The Markov Chain Imbedding Technique
Application to Scan Statistics

Alexandru Amǎrioarei

Laboratoire de Mathématiques Paul Painlevé
Département de Probabilités et Statistique
Université de Lille 1

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Compute the exact distribution of runs and patterns in a sequence of multi-state trial outcomes generated by an i.i.d. or Markov source.

Different approaches

- Traditional approach: combinatorial methods
  - i.i.d. case (Makri 1986 and Hirano 1990)
- Markov Chain Imbedding Technique (Fu and Koutras 1994)
  - i.i.d. case
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Given $X_1, X_2, \ldots, X_n$ a sequence of multi-state trials over the alphabet $S = \{b_1, \ldots, b_m\}$ we say that

- $\Lambda$ is a **simple pattern** if $\Lambda = b_{i_1} b_{i_2} \ldots b_{i_k}$ where $b_{i_j} \in S$ for all $j = 1, k$
- $\Lambda_1$ and $\Lambda_2$ are **distinct** if neither $\Lambda_1 \subset \Lambda_2$ nor $\Lambda_2 \subset \Lambda_1$
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- $X_n(\Lambda)$ denote the number of occurrences of the pattern $\Lambda$ in the sequence $X_1, X_2, \ldots, X_n$ using both overlapping and non-overlapping counting scheme

**Example**

Consider a simple pattern $\Lambda = ACA$ over the alphabet $S = \{A, C, G, T\}$ and the realization: $ATCACACATAGACAC\underline{AGTAC}$

- $X_{20}(\Lambda) = 2$ under non-overlapping scheme
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Definition

Given a compound pattern $\Lambda$ we say that $X_n(\Lambda)$ is finite Markov chain imbeddable if:

- there exists a finite Markov chain $\{Y_t| t = 0, 1, \ldots, n\}$ defined on a finite state space $\Omega = \{a_1, a_2, \ldots, a_s\}$ with initial probability vector $\xi_0$
- there exists a finite partition $\{C_x| x = 0, 1, \ldots, l_n\}$ on the state space
- for every $x = 0, 1, \ldots, l_n$ we have

$$P(X_n(\Lambda) = x) = P(Y_n \in C_x|\xi_0)$$
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An application of Chapman-Kolmogorov equations leads to:

**Theorem**

*If $X_n(\Lambda)$ is finite Markov chain imbeddable, then*

$$P(X_n(\Lambda) = x) = \xi_0 M^n U^T(C_x)$$

- $\xi_0 = P(Y_0 = a_1, Y_0 = a_2, \ldots, Y_0 = a_s)$ is the initial probability vector
- $M$ is the transition probability matrix of $(Y_t)_{t=0, n}$
- $U(C_x) = \sum_{a_j \in C_x} e_j$ and $e_j = (0, \ldots, 1, \ldots, 0)_{1 \times s}$ is an unit vector corresponding to $a_j$

The imbedded chain may be
- homogeneous
- non-homogeneous and $M^n \to \prod_{t=1}^n M_t$
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Can we always imbed a random variable associated with a specified pattern into a Markov chain?

...one way is by using *forward-backward* procedure developed by Fu (1996) based on

- a proper understanding of the structure of the specified pattern
- the counting procedure applied throughout the sequence
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Non-overlap counting

Given

- \((X_t)_{t=1}^{n}\) - Markov dependent
  
  \[
  A = \begin{pmatrix}
  p_{11} & p_{12} & p_{13} \\
  p_{21} & p_{22} & p_{23} \\
  p_{31} & p_{32} & p_{33}
  \end{pmatrix}
  \]

- the alphabet \(S = \{b_1, b_2, b_3\}\)
- the simple pattern \(\Lambda = b_1 b_1 b_1 b_2\)
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We will give the method in five steps:

**Step 1**
Define $S(\Lambda) = \{b_1, b_1 b_1, b_1 b_1 b_1, b_1 b_1 b_1 b_2\}$ the set of all sequential sub-patterns and

$$\mathcal{E} = S \cup S(\Lambda) = \{b_1, b_2, b_3, b_1 b_1, b_1 b_1 b_1, b_1 b_1 b_1 b_2\}$$

**Step 2**
Define the state space

$$\Omega = \{(u, v) | u = 0, 1, \ldots, [n/4], v \in \mathcal{E}\} \cup \{\emptyset\} \setminus \{(0, b_1 b_1 b_1 b_2)\}$$
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Step 3: define the Markov chain

\[ Y_t = (X_t(\Lambda), E_t), \quad t = 1, 2, \ldots, n \]

such that \( Y_t(\omega) = (u, v) \in \Omega \), where

- \( u = X_t(\Lambda)(\omega) \) - the total number of non-overlapping occurrences of the pattern \( \Lambda \) in the first \( t \) trials, counting forward from the first to the \( t \)-th trial
- \( v = E_t(\omega) \) - the longest ending block in \( E \), counting backward from \( X_t \).
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Considering the realization:

\[ \omega = (b_2 b_3 b_1 b_1 b_2 b_1 b_1 b_2 b_1 b_3 b_1) \]

| \( Y_1(\omega) = (0, b_2) \) | \( Y_5(\omega) = (0, b_2) \) | \( Y_9(\omega) = (1, b_1 b_1 b_1 b_2) \) |
| \( Y_2(\omega) = (0, b_3) \) | \( Y_6(\omega) = (0, b_1) \) | \( Y_{10}(\omega) = (1, b_1) \) |
| \( Y_3(\omega) = (0, b_1) \) | \( Y_7(\omega) = (0, b_1 b_1) \) | \( Y_{11}(\omega) = (1, b_3) \) |
| \( Y_4(\omega) = (0, b_1 b_1) \) | \( Y_8(\omega) = (0, b_1 b_1 b_1) \) | \( Y_{12}(\omega) = (1, b_1) \) |
Step 4  the transition matrix $M$ can be determined for example by

$$(0, b_1 b_1 b_1) \rightarrow \begin{cases} 
(0, b_1 b_1 b_1), & X_9 = b_1, \text{probability is } p_{11} \\
(1, b_1 b_1 b_1 b_2), & X_9 = b_2, \text{probability is } p_{12} \\
(0, b_3), & X_9 = b_3, \text{probability is } p_{13}
\end{cases}$$

- $\emptyset$ - the dummy state
- $P(Y_1 = b_i|Y_0 = \emptyset) = p_i$ with $i = 1, 2, 3$ the initial distribution

Step 5  the partition

$$C_x = \begin{cases} 
C_{\emptyset} = \{\emptyset\} \\
C_0 = \{(0, b_1), (0, b_2), (0, b_3), (0, b_1 b_1), (0, b_1 b_1 b_1)\} \\
C_z = \{(z, v)|v \in E, z = 1, \ldots, [n/4]\}.
\end{cases}$$
Step 4  the transition matrix $M$ can be determined for example by

$$(0, b_1 b_1 b_1) \rightarrow \begin{cases} 
(0, b_1 b_1 b_1), & X_9 = b_1, \text{probability is } p_{11} \\
(1, b_1 b_1 b_1 b_2), & X_9 = b_2, \text{probability is } p_{12} \\
(0, b_3), & X_9 = b_3, \text{probability is } p_{13} 
\end{cases}$$

- $\emptyset$ - the dummy state
- $\mathbb{P}(Y_1 = b_i | Y_0 = \emptyset) = p_i$ with $i = 1, 2, 3$ the initial distribution

Step 5  the partition

$$C_x = \begin{cases} 
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Step 5  the partition

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C_z = \{(z, v) | v \in \mathcal{E}, z = 1, \ldots, \lfloor n/4 \rfloor\}.
\end{cases}$$
The transition matrix \((n = 5)\) \(M:\)

\[
\begin{pmatrix}
\emptyset & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} & a_{11} \\
0 & p_1 & p_2 & p_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & p_{12} & p_{13} & p_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & p_{21} & p_{22} & p_{23} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & p_{31} & p_{32} & p_{33} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & p_{12} & p_{13} & 0 & p_{11} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & p_{13} & 0 & p_{11} & p_{12} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & p_{21} & p_{22} & p_{23} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & p_{12} & p_{13} & p_{11} & 0 & 0 \\
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0 & 0 & 0 & 0 & 0 & 0 & 0 & p_{12} & p_{13} & 0 & p_{11} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 
\end{pmatrix}
\]

A. Amarioarei (Laboratoire P. Painlevé)
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2 Description of the method
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   ● The forward-backward principle

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   ● Numerical example

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6 References
Definition

- the waiting time for a simple pattern $\Lambda = b_{i_1}b_{i_2} \ldots b_{i_k}$

$$W(\Lambda) = \inf \{ n | X_{n-k+1} = b_{i_1}, \ldots, X_n = b_{i_k} \}$$

- the waiting time of a compound pattern $\Lambda = \cup_{i=1}^{l} \Lambda_i$

$W(\Lambda) =$ minimum number of trials required to observe the occurrence of one of the simple patterns $\Lambda_1, \ldots, \Lambda_l$

- the waiting time of the $r$-th occurrence of the pattern $\Lambda$

$W(r, \Lambda) =$ minimum number of trials required to observe the $r$-th occurrence of the pattern $\Lambda$

The duality property:

$$\mathbb{P}(X_n(\Lambda) < r) = \mathbb{P}(W(r, \Lambda) > n).$$
Definition

- The waiting time for a simple pattern \( \Lambda = b_{i_1} b_{i_2} \ldots b_{i_k} \)

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Waiting time distributions

Definitions and main results

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The duality property:

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\mathbb{P}(X_n(\Lambda) < r) = \mathbb{P}(W(r, \Lambda) > n).
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Given:

- the Markov chain \((X_t)_{1,\infty}\) over the alphabet \(S = \{b_1, \ldots, b_m\}\)
- compound pattern \(\Lambda = \bigcup_{i=1}^l \Lambda_i\)

we have using the *forward-backward* principle:

- the state space \(\Omega = \{\emptyset\} \cup S \cup \bigcup_{i=1}^l S(\Lambda_i)\)
- \(A = \{\alpha_1, \ldots, \alpha_l\}\) the set of absorbing states corresponding to the simple pattern \(\Lambda_i\)
- for \(Y_{t-1} = u \in \Omega \setminus A \setminus \{\emptyset\}\) and \(X_t = z \in S\) we define the longest ending block

\[v = \langle u, z \rangle_{\Omega}\]

and the set

\[[u : S] = \{v \mid v \in \Omega, v = \langle u, z \rangle_{\Omega}, z \in S\}\]
Given:

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Theorem

1. The transition probabilities of the imbedded Markov chain $Y_t$,

$$ p_{u,v} = \mathbb{P}(Y_t = v | Y_{t-1} = u) = \begin{cases} 
  p_z, & \text{if } u = \emptyset, v = z, z \in S \\
  p_{xz}, & \text{if } u \in \Omega \setminus A \setminus \{\emptyset\} \text{ and } v \in [u : S] \text{ and } X_t = z \\
  1, & \text{if } u \in A \text{ and } v = u \\
  0, & \text{otherwise} 
\end{cases} $$

where $x$ is the last symbol of $u$ and $p_z = \mathbb{P}(Y_1 = z | Y_0 = \emptyset)$

$$ M = \begin{pmatrix} 
  N^{(d-1) \times (d-1)} & C \\
  O & I 
\end{pmatrix}_{d \times d} $$

2. Given the initial distribution $\xi_0 = (\xi : 0)$

$$ \mathbb{P}(W(\Lambda) = n) = \xi N^{n-1}(I - N)1^T $$
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Waiting time of the $r$-th occurrence

For $W(r, \Lambda)$

- the state space

$$\Omega^{(r)} = \{\emptyset\} \cup \Omega_1 \cup \Omega_2 \cup A$$

- $A = \{\alpha_1, \ldots, \alpha_l\}$ is the set of all the absorbing states $\alpha_j$ corresponding to the $r$-th occurrence of the pattern $\Lambda_j$

$$\Omega_1 = \{(u, v) | u = 0, \ldots, r - 1; v \in S \cup S(\Lambda_1) \cdots \cup S(\Lambda_l) \setminus A\},$$

$$\Omega_2 = \{(u, v) | u = 1, \ldots, r - 1; v \in B\}$$

where $B$ is the collection of the last symbols of $\Lambda_i$, $i = 1, \ldots, l$ (we add some mark to distinguish from $S$)
Waiting time of the $r$-th occurrence

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Example

Given,

- the alphabet $\mathcal{S} = \{A, C, G, T\}$
- the Chi motif $\Lambda = GNTGGTG$ where $N \in \mathcal{S}$
- the transition matrix (estimated over *Escherichia Coli* genome)

\[
\begin{pmatrix}
  p_{AA} & p_{AC} & p_{AG} & p_{AT} \\
  p_{CA} & p_{CC} & p_{CG} & p_{CT} \\
  p_{GA} & p_{GC} & p_{GG} & p_{GT} \\
  p_{TA} & p_{TC} & p_{TG} & p_{TT}
\end{pmatrix} =
\begin{pmatrix}
  0.30 & 0.21 & 0.22 & 0.27 \\
  0.23 & 0.23 & 0.32 & 0.22 \\
  0.28 & 0.29 & 0.23 & 0.20 \\
  0.19 & 0.28 & 0.23 & 0.30
\end{pmatrix}
\]

and the stationary distribution

\[
\mu = (0.2501, 0.2524, 0.2502, 0.2473)
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Comparison between i.i.d. and Markov case:
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6. References
Scan Statistics

- \((X_t)_{t=1,n}\) - two-state Markov dependent

\[
P = \begin{pmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{pmatrix}
\]

- the scan statistic of window size \(r\)

\[
S_n(r) = \max_{r \leq t \leq n} \sum_{k=t-r+1}^{t} X_k.
\]

- the idea is to express the distribution of the \(S_n(r)\) in terms of the waiting time distribution of a special compound pattern
Scan Statistics

- \((X_t)_{t=1,n}\) - two-state Markov dependent

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Scan Statistics

- $(X_t)_{t=1,n}$ - two-state Markov dependent

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- the idea is to express the distribution of the $S_n(r)$ in terms of the waiting time distribution of a special compound pattern
Distribution of Scan Statistics in 4 Steps

1. define for $0 \leq k \leq r$

$$\mathcal{F}_{r,k} = \{ \Lambda_i | \Lambda_1 = \underbrace{1 \ldots 1}_k, \Lambda_2 = \underbrace{10 \ldots 1}_{k-1}, \ldots, \Lambda_l = \underbrace{1 \ldots 1}_{k-1} 0 \ldots 01 \}$$

$$|\mathcal{F}_{r,k}| = \sum_{j=0}^{r-k} \binom{k-2+j}{j}$$

2. the compound pattern $\Lambda = \bigcup_{i=1}^l \Lambda_i$, $\Lambda_i \in \mathcal{F}_{r,k}$

3. the dual property

$$\mathbb{P}(S_n(r) < k) = \mathbb{P}(W(\Lambda) \geq n + 1).$$

4. the matrix formula

$$\mathbb{P}(S_n(r) < k) = \xi N^T 1, \text{where } \xi = (1, 0, \ldots, 0)$$
Distribution of Scan Statistics in 4 Steps

1. Define for $0 \leq k \leq r$

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Applications to Scan Statistics

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1. Define for $0 \leq k \leq r$

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Distribution of Scan Statistics in 4 Steps

1. Define for $0 \leq k \leq r$

$$\mathcal{F}_{r,k} = \{\Lambda_i | \Lambda_1 = 1 \ldots 1, \Lambda_2 = 10 1 \ldots 1, \ldots, \Lambda_I = 1 \ldots 1 0 \ldots 01\}$$

$$|\mathcal{F}_{r,k}| = \sum_{j=0}^{r-k} \left(\begin{array}{c} k - 2 + j \\ j \end{array}\right)$$

2. The compound pattern $\Lambda = \bigcup_{i=1}^I \Lambda_i$, $\Lambda_i \in \mathcal{F}_{r,k}$

3. The dual property

$$\mathbb{P}(S_n(r) < k) = \mathbb{P}(W(\Lambda) \geq n + 1).$$

4. The matrix formula

$$\mathbb{P}(S_n(r) < k) = \xi N^n 1^T, \text{ where } \xi = (1, 0, \ldots, 0)$$
**Example**

- **an illustration for** $n = 20$ and $r = 3$

\[ S_{20}(3) = 1 \]

- **for** $r = 4$ and $k = 3$

\[ F_{4,3} = \{ \Lambda_1 = 111, \Lambda_2 = 1011, \Lambda_3 = 1101 \} \]

- **the state space**

\[ \Omega = \{ \emptyset, 0, 1, 10, 11, 101, 110, \alpha_1, \alpha_2, \alpha_3 \} \]
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\begin{array}{ccccccccccccccc}
0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0
\end{array}
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$S_{20}(3) = 2$

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\( S_{20}(S(3)|3) = 2 \)

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the transition matrix $M$:

$$
\begin{pmatrix}
0 & q & p & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & p_{00} & p_{01} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & p_{10} & p_{11} & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & p_{00} & 0 & 0 & 0 & p_{01} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & p_{10} & \cdots & p_{11} & 0 & 0 \\
0 & 0 & 0 & p_{10} & 0 & 0 & 0 & \cdots & 0 & p_{11} & 0 \\
0 & p_{00} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & p_{01} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\
\end{pmatrix}
$$
Outline

1 Introduction
   • Problem

2 Description of the method
   • Definitions and main results
   • The forward-backward principle

3 Waiting time distributions
   • Definitions and main results
   • An example

4 Applications to Scan Statistics
   • Model
     • Numerical example

5 Conclusions

6 References
An example for windows size $r = 10$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$k$</th>
<th>$(p, q) = (0.4091, 0.5909)$</th>
<th>$p_{11} = 0.35, p_{21} = 0.45$</th>
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<tr>
<td>100</td>
<td>5</td>
<td>$2.3233 \times 10^{-4}$</td>
<td>$2.0318 \times 10^{-4}$</td>
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<tr>
<td></td>
<td>6</td>
<td>0.0166</td>
<td>0.0233</td>
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<td></td>
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<td>0.1953</td>
<td>0.2801</td>
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<td>8</td>
<td>0.6204</td>
<td>0.7488</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.9168</td>
<td>0.9638</td>
</tr>
<tr>
<td>300</td>
<td>5</td>
<td>$5.8339 \times 10^{-12}$</td>
<td>$3.7279 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>$2.9108 \times 10^{-6}$</td>
<td>$8.1662 \times 10^{-6}$</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>0.0060</td>
<td>0.0185</td>
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<tr>
<td></td>
<td>8</td>
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<tr>
<td></td>
<td>9</td>
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<td>0.8896</td>
</tr>
<tr>
<td>500</td>
<td>5</td>
<td>$1.4649 \times 10^{-19}$</td>
<td>$6.8399 \times 10^{-20}$</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>$5.1014 \times 10^{-10}$</td>
<td>$2.8665 \times 10^{-9}$</td>
</tr>
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<td>7</td>
<td>$1.8544 \times 10^{-4}$</td>
<td>0.0012</td>
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<td>8</td>
<td>0.0796</td>
<td>0.2151</td>
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<tr>
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<td>0.6292</td>
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Comparison between i.i.d. and Markov case:
Conclusions:

- **Advantages:**
  - The method gives exact results for the distribution of $X_n(\Lambda)$.
  - The method is simpler than the traditional approach.
  - The method can be used for both i.i.d. and Markov chain sources.

- **Disadvantages:**
  - For big $n$, the order of the state space and the transition matrix become very large, and in this case, the need for approximations methods is mandatory.
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