The Markov Chain Imbedding Technique

Application to Scan Statistics

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Outline

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Problem

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

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

- Λ is a *simple pattern* if $\Lambda = b_{i_1} b_{i_2} \ldots b_{i_k}$ where $b_{i_j} \in \mathcal{S}$ for all $j = \overline{1, k}$
- Λ_1 and Λ_2 are *distinct* if neither $\Lambda_1 \subset \Lambda_2$ nor $\Lambda_2 \subset \Lambda_1$
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Example

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

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

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

- there exists a finite Markov chain $\{Y_t | t = 0, 1, \dots, n\}$ defined on a finite state space $\Omega = \{a_1, a_2, \dots, a_s\}$ with initial probability vector ξ_0
- there exists a finite partition $\{C_x | x = 0, 1, \dots, l_n\}$ on the state space
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$$\mathbb{P}(X_n(\Lambda) = x) = \mathbb{P}(Y_n \in C_x | \xi_0)$$

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- $\boldsymbol{U}(C_x) = \sum_{a_j \in C_x} e_j$ *and* $e_j = (0, \dots, 1, \dots, 0)_{1\times s}$ *is an unit vector corresponding to* a_j

The imbedded chain may be

- homogeneous
- non-homogeneous and $\boldsymbol{M}^n \to \prod_{t=1}^{n} \boldsymbol{M_t}$

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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
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Non-overlap counting

Given

- $(X_t)_{t=\overline{1,n}}$ - Markov dependent

$$\boldsymbol{A} = \begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{pmatrix}$$

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We will give the method in five steps:

Step1 define $\mathcal{S}(\Lambda) = \{b_1, b_1 b_1, b_1 b_1 b_1, b_1 b_1 b_1 b_2\}$ the set of all sequential sub-patterns and

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

Step2 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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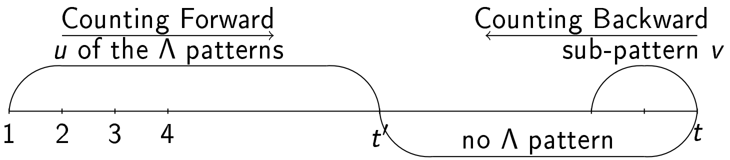


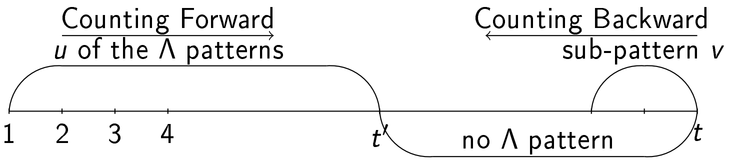
Step3 define the Markov chain

$$Y_t = (X_t(\Lambda), E_t),\ t = 1, 2, \ldots, n$$

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 Λ in the first t trials, counting *forward* from the first to the t-th trial

$v =$ $E_t(\omega)$ - the longest ending block in $\mathcal{E}$, counting *backward* from X_t.



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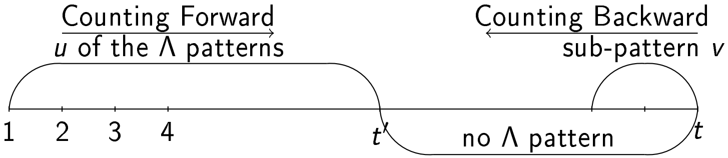

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Considering the realization:

$$\omega = (b_2 b_3 b_1 b_1 b_2 b_1 b_1 b_1 b_2 b_1 b_3 b_1)$$

$Y_1(\omega) = (0, b_2)$	$Y_5(\omega) = (0, b_2)$	$Y_9(\omega) = (1, b_1 b_1 b_1 b_2)$
$Y_2(\omega) = (0, b_3)$	$Y_6(\omega) = (0, b_1)$	$Y_{10}(\omega) = (1, b_1)$
$Y_3(\omega) = (0, b_1)$	$Y_7(\omega) = (0, b_1 b_1)$	$Y_{11}(\omega) = (1, b_3)$
$Y_4(\omega) = (0, b_1 b_1)$	$Y_8(\omega) = (0, b_1 b_1 b_1)$	$Y_{12}(\omega) = (1, b_1)$

Step4 the transition matrix $\boldsymbol{M}$ 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

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$$C_x = \begin{cases} C_\emptyset = \{\emptyset\} \\ C_0 = \{(0, b_1), (0, b_2), (0, b_3), (0, b_1 b_1), (0, b_1 b_1 b_1)\} \\ C_z = \{(z, v) | v \in \mathcal{E}, z = 1, \dots, [n/4]\}. \end{cases}$$

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The transition matrix ($n = 5$) M:

$$
\begin{array}{c}
\begin{array}{cccccccccccc}
\emptyset & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & a_7 & a_8 & a_9 & a_{10} & a_{11}
\end{array} \\
\begin{pmatrix}
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 \\
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0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
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Outline

Definition

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

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

- 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 $\Lambda_1, \dots, \Lambda_l$
- the waiting time of the r-th occurrence of the pattern Λ
  $W(r, \Lambda)$ = minimum number of trials required to observe the r-th occurrence of the pattern Λ

The duality property:

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

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Given:

- the Markov chain $(X_t)_{\overline{1,\infty}}$ over the alphabet $\mathcal{S} = \{b_1, \ldots, b_m\}$
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we have using the *forward-backward* principle:

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

1. *the transition probabilities of the imbedded Markov chain Y_t,*

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

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

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

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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 α_j corresponding to the r-th occurrence of the pattern Λ_j
- $$\Omega_1 = \{(u, v) | u = 0, \ldots, r-1; v \in \mathcal{S} \cup \mathcal{S}(\Lambda_1) \cdots \cup \mathcal{S}(\Lambda_l) \setminus A\},$$
$$\Omega_2 = \{(u, v) | u = 1, \ldots, r-1; v \in \mathcal{B}\}$$
where $\mathcal{B}$ is the collection of the last symbols of Λ_i, $i = 1, \ldots, l$ (we add some mark to distinguish from $\mathcal{S}$)

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Outline

Example

Given,

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

$$\begin{array}{cccc} A & C & G & T \end{array} \qquad \begin{array}{cccc} A & C & G & T \end{array}$$

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

and the stationary distribution

$$\mu = (0.2501, 0.2524, 0.2502, 0.2473)$$

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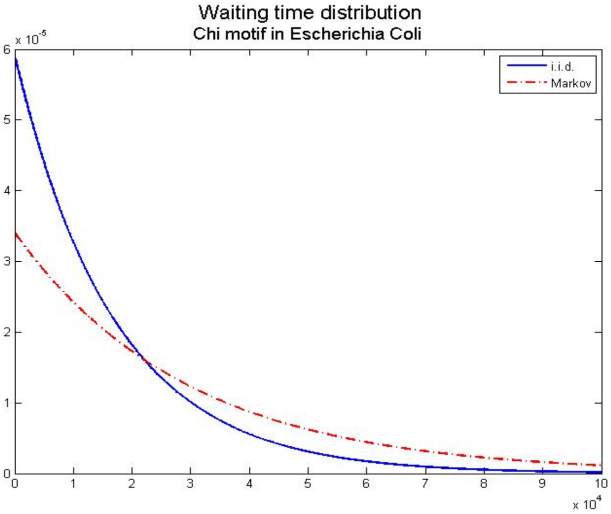
Comparison between i.i.d. and Markov case:



Outline

Scan Statisitcs

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

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

- the scan statistic of window size r

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

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Distribution of Scan Statistics in 4 Steps

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$$\mathcal{F}_{r,k} = \{\Lambda_i | \Lambda_1 = \underbrace{1\dots1}_{k}, \Lambda_2 = 10\underbrace{1\dots1}_{k-1}, \dots, \Lambda_l = \overbrace{\underbrace{1\dots1}_{k-1}0\dots01}^{r}\}$$

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

2. the compound pattern $\Lambda = \cup_{i=1}^{l} \Lambda_i, \ \Lambda_i \in \mathcal{F}_{r,k}$
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$$\mathbb{P}(S_n(r) < k) = \mathbb{P}(W(\Lambda) \geq n+1).$$

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

Distribution of Scan Statistics in 4 Steps

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

$$\mathcal{F}_{r,k} = \{\Lambda_i | \Lambda_1 = \underbrace{1\ldots1}_{k}, \Lambda_2 = 10\underbrace{1\ldots1}_{k-1}, \ldots, \Lambda_l = \overbrace{\underbrace{1\ldots1}_{k-1}0\ldots01}^{r}\}$$

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

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Example

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

0	0	1	0	1	0	1	1	1	0	1	1	0	1	0	1	0	1	1	0

$S_{20}(3) = 1$

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

$$\mathcal{F}_{4,3} = \{\Lambda_1 = 111, \Lambda_2 = 1011, \Lambda_3 = 1101\}$$

- the state space

$$\Omega = \{\emptyset, 0, 1, 10, 11, 101, 110, \alpha_1, \alpha_2, \alpha_3\}$$

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0	0	1	0	1	0	1	1	1	0	1	1	0	1	0	1	0	1	1	0

$S_{20}(3) = 2$

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- the transition matrix $\boldsymbol{M}$:

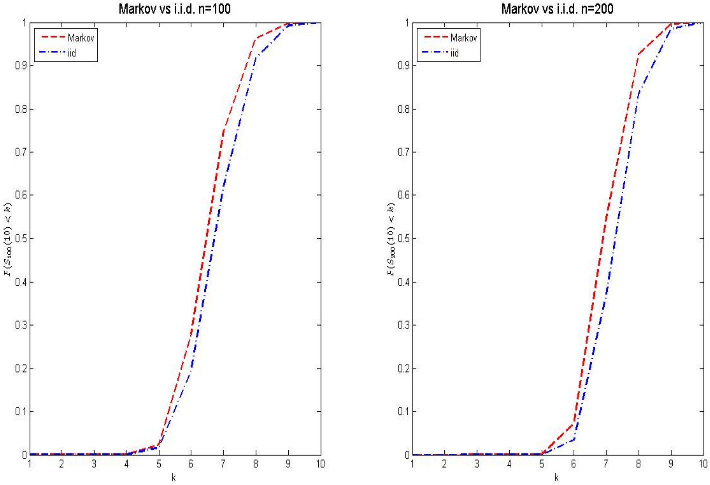
$$
\begin{pmatrix}
0 & q & p & 0 & 0 & 0 & 0 & \vdots & 0 & 0 & 0 \\
0 & p_{00} & p_{01} & 0 & 0 & 0 & 0 & \vdots & 0 & 0 & 0 \\
0 & 0 & 0 & p_{10} & p_{11} & 0 & 0 & \vdots & 0 & 0 & 0 \\
0 & p_{00} & 0 & 0 & 0 & p_{01} & 0 & \vdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & p_{10} & \vdots & p_{11} & 0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

Outline

An example for windows size $r = 10$

n	k	$(p,q) = (0.4091, 0.5909)$	$p_{11} = 0.35, p_{21} = 0.45$
100	5	2.3233×10^{-4}	2.0318×10^{-4}
	6	0.0166	0.0233
	7	0.1953	0.2801
	8	0.6204	0.7488
	9	0.9168	0.9638
300	5	5.8339×10^{-12}	3.7279×10^{-12}
	6	2.9108×10^{-6}	8.1662×10^{-6}
	7	0.0060	0.0185
	8	0.2223	0.4014
	9	0.7595	0.8896
500	5	1.4649×10^{-19}	6.8399×10^{-20}
	6	5.1014×10^{-10}	2.8665×10^{-9}
	7	1.8544×10^{-4}	0.0012
	8	0.0796	0.2151
	9	0.6292	0.8212

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 simple 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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