  $\eta$  of  $\xi$  is called a minimal cycle if  $\xi$  is a factor of  $\eta^\infty$  and  $\eta$  has the minimum length among them. We also obtain a minimum sufficient statistics. The sample mean  $(\xi_1 + \xi_2 + \dots + \xi_m)/m$  which is an unbiased estimator of  $\alpha$  is not admissible if  $m = 6$  or  $m \geq 8$  since it is not based on the minimum sufficient statistics.

**Keywords** Sturmian sequence · Irrational rotations · Minimum sufficient statistics · Admissible estimator · UMVUE

### 1 Introduction

Let  $\xi = \xi_1, \xi_2, \dots, \xi_m$  be a finite 0-1-sequence. We denote the length  $m$  of  $\xi$  by  $|\xi|$  and the number of 1s in  $\xi$  by  $|\xi|_1$ . We also denote  $\rho(\xi) := |\xi|_1/|\xi|$ , the relative frequency of 1s in  $\xi$ . Let  $\eta = \eta_1, \eta_2, \dots, \eta_n$  be a finite 0-1-sequence. We say that  $\eta$  is a *factor* of  $\xi$  if there exists an integer  $i$  with  $0 \leq i \leq m - n$  such that  $\eta_j = \xi_{i+j}$  ( $j = 1, 2, \dots, n$ ). In this case, we denote  $\eta < \xi$ . We say that  $\eta$  is a *prefix* of  $\xi$  if the above holds with  $i = 0$ .

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A finite 0-1-sequence is called *nontrivial* if it contains both 0 and 1.

For a finite 0-1-sequence  $\xi = \xi_1 \xi_2 \cdots \xi_m$ , we denote by  $\underline{\Omega}_\xi$  and  $\overline{\Omega}_\xi$  the set of  $(\alpha, \beta) \in [0, 1] \times [0, 1)$  satisfying

$$\xi_i = \lfloor i\alpha + \beta \rfloor - \lfloor (i - 1)\alpha + \beta \rfloor \quad (i = 1, 2, \dots, m), \tag{1}$$

and

$$\xi_i = \lceil i\alpha + \beta \rceil - \lceil (i - 1)\alpha + \beta \rceil \quad (i = 1, 2, \dots, m), \tag{2}$$

respectively. Here  $\lfloor \cdot \rfloor$  denotes the floor (rounding down) function, and  $\lceil \cdot \rceil$  denotes the ceiling (rounding up) function. Then, it holds for any finite 0-1-sequence  $\xi$  that  $\underline{\Omega}_\xi \neq \emptyset$  if and only if  $\overline{\Omega}_\xi \neq \emptyset$  (Lemma 1). We call  $\xi$  a (finite) *Sturmian* sequence if  $\underline{\Omega}_\xi \neq \emptyset$ . We denote by  $St_m$  the set of Sturmian sequences of length  $m$ .

An infinite sequence  $\xi_1 \xi_2 \xi_3 \cdots$  such that

$$\xi_i = \lfloor i\alpha + \beta \rfloor - \lfloor (i - 1)\alpha + \beta \rfloor \quad (\forall i) \quad (\text{or} \quad \xi_i = \lceil i\alpha + \beta \rceil - \lceil (i - 1)\alpha + \beta \rceil \quad (\forall i))$$

for a fixed pair  $(\alpha, \beta) \in [0, 1] \times [0, 1)$  with irrational  $\alpha$  is called an (infinite) *Sturmian* sequence which is a symbolic representation of the rotation  $\mathcal{R}_\alpha \theta = \theta + \alpha \pmod{1}$ . It determines  $\alpha$  as the relative frequency of 1 in  $\xi$ . Moreover, such sequences are characterized as the least complex sequences other than the eventually periodic sequences. Since the finite sequence  $\xi$  does not determine  $\alpha$ , it becomes a problem of statistical inference how to estimate  $\alpha$  from  $\xi$  under a suitable statistical model. Sturmian sequences appear in biological neuron model. Hata (1982) showed that aperiodic spike sequences generated by a single neuron model (Nagumo-Sato model, Nagumo and Sato, 1972) are Sturmian.

The partition of  $[0, 1] \times [0, 1)$  by  $\Omega_\xi$ s for  $m = 3$  is as follows, where the set  $\Omega_\xi$  is denoted simply by  $\xi$ :

We may consider  $\xi = \xi_1 \xi_2 \cdots \xi_m$  as a random variable defined by Eq. (1) with random element  $\beta$  in the Lebesgue measure space  $[0, 1)$  and unknown parameter  $\alpha$  in  $[0, 1]$ . The sample space is  $St_m$ . As usual the probability, expectation and variance under the parameter  $\alpha$  is denoted by  $P_\alpha$ ,  $E_\alpha$  and  $V_\alpha$ , respectively. Thus, we have a statistical model  $(St_m, P_\alpha, \alpha \in [0, 1])$ .

By Eq. (1),

$$|\xi|_1 = \lfloor m\alpha + \beta \rfloor = \begin{cases} \lfloor m\alpha \rfloor & (\beta < 1 - \{m\alpha\}) \\ \lfloor m\alpha \rfloor + 1 & (\beta \geq 1 - \{m\alpha\}), \end{cases}$$

where  $\{ \}$  denotes the fractional part. Hence, we have

$$\begin{aligned} E_\alpha(\rho(\xi)) &= (1/m)E_\alpha(|\xi|_1) \\ &= (1/m)(\lfloor m\alpha \rfloor(1 - \{m\alpha\}) + (\lfloor m\alpha \rfloor + 1)\{m\alpha\}) \\ &= (1/m)(\lfloor m\alpha \rfloor + \{m\alpha\}) \\ &= (1/m)(m\alpha) = \alpha \end{aligned} \tag{3}$$

$$\begin{aligned} V_\alpha(\rho(\xi)) &= (1/m^2)E_\alpha((|\xi|_1 - m\alpha)^2) \\ &= (1/m^2)((\lfloor m\alpha \rfloor - m\alpha)^2(1 - \{m\alpha\}) + (\lfloor m\alpha \rfloor + 1 - m\alpha)^2\{m\alpha\}) \\ &= (1/m^2)(\{m\alpha\}^2(1 - \{m\alpha\}) + (1 - \{m\alpha\})^2\{m\alpha\}) \\ &= (1/m^2)\{m\alpha\}(1 - \{m\alpha\}). \end{aligned} \tag{4}$$

Therefore, the sample mean  $\rho(\xi)$  is an unbiased estimator of  $\alpha$  having the variance given by Eq. (4). It is not admissible if  $m = 6$  or  $m \geq 8$  under the quadratic loss function since it is not based on a minimum sufficient statistics (Theorem 2).

The following theorem is well known.

**Theorem 1** (Morse and Hedlund, 1940) *For any finite 0-1-sequence  $\xi$ ,  $\xi$  is Sturmian if and only if it is balanced, i.e.,  $|\sum_i^{i+L} \xi_i - \sum_j^{j+L} \xi_j| \leq 1$  holds for any positive integers  $i, j, L$  such that  $1 \leq i + L \leq |\xi|, 1 \leq j + L \leq |\xi|$ .*

Let  $m$  be a positive integer. Then, we have the partition (see Fig. 1)

$$[0, 1] \times [0, 1) = \bigcup_{\xi \in \text{St}_m} \underline{\Omega}_\xi \text{ (disjoint).} \tag{5}$$

This partition is discussed in Yasutomi (1998) and Berstel and Pocchiola, (1996)

In Berstel and Pocchiola, (1996), it is proved that for any finite Sturmian sequence  $\xi$ , the domain  $\underline{\Omega}_\xi$  is surrounded by at most four pieces of line segments, at most two from above and at most two from below. Thus, there are only three cases as in Fig. 2 for the shape of  $\underline{\Omega}_\xi$ .

In this paper, we prove that in the third case in Fig. 2, the abscissas of  $A$  and  $B$  coincide (Lemma 7), which implies that the graph of  $P_\alpha(\xi)$  with respect to  $\alpha$  given  $\xi$  is of triangular shape as in Fig. 3. The value  $\hat{\alpha} = \hat{\alpha}(\xi)$  which maximize  $P_\alpha(\xi)$  is the *maximum likelihood estimator*. That is,

$$P_{\hat{\alpha}}(\xi) = \max_{\alpha \in [0,1]} P_\alpha(\xi). \tag{6}$$

In Takahashi (2002) and Takahashi and Aihara (2003), it is proved that  $|\alpha_1 - \alpha_2| \leq 2m - 1/m(m - 1)$  for any  $m = 2, 3, \dots$  and  $\xi \in \text{St}_m$ , where  $\alpha_1$  and

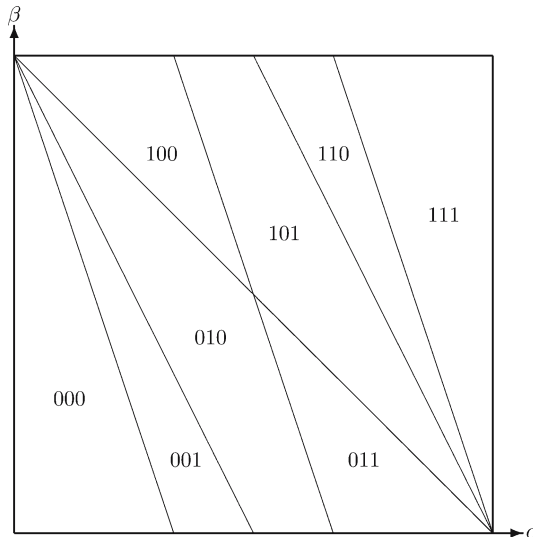


Fig. 1 Partition by  $\underline{\Omega}_\xi$ s for  $m = 3$

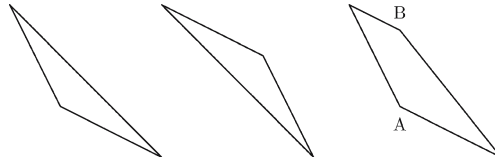


Fig. 2 Shape of  $\Omega_\xi$

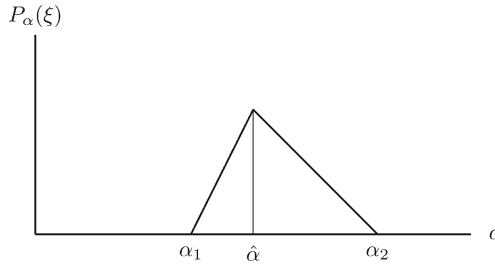


Fig. 3 Likelihood function

$\alpha_2$  are such that  $[\alpha_1, \alpha_2]$  is the support of the likelihood function  $P_\alpha(\xi)$  (Fig. 3). This implies that the maximum likelihood estimator  $\hat{\alpha}$  as a function of  $(\alpha, \beta) \in [0, 1] \times [0, 1)$  and  $m$  through  $\xi \in St_m$  defined by Eq. (1) converge to  $\alpha$  as  $m \rightarrow \infty$  for any  $\beta \in [0, 1)$ , i.e.,  $\hat{\alpha}$  always converges to  $\alpha$  without exception, which is a stronger property than the strong consistency, i.e.,  $\lim_{m \rightarrow \infty} \hat{\alpha} = \alpha$  ( $P_\alpha - a.e.$ ).

Let  $\xi = \xi_1 \xi_2 \cdots \xi_m$  be a 0-1-sequence. A positive integer  $p$  is called a *period* of  $\xi$  if

$$\xi_i = \xi_{i+p} \quad (i = 1, 2, \dots, m - p). \tag{7}$$

This is equivalent to saying that for any factor  $\eta$  of  $\xi$  with  $|\eta| = p$ ,  $\xi < \eta^\infty$  holds, where  $\eta^\infty$  implies the infinite time concatenation of  $\eta$ .

The minimum positive integer  $p$  as Eq. (7) is denoted by  $\text{per}(\xi)$ . Note that  $\text{per}(\xi)$  always exists since  $|\xi|$  is clearly a period of  $\xi$ . A factor  $\eta$  of  $\xi$  is called a *minimal cycle* of  $\xi$  if  $|\eta| = \text{per}(\xi)$ . We define  $\hat{\rho}(\xi) := \rho(\eta)$ , where  $\eta$  is any minimal cycle of  $\xi$ .

For example, let  $\xi = 0100100100$  then  $m = |\xi| = 10$ , periods of  $\xi$  are 3, 6, 9,  $\text{per}(\xi) = 3$  and factors are 0, 1, 01, 10, 00, 001, 010, 100,  $\dots$ . We see that  $\eta = 010$  is a minimum cycle,  $\hat{\rho}(\xi) = \rho(\eta) = 1/3$  and  $\rho(\xi) = 3/10$ .

Recall that a statistics  $T = T(\xi)$  is called *sufficient* if for any  $\xi \in St_m$  and  $t$ , the conditional distribution  $P_\alpha(\xi | T = t)$  does not depend on  $\alpha \in [0, 1]$  as long as  $P_\alpha(T = t) > 0$ .

This condition of sufficiency is equivalent to the following: for any  $\xi, \xi' \in St_m$ ,  $T(\xi) = T(\xi')$  holds if and only if  $\hat{\alpha}(\xi) = \hat{\alpha}(\xi')$ ,  $\alpha_1(\xi) = \alpha_1(\xi')$  and  $\alpha_2(\xi) = \alpha_2(\xi')$  holds (Fig. 3). A sufficient statistics  $T$  is called a *minimum sufficient statistics* if for any sufficient statistics  $T'$ , the partition on  $St_m$  induced by  $T'$  is finer than that induced by  $T$ . Note that a minimum sufficient statistics is unique in the sense of the partition induced on  $St_m$ . Clearly, the triple  $(\hat{\alpha}, \alpha_1, \alpha_2)$  is a minimum sufficient statistics.

For  $\xi \in \text{St}_m$ , we define

$$\underline{I}(\xi) := \left\{ i \in \{0, 1, \dots, m\}; \Xi_i - i\hat{\rho}(\xi) = \min_{0 \leq j \leq m} (\Xi_j - j\hat{\rho}(\xi)) \right\}$$

$$\bar{I}(\xi) := \left\{ i \in \{0, 1, \dots, m\}; \Xi_i - i\hat{\rho}(\xi) = \max_{0 \leq j \leq m} (\Xi_j - j\hat{\rho}(\xi)) \right\},$$

where  $\Xi_i := \xi_1 + \dots + \xi_i$  ( $i = 0, 1, \dots, n$ ). The maximum or minimum value in  $\bar{I}(\xi)$  or  $\underline{I}(\xi)$  considered as a function of  $\xi$  is denoted by  $\max \bar{I}(\xi)$ ,  $\min \bar{I}(\xi)$ ,  $\max \underline{I}(\xi)$  or  $\min \underline{I}(\xi)$ . We prove that  $\max \bar{I}(\xi) - \min \underline{I}(\xi)$  is the slope of the left line segment and  $\max \underline{I}(\xi) - \min \bar{I}(\xi)$  is minus of the slope of the right line segment in Fig. 3.

In this paper, we prove the following theorem.

**Theorem 2** *For the statistical model  $(\text{St}_m, P_\alpha, \alpha \in [0, 1])$  with the quadratic loss function, we have*

1. *The maximum likelihood estimator  $\hat{\alpha}$  satisfies that  $\hat{\alpha}(\xi) = \hat{\rho}(\xi)$  and the likelihood at  $\hat{\alpha}$  satisfies that  $P_{\hat{\alpha}}(\xi) = 1/\text{per}(\xi)$ .*
2. *As for  $\alpha_1$  and  $\alpha_2$  in Fig. 3, it holds for any nontrivial  $\xi \in \text{St}_m$  that*

$$\alpha_1 = \hat{\alpha} - \frac{1}{(\max \bar{I}(\xi) - \min \underline{I}(\xi))\text{per}(\xi)}$$

$$\alpha_2 = \hat{\alpha} + \frac{1}{(\max \underline{I}(\xi) - \min \bar{I}(\xi))\text{per}(\xi)}$$

3. *The statistics  $(\hat{\rho}, \max \bar{I} - \min \underline{I}, \max \underline{I} - \min \bar{I})$  is a minimum sufficient statistics.*
4. *The sample mean  $\rho = \rho(\xi)$  is not based on the minimum sufficient statistics and is not admissible if  $m = 6$  or  $m \geq 8$ .*
5. *The Bayes estimate  $\alpha_3$  with respect to the uniform prior distribution on  $\alpha \in [0, 1]$  is determined by*

$$\alpha_3 = \frac{\hat{\alpha} + \alpha_1 + \alpha_2}{3}$$

6. *There is no UMVUE (uniformly minimum variance unbiased estimator) for  $\alpha$  if  $m \geq 3$ .*

*Remark 1* For  $m = 1, 2, 3, 4, 5$  and  $7$ , the sample mean  $\rho$  is based on the above minimum sufficient statistics. But we do not know whether it is admissible or not except for rather trivial cases  $m = 1, 2$  where  $\rho$  is admissible.

## 2 Prime segments

Let  $\xi = \xi_1, \xi_2 \dots \xi_m$  be a 0-1-sequence. We denote

$$\Xi_0 := 0 \text{ and } \Xi_i := \sum_{j=1}^i \xi_j \quad (i = 1, 2, \dots, m). \tag{8}$$

**Lemma 1** Let  $\xi = \xi_1\xi_2 \cdots \xi_m$  be a 0-1-sequence.

1.  $\underline{\Omega}_\xi \neq \emptyset$  if and only if  $\overline{\Omega}_\xi \neq \emptyset$ .
2. For  $(\alpha, \beta) \in [0, 1] \times [0, 1)$ , the condition (1) is equivalent to the following condition:

$$\Xi_i \leq i\alpha + \beta < \Xi_i + 1 \quad (i = 0, 1, \dots, m). \tag{9}$$

3. For  $(\alpha, \beta) \in [0, 1] \times (0, 1]$ , the condition (2) is equivalent to the following condition:

$$\Xi_i < i\alpha + \beta \leq \Xi_i + 1 \quad (i = 0, 1, \dots, m). \tag{10}$$

4. If  $\xi$  is nontrivial, then  $\underline{\Omega}_\xi$  is the set of  $(\alpha, \beta)$  satisfying Eq. 9.
5. If  $\xi$  is nontrivial, then  $\overline{\Omega}_\xi$  is the set of  $(\alpha, \beta)$  satisfying Eq. 10.

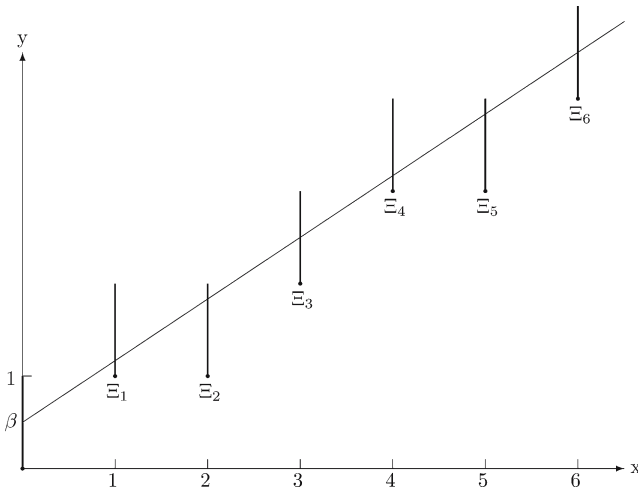
*Proof* 1. If  $\underline{\Omega}_\xi \neq \emptyset$ , then there exists  $(\alpha, \beta) \in [0, 1] \times [0, 1)$  satisfying Eq. (1). Then, there exists  $\beta'$  with  $\beta \leq \beta' < 1$  satisfying Eq. (1) such that  $i\alpha + \beta'$  is not an integer for any  $i = 0, 1, \dots, m$ . Then, we have

$$\xi_i = \lfloor i\alpha + \beta' \rfloor - \lfloor (i - 1)\alpha + \beta' \rfloor = \lceil i\alpha + \beta' \rceil - \lceil (i - 1)\alpha + \beta' \rceil.$$

Thus,  $(\alpha, \beta') \in \overline{\Omega}_\xi$  and  $\overline{\Omega}_\xi \neq \emptyset$ . The converse is proved similarly (Fig. 4).

2. If  $(\alpha, \beta) \in [0, 1] \times [0, 1)$  satisfies Eq. (1), then for  $i = 1, 2, \dots, m$ , we have

$$\begin{aligned} \Xi_i &= \sum_{j=1}^i \xi_j \\ &= \sum_{j=1}^i (\lfloor j\alpha + \beta \rfloor - \lfloor (j - 1)\alpha + \beta \rfloor) \\ &= \lfloor i\alpha + \beta \rfloor. \end{aligned}$$



**Fig. 4** The graph of  $y = \alpha x + \beta$  with  $(\alpha, \beta) \in \underline{\Omega}_\xi$

Hence, we have Eq. (9).

Conversely, if  $(\alpha, \beta) \in [0, 1] \times [0, 1)$  satisfies Eq. (9), then for  $i = 1, 2, \dots, m$ , we have

$$\lfloor i\alpha + \beta \rfloor - \lfloor (i - 1)\alpha + \beta \rfloor = \Xi_i - \Xi_{i-1} = \xi_i.$$

3. The proof is similar to 2.
4. Assume that Eq. (9) holds for  $(\alpha, \beta)$ . Then, we have  $0 = \Xi_0 \leq \beta < \Xi_0 + 1 = 1$ . Moreover, since  $\xi$  is nontrivial, we have  $1 \leq \Xi_m \leq m - 1$ .

Hence,  $m\alpha \geq \Xi_m - \beta > 0$  and  $m\alpha < \Xi_m + 1 - \beta \leq m$ , so that  $\alpha \in (0, 1)$ . Thus,  $(\alpha, \beta) \in [0, 1] \times [0, 1)$ . Then by 1.,  $(\alpha, \beta) \in \Omega_\xi$ . The converse follows from 1.

5. The proof is similar to 4. □

Let  $\xi = \xi_1 \xi_2 \dots \xi_m$  be a Sturmian sequence, which is fixed throughout this section. Let  $\underline{\Gamma}_\xi$  and  $\overline{\Gamma}_\xi$  be the minimal concave function and the maximal convex function, respectively, defined on the interval  $[0, m]$  satisfying that

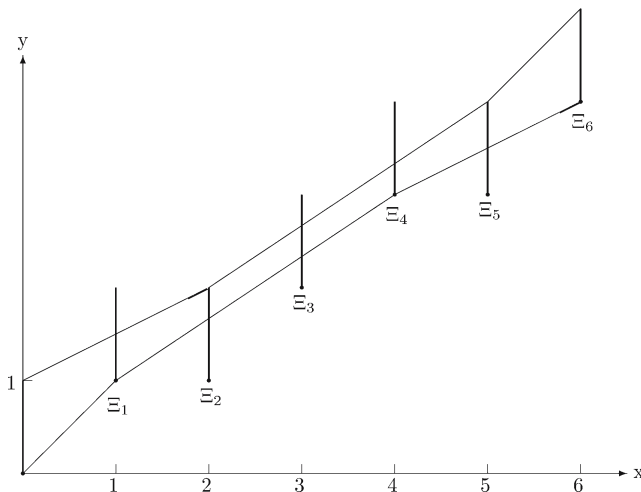
$$\underline{\Gamma}_\xi(i) \geq \Xi_i \quad (i = 0, 1, \dots, m) \tag{11}$$

and

$$\overline{\Gamma}_\xi(i) \leq \Xi_i + 1 \quad (i = 0, 1, \dots, m), \tag{12}$$

respectively. Clearly, they are piecewise linear functions such that  $\underline{\Gamma}_\xi(0) = 0$ ,  $\underline{\Gamma}_\xi(m) = \Xi_m$ ,  $\overline{\Gamma}_\xi(0) = 1$  and  $\overline{\Gamma}_\xi(m) = \Xi_m + 1$  (Fig. 5).

A point  $(i, j)$  in  $[0, m] \times [0, \infty)$  is called an *integer point* if both  $i$  and  $j$  are integers. A closed line segment  $AB$  with  $A = (A_x, A_y)$ ,  $B = (B_x, B_y)$  and  $A_x < B_x$  contained in the graph of  $\overline{\Gamma}_\xi$  such that the set of integer points on  $AB$  is  $\{A, B\}$  is called a *prime segment* of  $\overline{\Gamma}_\xi$ . A maximal closed line segment  $AB$  with  $A_x < B_x$  contained in the graph of  $\overline{\Gamma}_\xi$  is called a *maximal segment* of  $\overline{\Gamma}_\xi$ . In the same way, we define a *prime segment* of  $\underline{\Gamma}_\xi$  and a *maximal segment* of  $\underline{\Gamma}_\xi$ .



**Fig. 5** The graph of  $\underline{\Gamma}_\xi$  and  $\overline{\Gamma}_\xi$

- Lemma 2** 1. For any  $(\alpha, \beta) \in [0, 1] \times [0, 1]$ ,  $(\alpha, \beta) \in \underline{\Omega}_\xi$  holds if and only if  $\underline{\Gamma}_\xi(x) \leq x\alpha + \beta < \overline{\Gamma}_\xi(x)$  for any  $x \in [0, m]$ . In particular,  $\underline{\Gamma}_\xi(x) < \overline{\Gamma}_\xi(x)$  holds for any  $x \in [0, m]$ .
2. For any  $(\alpha, \beta) \in [0, 1] \times (0, 1]$ ,  $(\alpha, \beta) \in \overline{\Omega}_\xi$  holds if and only if  $\underline{\Gamma}_\xi(x) < x\alpha + \beta \leq \overline{\Gamma}_\xi(x)$  for any  $x \in [0, m]$ .
3. Any integer point  $A$  on the graph of  $\underline{\Gamma}_\xi$  (or  $\overline{\Gamma}_\xi$ ) satisfies that  $A = (i, \Xi_i)$  [or  $A = (i, \Xi_i + 1)$ ], respectively] for some  $i = 0, 1, \dots, m$ .
4. There is no integer point in the domain

$$\{(x, y); 0 \leq x \leq m, \underline{\Gamma}_\xi(x) < y < \overline{\Gamma}_\xi(x)\}.$$

5. For a maximal segment  $CD$  of  $\underline{\Gamma}_\xi$  (or  $\overline{\Gamma}_\xi$ ), both  $C$  and  $D$  are integer points. Moreover, there exists a positive integer  $k$  such that for any prime segment  $AB$  of  $\underline{\Gamma}_\xi$  (or  $\overline{\Gamma}_\xi$ ) contained in  $CD$ , we have  $\overrightarrow{CD} = k\overrightarrow{AB}$ , where  $\overrightarrow{AB}$  implies the vector from  $A$  to  $B$ .

*Proof* 1. Let  $(\alpha, \beta) \in \underline{\Omega}_\xi$ . Then by Lemma 1, we have Eq. (9). Therefore, there exists  $\beta' > \beta$  such that

$$\Xi_i \leq i\alpha + \beta < i\alpha + \beta' \leq \Xi_i + 1 \quad (i = 0, 1, \dots, m). \tag{13}$$

Since the functions  $x\alpha + \beta$  and  $x\alpha + \beta'$  of  $x \in [0, m]$  are concave and convex at the same time satisfying Eq. (13), we have

$$\underline{\Gamma}_\xi(x) \leq x\alpha + \beta < x\alpha + \beta' \leq \overline{\Gamma}_\xi(x) \tag{14}$$

for any  $x \in [0, m]$  by the minimality and the maximality of  $\underline{\Gamma}_\xi$  or  $\overline{\Gamma}_\xi$ , respectively.

Conversely, if  $\underline{\Gamma}_\xi(x) \leq x\alpha + \beta < \overline{\Gamma}_\xi(x)$  holds for any  $x \in [0, m]$ . Then, we have Eq. (9) since

$$\Xi_i \leq \underline{\Gamma}_\xi(i) \leq i\alpha + \beta < \overline{\Gamma}_\xi(i) \leq \Xi_i + 1 \quad (i = 0, 1, \dots, m).$$

Then by 2 of Lemma 1, we have  $(\alpha, \beta) \in \underline{\Omega}_\xi$ .

Finally, since there exists  $(\alpha, \beta) \in \underline{\Omega}_\xi$ , we have  $\underline{\Gamma}_\xi(x) < \overline{\Gamma}_\xi(x)$  for any  $x \in [0, m]$  by Eq. (14).

2. The proof is same as 1.
3. Let  $(i, j)$  be an integer point on  $\underline{\Gamma}_\xi$ . Then, by 1, we have

$$\Xi_i \leq \underline{\Gamma}_\xi(i) = j < \overline{\Gamma}_\xi(i) \leq \Xi_i + 1,$$

which implies  $j = \Xi_i$ .

The proof is similar for  $\overline{\Gamma}_\xi$ .

4. Suppose that there exists an integer point  $(i, j)$  satisfying  $0 \leq i \leq m$  and  $\underline{\Gamma}_\xi(i) < j < \overline{\Gamma}_\xi(i)$  then we have

$$\Xi_i \leq \underline{\Gamma}_\xi(i) < j < \overline{\Gamma}_\xi(i) \leq \Xi_i + 1,$$

which is a contradiction since both  $\Xi_i$  and  $j$  are integers.



5. If either  $C$  or  $D$  is not an integer point, then we can decrease the function  $\Gamma_\xi$  near the point  $C$  or  $D$ , respectively, keeping the concavity and the inequality (11), which contradicts with the minimality. Thus,  $C$  and  $D$  are integer points.

Let  $C = (C_x, C_y)$ ,  $D = (D_x, D_y)$  be their coordinates and let  $k$  be the greatest common divisor of  $D_x - C_x$  and  $D_y - C_y$ . Then, any prime segment  $AB$  contained in  $CD$  satisfies that  $\vec{CD} = k\vec{AB}$  since  $B$  is the nearest integer point on  $CD$  to the right of  $A$ .

The proof is similar for  $\bar{\Gamma}_\xi$ .

Let  $CD$  be a maximal segment of  $\Gamma_\xi$ . We call  $CD$  *central* if there exists  $(\alpha, \beta) \in \underline{\Omega}_\xi$  such that  $CD$  is on the graph  $y = x\alpha + \beta$ . Let  $CD$  be a maximal segment of  $\bar{\Gamma}_\xi$ . We call  $CD$  *central* if there exists  $(\alpha, \beta) \in \bar{\Omega}_\xi$  such that  $CD$  is on the graph  $y = x\alpha + \beta$ . A prime segment  $CD$  of  $\Gamma_\xi$  (or  $\bar{\Gamma}_\xi$ ) is called *central* if it is contained in a central maximal segment of  $\Gamma_\xi$  (or  $\bar{\Gamma}_\xi$ , respectively).

**Lemma 3** 1. Let  $AB$  be a central maximal segment of  $\Gamma_\xi$  (or  $\bar{\Gamma}_\xi$ ), then we have  $B_x > 2A_x$  and  $2B_x - A_x > m$ .

2. A central maximal segment of  $\Gamma_\xi$  (or  $\bar{\Gamma}_\xi$ ) is unique if it exists.

*Proof* 1. Suppose to the contrary that either  $B_x \leq 2A_x$  or  $2B_x - A_x \leq m$  holds.

Without loss of generality, we assume  $2B_x - A_x \leq m$ . Define  $B'$  by  $\vec{AB}' = 2\vec{AB}$ . Then, we have  $B'_x \leq m$ .

Since by 5 of Lemma 2, both  $A$  and  $B$  are integer points,  $B'$  is also an integer point. Since  $AB$  is central, there exist  $(\alpha, \beta) \in \underline{\Omega}_\xi$  such that  $AB$  is on the graph  $y = x\alpha + \beta$ . Since  $B'$  is also on this graph, we have  $\Xi_{B'_x} \leq B'_y < \Xi_{B'_x} + 1$ . Since  $B'$  is above the graph  $y = \Gamma_\xi(x)$ , we have  $B'_y > \Gamma_\xi(B'_x) \geq \Xi_{B'_x}$ . Thus,  $\Xi_{B'_x} < B'_y < \Xi_{B'_x} + 1$ . This is a contradiction since both  $\Xi_{B'_x}$  and  $B'_y$  are integers.

2. Suppose that there exist two distinct central maximal segments  $AB$  and  $CD$  of  $\Gamma_\xi$ . Assume that  $B_x \leq C_x$ . Since  $0 \leq A_x < B_x \leq C_x < D_x \leq m$ , either  $B_x \leq m/2$  or  $C_x \geq m/2$ . This implies that either  $2B_x - A_x \leq m$  or  $D_x \leq 2C_x$  which contradicts with 1. □

**Lemma 4** At least one of the central maximal segment of  $\bar{\Gamma}_\xi$  or the central maximal segment of  $\Gamma_\xi$  exists.

*Proof* Assume that the central maximal segment of  $\bar{\Gamma}_\xi$  does not exist. By 1 of Lemma 2, there exists  $(\alpha, \beta) \in \underline{\Omega}_\xi$  such that  $\Gamma_\xi(x) \leq x\alpha + \beta < \bar{\Gamma}_\xi(x)$  for any  $x \in [0, m]$ . Fixing  $\alpha$ , we increase  $\beta \in [0, 1)$  until  $\bar{\Gamma}_\xi(x) = x\alpha + \beta$  holds for some  $x \in [0, m]$  for the first time. If the equality holds for more than one point, then the equality holds for a maximal segment of  $\bar{\Gamma}_\xi$ , which is central since it is on the graph  $y = x\alpha + \beta$  with  $(\alpha, \beta) \in \bar{\Omega}_\xi$ , which contradicts with our assumption.

Hence,

$$\Gamma_\xi(x) < x\alpha + \beta \leq \bar{\Gamma}_\xi(x) \tag{15}$$

holds for any  $x \in [0, m]$  with the equality  $x\alpha + \beta = \overline{\Gamma}_\xi(x)$  for just one point  $x = x_0$ . Then,  $A = (x_0, \overline{\Gamma}_\xi(x_0)) = (x_0, x_0\alpha + \beta)$  is an integer point since it must be a broken point of the piecewise linear graph  $y = \overline{\Gamma}_\xi(x)$  by the uniqueness.

Let  $\alpha$  increase and  $\beta$  decrease keeping the value  $x_0\alpha + \beta$  invariant until the graph  $y = x\alpha + \beta$  touch the graph  $y = \overline{\Gamma}_\xi(x)$  for the first time. By the above argument with our assumption, the graph  $y = x\alpha + \beta$  does not touch the graph  $y = \overline{\Gamma}_\xi(x)$  at a different point from  $A$  before it touch the graph  $y = \overline{\Gamma}_\xi(x)$  for the first time. Let  $(\alpha_1, \beta_1)$  be the value of  $(\alpha, \beta)$  when the graph  $y = x\alpha + \beta$  touches the graph  $y = \overline{\Gamma}_\xi(x)$  for the first time. Then we have

$$\underline{\Gamma}_\xi(x) \leq x\alpha_1 + \beta_1 \leq \overline{\Gamma}_\xi(x) \tag{16}$$

for any  $x \in [0, m]$ , and  $\underline{\Gamma}_\xi(x) = x\alpha_1 + \beta_1$  holds for some  $x \in [0, m]$ , say  $x_1$ , while  $x\alpha_1 + \beta_1 = \overline{\Gamma}_\xi(x)$  holds if and only if  $x = x_0$  (Fig. 6).

Starting again from Eq. (15), let  $\alpha$  decrease and  $\beta$  increase keeping the value  $x_0\alpha + \beta$  invariant until the graph  $y = x\alpha + \beta$  touch the graph  $y = \underline{\Gamma}_\xi(x)$  for the first time and the value  $(\alpha, \beta)$  when it touch the graph  $y = \underline{\Gamma}_\xi(x)$  for the first time be  $(\alpha_2, \beta_2)$ . Then we have

$$\underline{\Gamma}_\xi(x) \leq x\alpha_2 + \beta_2 \leq \overline{\Gamma}_\xi(x) \tag{17}$$

for any  $x \in [0, m]$ , and  $\underline{\Gamma}_\xi(x) = x\alpha_2 + \beta_2$  holds for some  $x \in [0, m]$ , say  $x_2$ , while  $x\alpha_2 + \beta_2 = \overline{\Gamma}_\xi(x)$  holds if and only if  $x = x_0$ .

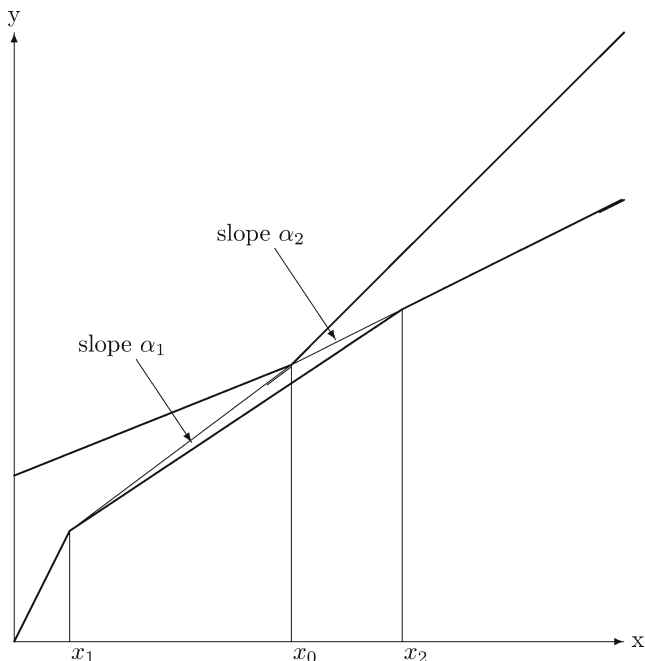


Fig. 6 Central maximal segment

Then, we have  $x_1 < x_0 < x_2$  and

$$\underline{\Gamma}_\xi(x_0) < \overline{\Gamma}_\xi(x_0) = x_0\alpha_1 + \beta_1 = x_0\alpha_2 + \beta_2.$$

Since

$$\frac{\underline{\Gamma}_\xi(x_0) - \underline{\Gamma}_\xi(x_1)}{x_0 - x_1} < \frac{\overline{\Gamma}_\xi(x_0) - \underline{\Gamma}_\xi(x_1)}{x_0 - x_1} = \alpha_1,$$

there exists  $x_3 \in (x_1, x_0)$  such that  $\underline{\Gamma}_\xi'(x_3) < \alpha_1$ . In the same way, there exists  $x_4 \in (x_0, x_2)$  such that  $\underline{\Gamma}_\xi'(x_4) > \alpha_2$ . Therefore, we have  $x_1 < x_3 < x_4 < x_2$  and

$$\underline{\Gamma}_\xi'(x_1 - 0) \geq \alpha_1 > \underline{\Gamma}_\xi'(x_3) \geq \underline{\Gamma}_\xi'(x_4) > \alpha_2 \geq \underline{\Gamma}_\xi'(x_2 + 0).$$

Hence, there exists a maximal segment  $BC$  of  $\underline{\Gamma}_\xi$  with the slope  $\alpha_3 := \underline{\Gamma}_\xi'(x_3)$  satisfying that  $\alpha_1 > \alpha_3 > \alpha_2$  and  $x_1 \leq B_x < C_x \leq x_2$ .

We prove that  $BC$  is central. Let  $y = x\alpha_3 + \beta_3$  be the graph which contains  $BC$ . Then, by 1 of Lemma 2, it is sufficient to prove that

$$\underline{\Gamma}_\xi(x) \leq x\alpha_3 + \beta_3 < \overline{\Gamma}_\xi(x) \quad (\forall x \in [0, m]).$$

Since  $\underline{\Gamma}_\xi(x) \leq x\alpha_3 + \beta_3$  holds for any  $x \in [0, m]$  by the concavity of  $\underline{\Gamma}_\xi$ , it is sufficient to prove that

$$x\alpha_3 + \beta_3 < \overline{\Gamma}_\xi(x) \quad (\forall x \in [0, m]). \tag{18}$$

Since  $BC$  is below the graph  $y = x\alpha_1 + \beta_1$  except possibly for  $B$  and  $\alpha_3 < \alpha_1$ , we have

$$x\alpha_3 + \beta_3 < x\alpha_1 + \beta_1 \leq \overline{\Gamma}_\xi(x)$$

for any  $x \in (B_x, m]$ . In the same way, we have

$$x\alpha_3 + \beta_3 < x\alpha_2 + \beta_2 \leq \overline{\Gamma}_\xi(x)$$

for any  $x \in [0, C_x)$ . Thus, we have Eq. (18). □

**Lemma 5** *Assume that a central prime segment of  $\underline{\Gamma}_\xi$  and a central prime segment of  $\overline{\Gamma}_\xi$  exist at the same time. Then, their lengths and slopes coincide.*

*Proof* Let  $AB$  and  $CD$  be the central prime segments of  $\underline{\Gamma}_\xi$  and of  $\overline{\Gamma}_\xi$ , respectively. Suppose that either their slopes or lengths do not coincide.

Let  $y = x\alpha + \beta$  and  $y = x\alpha' + \beta'$  be the graphs containing  $AB$  or  $CD$ , respectively. Let  $x_1 = A_x \wedge C_x$  and  $x_2 = B_x \vee D_x$ . Denote

$$\Lambda := \{(x, y); x_1 \leq x \leq x_2, x\alpha + \beta \leq y \leq x\alpha' + \beta'\}.$$

Since both  $AB$  and  $CD$  are central,  $\Lambda \setminus (AB \cup CD)$  is contained in the domain  $\{(x, y); 0 \leq x \leq m, \underline{\Gamma}_\xi(x) < y < \overline{\Gamma}_\xi(x)\}$  and has no integer point by 4 of Lemma 2.

Assume that the slopes of  $AB$  and  $CD$  do not coincide. Without loss of generality, assume that the slope of  $AB$  is less than the slope of  $CD$ . Let  $F$  be the point such that  $\overrightarrow{DF} = \overrightarrow{CA}$  if  $A_x \leq C_x$ , and  $\overrightarrow{BF} = \overrightarrow{AC}$  if  $A_x > C_x$ . Then,  $F$  is an integer

point since  $A, B, C, D$  are integer points. Moreover, we have  $F \in \Lambda \setminus (AB \cup CD)$ , which contradicts the fact that  $\Lambda \setminus (AB \cup CD)$  has no integer point.

Assume that  $AB$  and  $CD$  have the same slope but different lengths, say  $|\vec{AB}| < |\vec{CD}|$ . Let  $F$  be the point such that  $\vec{BF} = \vec{AC}$ . Then,  $F$  is an integer point since  $A, B, C, D$  are integer points. Moreover,  $F$  is in the interior of the line segment  $CD$ , which contradicts with that  $CD$  is a prime segment of  $\bar{\Gamma}_\xi$ .

Thus, we have  $\vec{AB} = \vec{CD}$ , which implies that a central prime segment of  $\underline{\Gamma}_\xi$  and a central prime segments of  $\bar{\Gamma}_\xi$  have the same length and slope. □

### 3 Shape of $\underline{\Omega}_\xi$

Let  $\xi = \xi_1 \xi_2 \dots \xi_m$  be a Sturmian sequence, which we fix throughout this section. In Berstel and Pocchiola, (1996), the duality between the domains

$$\begin{aligned} \underline{\Sigma}_\xi &:= \{(x, y); 0 \leq x \leq m, \underline{\Gamma}_\xi(x) \leq y < \bar{\Gamma}_\xi(x)\} \\ \bar{\Sigma}_\xi &:= \{(x, y); 0 \leq x \leq m, \underline{\Gamma}_\xi(x) < y \leq \bar{\Gamma}_\xi(x)\} \end{aligned}$$

and the domains  $\underline{\Omega}_\xi$  and  $\bar{\Omega}_\xi$  is discussed, although the notations used there are slightly different from ours. We reproduce their results there in our framework.

For  $(x, y) \in [0, m] \times [0, \infty)$ , denote

$$\begin{aligned} (x, y)^* &= \{(\alpha, \beta) \in [0, 1] \times [0, 1]; x\alpha + \beta = y\} \\ (x, y)^+ &= \{(\alpha, \beta) \in [0, 1] \times [0, 1]; x\alpha + \beta < y\} \\ (x, y)^- &= \{(\alpha, \beta) \in [0, 1] \times [0, 1]; x\alpha + \beta > y\} \\ (x, y)^{*+} &= (x, y)^+ \cup (x, y)^* \\ (x, y)^{-*} &= (x, y)^- \cup (x, y)^*. \end{aligned}$$

Thus,  $(x, y)^*$  is a straight line in the domain  $[0, 1] \times [0, 1]$ . Conversely, for  $(\alpha, \beta) \in [0, 1] \times [0, 1]$ , denote

$$(\alpha, \beta)^* = \{(x, y) \in [0, m] \times [0, \infty); x\alpha + \beta = y\},$$

so that  $(\alpha, \beta)^*$  is a straight line in  $[0, m] \times [0, \infty)$ . For a subset  $S$  of  $[0, m] \times [0, \infty)$  or a subset  $T$  of  $[0, 1] \times [0, 1]$ , we denote

$$S^* = \bigcap_{(x,y) \in S} (x, y)^*$$

and

$$T^* = \bigcap_{(\alpha,\beta) \in T} (\alpha, \beta)^*.$$

Then we have the dualities:  $((x, y)^*)^* = (x, y)$ , for any  $(x, y) \in [0, m] \times [0, \infty)$ ;  $((\alpha, \beta)^*)^* = (\alpha, \beta)$ , for any  $(\alpha, \beta) \in [0, 1] \times [0, 1]$ .

**Lemma 6** *We have*

$$\underline{\Omega}_\xi = \bigcap_{i=0}^m (i, \Xi_i)^{*+} \cap \bigcap_{i=0}^m (i, \Xi_i + 1)^-.$$

and

$$\overline{\Omega}_\xi = \bigcap_{i=0}^m (i, \Xi_i)^+ \cap \bigcap_{i=0}^m (i, \Xi_i + 1)^{*-}.$$

*In particular, both  $\underline{\Omega}_\xi$  and  $\overline{\Omega}_\xi$  are convex domains surrounded by a finite number of line segments with nonpositive slopes.*

*Proof* Clear from Lemma 1. □

Let  $\underline{\Omega}_\xi^{\text{cl}}$  be the closure of  $\underline{\Omega}_\xi$ , which is a compact convex set surrounded by line segments with nonpositive slopes. Let  $\text{ex}(\underline{\Omega}_\xi^{\text{cl}})$  be the set of extremal points of  $\underline{\Omega}_\xi^{\text{cl}}$ . Take a point on a boundary of  $\underline{\Omega}_\xi^{\text{cl}}$  and move it around the boundary counter-clockwise. Then, the direction of the movement changed when it arrives at extremal points. There is a unique extremal point such that the horizontal component of the direction changes from negative to positive at this point, which is called the *left vertex*. Also, there is a unique extremal point such that the horizontal component of the direction changes from positive to negative at this point, which is called the *right vertex*. The other extremal points are either upper or lower as defined below.

An *upper edge* of  $\underline{\Omega}_\xi$  is defined as  $\underline{\Omega}_\xi \cap (i, \Xi_i + 1)^*$  for some  $i = 0, 1, \dots, m$  if it contains at least two points. A *lower edge* of  $\underline{\Omega}_\xi$  is defined as  $\underline{\Omega}_\xi \cap (i, \Xi_i)^*$  for some  $i = 0, 1, \dots, m$  if it contains at least two points. An *upper vertex* is an intersection of two distinct upper edges belonging to  $\overline{\Omega}_\xi$ . A *lower vertex* is an intersection of two distinct upper edges belonging to  $\underline{\Omega}_\xi$ .

- Lemma 7** 1. *For  $Q \in [0, 1] \times (0, 1]$ ,  $Q$  is an upper vertex of  $\underline{\Omega}_\xi$  if and only if  $Q^*$  contains the central maximal segment of  $\overline{\Gamma}_\xi$ . In this case, the slope of the central maximal segment of  $\overline{\Gamma}_\xi$  is  $Q_\alpha$ , where  $Q = (Q_\alpha, Q_\beta)$ . Moreover, an upper vertex is unique if it exists.*
2. *For  $Q \in [0, 1] \times [0, 1)$ ,  $Q$  is a lower vertex of  $\underline{\Omega}_\xi$  if and only if  $Q^*$  contains the central maximal segment of  $\underline{\Gamma}_\xi$ . In this case, the slope of the central maximal segment of  $\underline{\Gamma}_\xi$  is  $Q_\alpha$ . Moreover, a lower vertex is unique if it exists.*
3. *Either the upper vertex or the lower vertex of  $\underline{\Omega}_\xi$  exists. Moreover, if both of the upper vertex  $P$  and the lower vertex  $Q$  exist, then we have  $P_\alpha = Q_\alpha$ .*
4. *If the central maximal segment of  $\underline{\Gamma}_\xi$  or the central maximal segment of  $\overline{\Gamma}_\xi$  exists, then their slopes coincide with the maximum likelihood estimator  $\hat{\alpha}(\xi)$  (Fig. 3).*

*Proof* 1. Let  $Q \in \overline{\Omega}_\xi$  be an upper vertex of  $\underline{\Omega}_\xi$ . It is the intersection of two distinct upper edges, say  $PQ$  and  $QR$ , where  $P_\alpha < Q_\alpha < R_\alpha$ . Since  $PQ$  is an upper edge, there exists  $i = 0, 1, \dots, m$  such that the graph  $y = x\alpha + \Xi_i + 1 - i\alpha$  in  $[0, m] \times [0, \infty)$  passing  $(i, \Xi_i + 1)$  is contained in the domain  $\overline{\Omega}_\xi$  for any  $\alpha$  with  $P_\alpha \leq \alpha \leq Q_\alpha$ . Also, there exists  $j = 0, 1, \dots, m$  such that the graph

$y = x\alpha + \Xi_j + 1 - j\alpha$  in  $[0, m] \times [0, \infty)$  passing  $(j, \Xi_j + 1)$  is contained in the domain  $\overline{\Sigma}_\xi$  for any  $\alpha$  with  $Q_\alpha \leq \alpha \leq R_\alpha$ .

For  $\alpha = Q_\alpha$ , the graphs  $y = x\alpha + \Xi_i + 1 - i\alpha$  and  $y = x\alpha + \Xi_j + 1 - j\alpha$  should coincide, since otherwise, one of them is above the point  $(i, \Xi_i + 1)$  or  $(j, \Xi_j + 1)$  and is not in the domain  $\overline{\Sigma}_\xi$ , which is a contradiction. Therefore, those graphs coincide and pass both points  $(i, \Xi_i + 1)$  and  $(j, \Xi_j + 1)$ . Since this graph is contained in  $\overline{\Sigma}_\xi$ , these points are on the central maximal segment of  $\overline{\Gamma}_\xi(x)$  with the slope  $Q_\alpha$ .

Conversely, if  $Q^*$  contains the central maximal segment of  $\overline{\Gamma}_\xi(x)$ , say  $AB$ . Then, the graph  $y = xQ_\alpha + Q_\beta$  contains  $AB$  and is contained in the domain  $\overline{\Sigma}_\xi$ . Starting from  $\alpha = Q_\alpha$  and  $\beta = Q_\beta$ , we can decrease  $\alpha$  and increase  $\beta$  keeping the graph in the domain  $\overline{\Sigma}_\xi$  and keeping the equation  $A_x\alpha + \beta = A_y$ . Hence,  $\overline{\Omega}_\xi \cap A^*$  contains at least two points including  $Q$ . The same thing holds for  $\overline{\Omega}_\xi \cap B^*$ . Hence, they are distinct upper edges whose intersection is  $Q$ . Thus,  $Q$  is an upper edge.

2. The proof is similar to 1.
3. It follows from 1, 2 and Lemma 5.
4. Clear from 1 and 2 and the shape of the domain  $\underline{\Omega}_\xi$  (Fig. 2). □

### 4 Main results

Let  $\xi = \xi_1, \xi_2 \dots \xi_m$  be a Sturmian sequence, which we fix throughout this section.

For a pair of positive integers  $(u, v)$  with  $v \leq u$ , we denote by  $\underline{\lambda}(u, v)$  the 0-1-sequence of length  $u$  such that

$$\underline{\lambda}(u, v)_i = \lfloor iv/u \rfloor - \lfloor (i-1)v/u \rfloor \quad (i = 1, 2, \dots, u),$$

and by  $\overline{\lambda}(u, v)$  the 0-1-sequence of length  $u$  such that

$$\overline{\lambda}(u, v)_i = \lceil iv/u \rceil - \lceil (i-1)v/u \rceil \quad (i = 1, 2, \dots, u).$$

For integers  $i, j$  with  $0 \leq i < j \leq m$ , we denote

$$\xi[i, j] := \xi_{i+1}\xi_{i+2} \cdots \xi_j.$$

- Lemma 8** *1. Let  $AB$  be a prime segment of  $\underline{\Gamma}_\xi$ . Then, we have  $A_y = \Xi_{A_x}$ ,  $B_y = \Xi_{B_x}$  and  $\xi[A_x, B_x] = \underline{\lambda}(B_x - A_x, B_y - A_y)$ . Moreover,  $B_x - A_x$  and  $B_y - A_y$  are coprime.*
- 2. Let  $AB$  be a prime segment of  $\overline{\Gamma}_\xi$ . Then, we have  $A_y = \Xi_{A_x} + 1$ ,  $B_y = \Xi_{B_x} + 1$  and  $\xi[A_x, B_x] = \overline{\lambda}(B_x - A_x, B_y - A_y)$ . Moreover,  $B_x - A_x$  and  $B_y - A_y$  are coprime.*
- 3. Let  $AB$  be a prime segment of  $\underline{\Gamma}_\xi$  ( $\overline{\Gamma}_\xi$ ). It is central if and only if  $B_x - A_x$  is a period of  $\xi$ . Moreover,  $B_x - A_x = \text{per}(\xi)$  holds in this case.*

*Proof* (1) Let  $AB$  be a prime segment of  $\underline{\Gamma}_\xi$ . Since  $A$  and  $B$  are integer points on the graph  $y = \underline{\Gamma}_\xi(x)$ , we have  $A_y = \Xi_{A_x}$  and  $B_y = \Xi_{B_x}$  by 3 of Lemma 2. Since  $AB$  is in the domain  $\underline{\Sigma}_\xi$ ,  $(i, \Xi_i)$  is on or below  $AB$  and  $(i, \Xi_i + 1)$  is above  $AB$  for any  $i$  with  $A_x \leq i \leq B_x$ . Therefore, we have

$$\Xi_i \leq (i - A_x)(B_y - A_y)/(B_x - A_x) + A_y < \Xi_i + 1, \tag{19}$$

or equivalently,

$$\Xi_i = \lfloor (i - A_x)(B_y - A_y)/(B_x - A_x) \rfloor + A_y \tag{20}$$

for any  $i$  with  $A_x \leq i \leq B_x$ . Hence, we have

$$\begin{aligned} \xi_{A_x+i} &= \Xi_{A_x+i} - \Xi_{A_x+i-1} \\ &= \lfloor i(B_y - A_y)/(B_x - A_x) \rfloor - \lfloor (i - 1)(B_y - A_y)/(B_x - A_x) \rfloor \\ &= \underline{\lambda}(B_x - A_x, B_y - A_y)_i \end{aligned}$$

for  $i = 1, 2, \dots, B_x - A_x$ , and hence  $\xi[A_x, B_x] = \underline{\lambda}(B_x - A_x, B_y - A_y)$ .

That  $B_x - A_x$  and  $B_y - A_y$  are coprime follows from the fact that  $AB$  contains no integer point other than the end points  $A$  and  $B$ .

2. The proof is similar to the proof in 1.
3. Let  $AB$  be a central prime segment of  $\Gamma_\xi$ . Then, the graph  $y = x\alpha + \beta$  ( $x \in [0, m]$ ) which contains  $AB$  is in  $\Sigma_\xi$ , so that for any  $i$  with  $0 \leq i \leq m$ ,  $(i, \Xi_i)$  is on or below the graph and  $(i, \Xi_i + 1)$  is above the graph. Therefore, we have Eq. (19), and hence, Eq. (20) for any  $i$  with  $0 \leq i \leq m$ . This implies that

$$\Xi_{i+B_x-A_x} = \Xi_i + B_y - A_y \quad (0 \leq i \leq m - (B_x - A_x)),$$

and hence,

$$\xi_{i+B_x-A_x} = \xi_i \quad (1 \leq i \leq m - (B_x - A_x)).$$

Thus,  $B_x - A_x$  is a period of  $\xi$ .

Conversely, let  $AB$  be a prime segment of  $\Gamma_\xi$  such that  $B_x - A_x$  is a period of  $\xi$ . Then, we have

$$\xi_{i+B_x-A_x} = \xi_i \quad (1 \leq i \leq m - (B_x - A_x)).$$

Since  $\Xi_{A_x} = A_y$  and  $\Xi_{B_x} = B_y$ , it follows that

$$\sum_{i=1}^{B_x-A_x} \xi_{\ell+i} = B_y - A_y$$

for any  $\ell$  with  $1 \leq \ell \leq m - (B_x - A_x)$ . Moreover since  $\xi[A_x, B_x] = \underline{\lambda}(B_x - A_x, B_y - A_y)$ , we have

$$\begin{aligned} \Xi_i &= A_y + \sum_{h=1}^j \underline{\lambda}(B_x - A_x, B_y - A_y)_h + k(B_y - A_y) \\ &= A_y + \lfloor j(B_y - A_y)/(B_x - A_x) \rfloor + k(B_y - A_y) \\ &= \lfloor (j + k(B_x - A_x))(B_y - A_y)/(B_x - A_x) \rfloor + A_y \\ &= \lfloor (i - A_x)(B_y - A_y)/(B_x - A_x) \rfloor + A_y \end{aligned}$$

for any  $i$  with  $0 \leq i \leq m$ , where  $j$  and  $k$  are integers with  $1 \leq j \leq B_x - A_x$  and  $i = A_x + j + k(B_x - A_x)$ . Therefore, the graph  $y = (x - A_x)(B_y - A_y)/(B_x - A_x) + A_y$  ( $x \in [0, m]$ ) which contains  $AB$  is in the domain  $\Sigma_\xi$ . Thus,  $AB$  is central.

Let  $AB$  be a prime segment of  $\Gamma_\xi$ . Suppose that  $p := \text{per}(\xi) < B_x - A_x$ . Let  $B_x - A_x = p + r$  with a positive integer  $r$ . Since  $(i, \Xi_i)$  is below the line segment  $AB$  for any  $i$  with  $A_x < i < B_x$ ,  $(A_x + p, \Xi_{A_x+p})$  and  $(A_x + r, \Xi_{A_x+r})$  are below  $AB$ . Hence, we have

$$\frac{\Xi_{A_x+p} - A_y}{p} < \frac{B_y - A_y}{B_x - A_x} \tag{21}$$

$$\frac{\Xi_{A_x+r} - A_y}{r} < \frac{B_y - A_y}{B_x - A_x}. \tag{22}$$

Moreover, since  $p$  is a period of  $\xi$ , we have

$$\begin{aligned} B_y - \Xi_{A_x+p} &= \Xi_{B_x} - \Xi_{A_x+p} \\ &= \Xi_{A_x+p+r} - \Xi_{A_x+p} \\ &= \Xi_{A_x+r} - \Xi_{A_x}. \end{aligned}$$

Then by Eqs. 21 and 22, we have a contradiction:

$$\begin{aligned} B_y - A_y &= (B_y - \Xi_{A_x+p}) + (\Xi_{A_x+p} - A_y) \\ &= (\Xi_{A_x+r} - \Xi_{A_x}) + (\Xi_{A_x+p} - A_y) \\ &< \frac{B_y - A_y}{B_x - A_x} r + \frac{B_y - A_y}{B_x - A_x} p \\ &= \frac{(B_y - A_y)(r + p)}{B_x - A_x} = B_y - A_y. \end{aligned}$$

Thus,  $B_x - A_x \leq \text{per}(\xi)$  holds for any prime segment of  $\Gamma_\xi$ , and  $B_x - A_x = \text{per}(\xi)$  holds for any central prime segment of  $\Gamma_\xi$  since in this case,  $B_x - A_x$  is a period of  $\xi$  as is proved in the above.

The proof is similar for a prime segment in  $\overline{\Gamma}_\xi$ . □

Let  $AB$  be a central prime segment of  $\Gamma_\xi$ . Then, the factor  $\xi[A_x, B_x]$  of  $\xi$  is called a *convex kernel* of  $\xi$ . Also, for a central prime segment  $AB$  of  $\overline{\Gamma}_\xi$ , the factor  $\xi[A_x, B_x]$  of  $\xi$  is called a *concave kernel* of  $\xi$ .

- Lemma 9** 1. For a convex kernel  $\eta$  of  $\xi$ , we have  $\eta = \underline{\lambda}(u, v)$  with  $u := |\eta| = \text{per}(\xi)$  and  $v := |\eta|_1 = \text{per}(\xi)\hat{\rho}(\xi)$ . Hence, a convex kernel of  $\xi$  is unique if it exists.
2. For a concave kernel  $\zeta$  of  $\xi$ , we have  $\eta = \overline{\lambda}(u, v)$  with  $u := |\zeta| = \text{per}(\xi)$  and  $v := |\zeta|_1 = \text{per}(\xi)\hat{\rho}(\xi)$ . Hence, a concave kernel of  $\xi$  is unique if it exists.
3. Either the convex kernel of  $\xi$  or the concave kernel of  $\xi$  exists.
4. For the maximum likelihood estimator, we have  $\hat{\alpha}(\xi) = \hat{\rho}(\xi)$ .
5. For the convex kernel  $\eta$  of  $\xi$ , we have

$$\min \{|\theta|_1 - |\theta|\rho(\eta)\} = -1 + \frac{1}{|\eta|}, \tag{23}$$

and for the concave kernel  $\zeta$  of  $\xi$ , we have

$$\max \{|\theta|_1 - |\theta|\rho(\zeta)\} = 1 - \frac{1}{|\zeta|},$$

where “min” and “max” are for all prefixes  $\theta$  of  $\eta$  or  $\zeta$ , respectively.



*Proof* 1. Follows from Lemma 8 and the fact that

$$|\eta|_1 = \text{per}(\xi)\rho(\eta) = \text{per}(\xi)\hat{\rho}(\xi).$$

2. Similar to 1.
3. Follows from Lemma 4.
4. Follows from 4 of Lemma 7.
5. Let  $u := |\eta|$  and  $v := |\eta|_1$ . Then,  $u$  and  $v$  coprime by Lemma 8. Since  $\eta = \underline{\lambda}(u, v)$ , we have

$$|\eta_1, \eta_2 \dots \eta_i|_1 - |\eta_1, \eta_2 \dots \eta_i|\rho(\eta) = [iv/u] - iv/u = -j/u$$

for any  $i = 0, 1, \dots, u$ , where  $j \equiv iv \pmod{u}$  with  $0 \leq j \leq u - 1$ . Since  $u$  and  $v$  are coprime, there exists  $i = 0, 1, \dots, u$  such that  $j = u - 1$  holds in the above. Thus, we have Eq. (23).

The other part is proved in the same way. □

*Proof of Theorem 2* 1. We have already proved that  $\hat{\alpha}(\xi) = \hat{\rho}(\xi)$  in Lemma 9.

To prove that  $P_{\hat{\alpha}}(\xi) = 1/\text{per}(\xi)$ , we may assume without loss of generality that there exists the convex kernel  $\eta$  of  $\xi$  such that  $\eta = \xi[i, i+u]$  with  $u = \text{per}(\xi)$ . Then,  $AB$  is a central prime segment of  $\overline{\Gamma}_\xi$ , where  $A = (i, \Xi_i)$  and  $B = (i+u, \Xi_{i+u})$ . Let  $AB$  be on the graph  $y = x\alpha + \beta_1$  ( $x \in [0, m]$ ). Then, by Lemma 7,  $\alpha = \hat{\alpha} = \hat{\alpha}(\xi)$ . Let  $\beta_2$  be the maximum value of  $\beta$  such that the graph  $y = x\alpha + \beta$  ( $x \in [0, m]$ ) is in the domain  $\overline{\Sigma}_\xi$ . Then,  $y = x\hat{\alpha} + \beta$  ( $x \in [0, m]$ ) is in the domain  $\underline{\Sigma}_\xi$  if and only if  $\beta_1 \leq \beta < \beta_2$ . Hence by 1 of Lemma 2,  $P_{\hat{\alpha}}(\xi) = \beta_2 - \beta_1$ .

Since the graph  $y = x\hat{\alpha} + \beta_2$  ( $x \in [0, m]$ ) is in the domain  $\overline{\Sigma}_\xi$ , any point  $(h, \Xi_h + 1)$  for  $h = 0, 1, \dots, m$  is on or above the graph. Moreover, by the maximality of  $\beta_2$ , there exists an integer  $h$  with  $h \in [0, m]$  such that  $(h, \Xi_h + 1)$  is on the graph  $y = x\hat{\alpha} + \beta_2$ . Since  $u = \text{per}(\xi)$  and  $\hat{\alpha} = \rho(\eta)$ , such an  $h$  can be found in the interval  $[i, i+u]$ . Therefore, we have

$$\beta_2 = \Xi_h + 1 - h\hat{\alpha} = \min_{i \leq j \leq i+u} \{ \Xi_j + 1 - j\hat{\alpha} \}.$$

Since  $\beta_1 = \Xi_i - i\hat{\alpha}$ , we have

$$\begin{aligned} \beta_2 - \beta_1 &= \min_{i \leq j \leq i+u} \{ (\Xi_j + 1 - j\hat{\alpha}) - (\Xi_i - i\hat{\alpha}) \} \\ &= 1 + \min_{i \leq j \leq i+u} \{ |\xi_{i+1}\xi_{i+2} \dots \xi_j|_1 - |\xi_{i+1}\xi_{i+2} \dots \xi_j|\rho(\eta) \}. \end{aligned}$$

Hence, by Eq. 24,

$$P_{\hat{\alpha}}(\xi) = \beta_2 - \beta_1 = \frac{1}{|\eta|} = \frac{1}{\text{per}(\xi)},$$

which completes the proof of 1.

2. Let  $\xi \in \text{St}_m$  be nontrivial. Let  $\alpha = \hat{\alpha} - \varepsilon$  for a sufficiently small  $\varepsilon > 0$ . Let the graph  $y = x\alpha + \beta_1$  ( $0 \leq x \leq m$ ) be in  $\underline{\Sigma}_\xi$  but not in  $\overline{\Sigma}_\xi$  and let the graph  $y = x\alpha + \beta_2$  ( $0 \leq x \leq m$ ) be in  $\overline{\Sigma}_\xi$  but not in  $\underline{\Sigma}_\xi$ . Then, we have  $P_\alpha(\xi) = \beta_2 - \beta_1$ .

Let  $i := \max \bar{I}(\xi)$  and  $j := \min \underline{I}(\xi)$ . Then, the point  $(i, \Xi_i)$  is on  $y = x\alpha + \beta_1$  and the point  $(j, \Xi_j + 1)$  is on  $y = x\alpha + \beta_2$ . Therefore,

$$\begin{aligned} P_\alpha(\xi) &= \beta_2 - \beta_1 \\ &= (\Xi_j + 1 - j\alpha) - (\Xi_i - i\alpha) \\ &= (\Xi_j + 1 - j(\hat{\alpha} - \varepsilon)) - (\Xi_i - i(\hat{\alpha} - \varepsilon)) \\ &= (\Xi_j + 1 - j\hat{\alpha}) - (\Xi_i - i\hat{\alpha}) - (i - j)\varepsilon \\ &= P_{\hat{\alpha}}(\xi) - (\max \bar{I}(\xi) - \min \underline{I}(\xi))\varepsilon, \end{aligned}$$

which implies that the slope of the graph between  $\alpha_1$  and  $\hat{\alpha}$  in Fig. 3 is  $\max \bar{I}(\xi) - \min \underline{I}(\xi)$ . Since  $P_{\hat{\alpha}}(\xi) = 1/\text{per}(\xi)$ , this proved the formula for  $\alpha_1$ . Similarly, we can prove the formula for  $\alpha_2$ .

3. The statistics  $(\hat{\alpha}, \max \bar{I} - \min \underline{I}, \max \underline{I} - \min \bar{I})$  is the minimum sufficient statistics since it induces the same partition as  $(\hat{\alpha}, \alpha_1, \alpha_2)$  by the above formulas. Note that  $\text{per}(\xi)$  is a function of  $\hat{\alpha}$  since it is the denominator of the irreducible rational fraction equal to  $\hat{\alpha}$ .
4. Let  $T := (\hat{\alpha}, \max \bar{I} - \min \underline{I}, \max \underline{I} - \min \bar{I})$ .

Let  $m$  be an even number with  $m \geq 6$ . Let

$$\begin{aligned} \xi &= \bar{\lambda}(m - 1, 2) 1 \\ \eta &= \underline{\lambda}(m - 1, 2) 0. \end{aligned}$$

Then, we have  $|\xi| = |\eta| = m$ ,  $\text{per}(\xi) = \text{per}(\eta) = m - 1$  and  $\hat{\rho}(\xi) = \hat{\rho}(\eta) = 2/(m - 1)$  while  $\rho(\xi) = 3/m$  and  $\rho(\eta) = 2/m$ . Moreover, it is easily seen that

$$\begin{aligned} \bar{I}(\xi) &= \{m/2\} \\ \bar{I}(\eta) &= \{0, m - 1\} \\ \underline{I}(\xi) &= \{0, m - 1\} \\ \underline{I}(\eta) &= \{(m - 2)/2\}. \end{aligned}$$

Thus, we have

$$\begin{aligned} \max \bar{I}(\xi) - \min \underline{I}(\xi) &= (m/2) - 0 = m/2 \\ \max \bar{I}(\eta) - \min \underline{I}(\eta) &= (m - 1) - (m - 2)/2 = m/2 \\ \max \underline{I}(\xi) - \min \bar{I}(\xi) &= (m - 1) - (m/2) = (m - 2)/2 \\ \max \underline{I}(\eta) - \min \bar{I}(\eta) &= (m - 2)/2 - 0 = (m - 2)/2. \end{aligned}$$

Hence, we have  $T(\xi) = T(\eta)$  while  $\rho(\xi) \neq \rho(\eta)$ , which implies that  $\rho$  is not based on  $T$ .

Let  $m$  be an odd number with  $m \geq 9$ . Let

$$\begin{aligned} \xi &= \bar{\lambda}(m - 2, 2) 10 \\ \eta &= \underline{\lambda}(m - 2, 2) 00. \end{aligned}$$

Then, we have  $|\xi| = |\eta| = m$ ,  $\text{per}(\xi) = \text{per}(\eta) = m - 2$  and  $\hat{\rho}(\xi) = \hat{\rho}(\eta) = 2/(m - 2)$  while  $\rho(\xi) = 3/m$  and  $\rho(\eta) = 2/m$ . Moreover, it is easily seen that

$$\begin{aligned} \bar{I}(\xi) &= \{(m - 1)/2\} \\ \bar{I}(\eta) &= \{0, m - 2\} \\ \underline{I}(\xi) &= \{0, m - 2\} \\ \underline{I}(\eta) &= \{(m - 3)/2\}. \end{aligned}$$

Thus, we have

$$\begin{aligned} \max \bar{I}(\xi) - \min \underline{I}(\xi) &= (m - 1)/2 - 0 = (m - 1)/2 \\ \max \bar{I}(\eta) - \min \underline{I}(\eta) &= (m - 2) - (m - 3)/2 = (m - 1)/2 \\ \max \underline{I}(\xi) - \min \bar{I}(\xi) &= (m - 2) - (m - 1)/2 = (m - 3)/2 \\ \max \underline{I}(\eta) - \min \bar{I}(\eta) &= (m - 3)/2 - 0 = (m - 3)/2. \end{aligned}$$

Hence, we have  $T(\xi) = T(\eta)$  while  $\rho(\xi) \neq \rho(\eta)$ , which implies that  $\rho$  is not based on  $T$ .

- Since the Bayes estimate  $\alpha_3$  for the observation  $\xi$  with respect to the uniform prior distribution on  $\alpha \in [0, 1]$  is the mean of  $\alpha$  measured by the normalized likelihood function for  $\xi$  and the graph of the likelihood function is as in Fig. 3, we have

$$\alpha_3 = \frac{\hat{\alpha} + \alpha_1 + \alpha_2}{3}$$

- Suppose that there exists a UMVUE  $T$  for  $\alpha$ . Consider two unbiased estimators

$$\begin{aligned} \rho(\xi) &= \frac{\xi_1 + \xi_2 + \dots + \xi_m}{m} \\ \rho'(\xi) &:= \frac{\xi_1 + \xi_2 + \dots + \xi_{m-1}}{m - 1} \end{aligned}$$

of  $\alpha$ .

At first, assume that  $m$  is odd. Then for  $\alpha = (m + 1)/(2m)$ , we have  $V_\alpha(\rho) = 0$ , since  $P_\alpha$  is supported by the following  $m$  sample points:

$$1(01)(01) \dots (01), (01)1(01) \dots (01), \dots, (01)(01) \dots 1(01), (01)(01) \dots (01)1(10)(10) \dots (10), (10)1(10) \dots (10), \dots, (10)(10) \dots 1(10)$$

each point of which has the same weight  $1/m$ . On the other hand, if  $\alpha = 1/2$ , then we have  $V_\alpha(\rho') = 0$ , since  $P_\alpha$  is supported by the following two sample points:

$$0101 \dots 010, 1010 \dots 101$$

each point of which has the same weight  $1/2$ . Note that the sample point  $1010 \dots 101$  belongs to the both sets. Since  $T$  is UMVUE, we have

$$V_{(m-1)/(2m)}(T) \leq V_{(m-1)/(2m)}(\rho) = 0 \tag{24}$$

$$V_{1/2}(T) \leq V_{1/2}(\rho') = 0. \tag{25}$$

It follows from Eq. (24) that  $T(1010 \cdots 101) = (m - 1)/(2m)$ , while by Eq. (25), we have  $T(1010 \cdots 101) = 1/2$ , which is a contradiction. Thus, UMVUE does not exist.

For the case that  $m$  is even, we can do the same argument for  $\alpha = 1/2$  and  $m/(2m - 2)$  to lead a contradiction.

□

*Example 1*  $St_6$  consists of the following 36 elements:

```

000000 100000 010000 001000 000100 100100
010100 000010 100010 010010 001010 101010
011010 010110 110110 101110 011110 111110
000001 100001 010001 001001 101001 100101
010101 110101 101101 011101 111101 101011
011011 111011 110111 101111 011111 111111
    
```

where 010100, 001010, 101001 and 100101 have the same  $(\hat{\alpha}, \alpha_1, \alpha_2) = (2/5, 1/3, 1/2)$ , and 101011, 110101, 010110 and 011010 have the same  $(\hat{\alpha}, \alpha_1, \alpha_2) = (3/5, 1/2, 2/3)$ . In the other cases, the sample mean coincides if the minimum sufficient statistics coincides. Since  $\rho(010100) = \rho(001010) = 1/3$ ,  $\rho(101001) = \rho(100101) = 1/2$ ,  $\rho(101011) = \rho(110101) = 2/3$  and  $\rho(010110) = \rho(011010) = 1/2$ , we have

$$U(\xi) := E(\rho|\hat{\alpha}, \alpha_1, \alpha_2)(\xi) = \begin{cases} 5/12 & \xi \in \{010100, 001010, 101001, 100101\} \\ 7/12 & \xi \in \{101011, 110101, 010110, 011010\} \\ \rho(\xi) & \text{otherwise.} \end{cases}$$

Clearly,  $U$  is an unbiased estimator of  $\alpha$ . For any  $\alpha$  with  $1/3 < \alpha \leq 2/5$ , since we have

$$P_\alpha(010100) = P_\alpha(001010) = P_\alpha(101001) = P_\alpha(100101) = 3\alpha - 1,$$

it holds that

$$\begin{aligned} V_\alpha(U) &= V_\alpha(\rho) - 4(3\alpha - 1) \left( \frac{1}{2} \left( \frac{1}{3} - \frac{5}{12} \right)^2 + \frac{1}{2} \left( \frac{1}{2} - \frac{5}{12} \right)^2 \right) \\ &= V_\alpha(\rho) - 4(1/2)\{6\alpha\}/144 \\ &= \{6\alpha\}(1 - \{6\alpha\})/36 - \{6\alpha\}/72 \\ &= \{6\alpha\}(1/2 - \{6\alpha\})/36 \end{aligned}$$

In the same way, we have

$$V_\alpha(U) = \begin{cases} \{6\alpha\}(1/2 - \{6\alpha\})/36 & 1/3 < \alpha \leq 2/5 \\ (\{6\alpha\} - 1/3)(1 - \{6\alpha\})/36 & 2/5 \leq \alpha < 1/2 \\ \{6\alpha\}(2/3 - \{6\alpha\})/36 & 1/2 < \alpha \leq 3/5 \\ (\{6\alpha\} - 1/2)(1 - \{6\alpha\})/36 & 3/5 \leq \alpha \leq 2/3 \\ \{6\alpha\}(1 - \{6\alpha\})/36 & \text{otherwise.} \end{cases}$$

*Example 2*  $St_7$  consists of the following 36 elements:

```

000000 100000 010000 001000 000100 100100
010100 000010 100010 010010 001010 101010
011010 010110 110110 101110 011110 111110
000001 100001 010001 001001 101001 100101
010101 110101 101101 011101 111101 101011
011011 111011 110111 101111 011111 111111

```

where 010100, 001010, 101001 and 100101 have the same  $(\hat{\alpha}, \alpha_1, \alpha_2) = (2/5, 1/3, 1/2)$  and 101011, 110101, 010110 and 011010 have the same  $(\hat{\alpha}, \alpha_1, \alpha_2) = (3/5, 1/2, 2/3)$ . In the other cases, the sample mean coincides if the minimum sufficient statistics coincides.

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