A BWT-based algorithm for random de Bruijn sequence construction

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(joint work with Luca Parmigiani[2])

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Def. A binary de Bruijn sequence (dB sequence) of order k is a (circular) string in which every k-mer (string of length k) occurs exactly once as a substring.

Ex. $t = \underset{0\,1\,2\,3\,4\,5\,6\,7}{\text{aaababbb}}$

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aab	1
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abb	4
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bab	3
bba	6
bbb	5

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Clearly, a dB sequence of order k has length 2^k.

de Bruijn sequences

- de Bruijn sequences exist for every k (Fly Sainte-Marie, 1894)
- There are $2^{2^{k-1}-k}$ dB sequences of order k (de Bruijn, 1946)

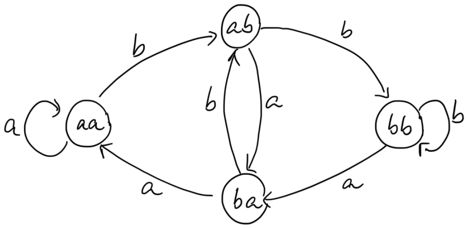
k	1	2	3	4	5	6	7	10	15
#dBseqs	1	1	2	16	2048	67 108 864	$1.44 \cdot 10^{17}$	$1.3 \cdot 10^{151}$	$3.63 \cdot 10^{4927}$

- $k = 1$: ab, $k = 2$: aabb, $k = 3$: aaababbb, aaabbbab
- dB sequences correspond to Euler cycles in the dB graph

de Bruijn graphs

Def. The (binary) de Bruijn graph of order k is a directed graph (V, E) s.t. $V = \{a, b\}^k$, and $(u, v) \in E$ iff there is $w \in \{a, b\}^{k+1}$ with prefix u and suffix v.[1]

Ex. $k = 2$:



We write the new character x on edge (u, v): $w = ux$.

[1] In the bioinformatics literature these are called dB graphs of order $k + 1$.

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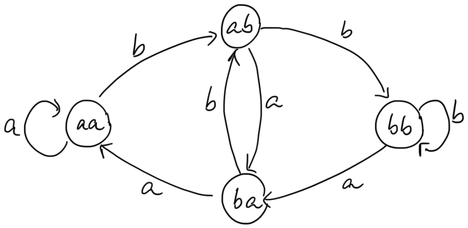

We write the new character x on edge (u, v): $w = ux$.

So we have a 1-to-1 correspondence between E and $\{a, b\}^{k+1}$, and every walk in the dB graph spells a string (concatenate the new characters).

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de Bruijn graphs

- de Bruijn graphs are connected and balanced (all v: indeg = outdeg)
- By Euler's theorem, they are Eulerian (have Euler cycles).
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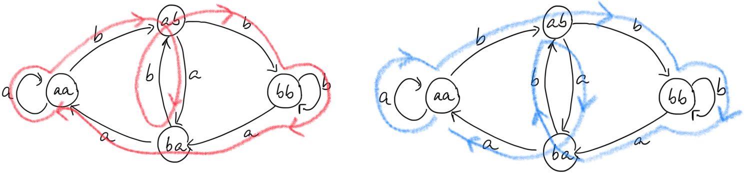

aaababbb

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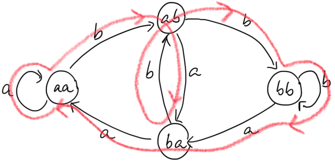
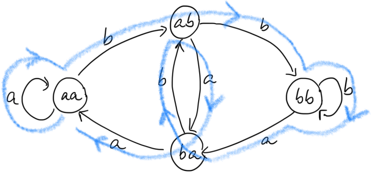


aaababbb



aaabbbab

- Tatyana Ehrenfest and Nicolaas de Bruijn gave the exact number of Euler cycles in directed Eulerian graphs (BEST theorem, 1951).

Applications of de Bruijn sequences

- pseudo-random bit generators

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Related work

Many algorithms exist for constructing dB sequences (see the classic book [Golomb 1968], the survey [Fredricksen 1982], Joe Sawada's website `debruijnsequence.org`). Most construct:

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- The only algorithms able to construct **any** dB sequence are based on finding Eulerian cycles in de Bruijn graphs (Hierholzer, Fleury)

Construction of random dB sequences

- Surprisingly, there appear to be no practical algorithm for random dB sequence construction that can output **any** dB sequence with positive probability.
- Our algorithm does just that!

The Burrows-Wheeler Transform

Def. The Burrows-Wheeler Transform (BWT) of a string t is the concatenation of the last characters of its rotations, taken in lexicographical order.

Ex. $t = \text{aaababbb}$

							bwt(t)
a	a	a	b	a	b	b	b
a	a	b	a	b	b	b	a
a	b	a	b	b	b	a	a
a	b	b	b	a	a	a	b
b	a	a	a	b	a	b	b
b	a	b	b	b	a	a	a
b	b	a	a	a	b	a	b
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b	a	a	a	b	a	b	b
b	a	b	b	b	a	a	a
b	b	a	a	a	b	a	b
b	b	b	a	a	a	b	a

bwt(aaababbb) $=$ baabbaba

Reversing the BWT

Def. Given a string v, its standard permutation π_v is defined by: $\pi_v(i) < \pi_v(j)$ if (i) $v_i < v_j$, or (ii) $v_i = v_j$ and $i < j$.

(When v is a BWT, then π_v is also called LF-mapping, which can be used to recover t from $\text{bwt}(t)$ back-to-front.)

Ex. $v = \text{baabbaba}$

$$\pi_v = \left(\begin{smallmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 4 & 0 & 1 & 5 & 6 & 2 & 7 & 4 \end{smallmatrix}\right) = (0, 4, 6, 7, 3, 5, 2, 1)$$

Thm. (Folklore) A string v is the BWT of a primitive string u if and only if π_v is cyclic.

The BWT of a dB sequence

$t =$ aaababbb

							bwt(t)
a	a	a	b	a	b	b	b
a	a	b	a	b	b	b	a
a	b	a	b	b	b	a	a
a	b	b	b	a	a	a	b
b	a	a	a	b	a	b	b
b	a	b	b	b	a	a	a
b	b	a	a	a	b	a	b
b	b	b	a	a	a	b	a

bwt(aaababbb) $=$ baabbaba

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a	b	b	b	a	a	a	b
b	a	a	a	b	a	b	b
b	a	b	b	b	a	a	a
b	b	a	a	a	b	a	b
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The BWT of a dB sequence

$t =$ aaababbb

bwt(t)

a	a	a	b	a	b	b	b
a	a	b	a	b	b	b	a
a	b	a	b	b	b	a	a
a	b	b	b	a	a	a	b
b	a	a	a	b	a	b	b
b	a	b	b	b	a	a	a
b	b	a	a	a	b	a	b
b	b	b	a	a	a	b	a

$bwt(t) = u_0 u_1 \cdots u_{2^{k-1}-1}$, where each block $u_i \in \{ab, ba\}$

Question Is every string of the form $v \in \{\text{ab},\text{ba}\}^{2^{k-1}}$ the BWT of a dB sequence?

No! Ex. $v = \text{babababa}$, its standard perm. is

$$\pi_v = \left(\begin{smallmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 4 & 0 & 5 & 1 & 6 & 2 & 7 & 3 \end{smallmatrix}\right) = (0,4,6,7,3,1)(2,5)$$

The extended BWT (eBWT) is a generalization of the BWT, where every v is the eBWT of something (of a multiset of strings).

Ex. Here we get two strings, one for each cycle: $\{\text{aaabbb},\text{ab}\}$.

The extended BWT

Def. (Mantaci et al., 2007) Let $\mathcal{M}$ be a multiset of primitive strings. The extended BWT (eBWT) of $\mathcal{M}$ is the concatenation of the last characters of its rotations, taken in omega order.

$\mathcal{M} = \{$a,ab,aabbb$\}$

a	a
aabbb	b
ab	b
abbba	a
baabb	b
ba	a
bbaab	b
bbbaa	a

Def. (omega-order): $T <_\omega S$ if (i) $T^\omega <_{lex} S^\omega$, or (ii) $T^\omega = S^\omega$, $T = U^k, S = U^m$ and $k < m$.

The basic theorem

Thm (Higgins, 2012) $v \in \{ab, ba\}^{2^{k-1}}$ if and only if v is the eBWT of a de Bruijn set of order k.

Def. (Higgins, 2012) A binary de Bruijn set of order k is a multiset of total length 2^k such that every k-mer is the prefix of some rotation of some power of some string in $\mathcal{M}$.

Ex. $\mathcal{M}_1 = \{\text{aaabbb}, \text{ab}\}$, $\mathcal{M}_2 = \{\text{a}, \text{ab}, \text{aabbb}\}$.

Coro $v \in \{ab, ba\}^{2^{k-1}}$ is the BWT of a dB sequence if and only if π_v is cyclic.

Swapping characters in the eBWT

Lemma (Swap Lemma) Let $v \in \{\mathsf{a},\mathsf{b}\}^*, v_i \neq v_{i+1}$, and v' be the result of swapping v_i and v_{i+1}. If v_i and v_{i+1} belong to **distinct cycles** in the cycle decomposition of π_v then the number of cycles **decreases by one**; otherwise it **increases by one**.

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Ex.

$$v = \text{ba}\mathbf{ab}\text{baba} \qquad \pi_v = \left(\begin{smallmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 4 & 0 & \mathbf{1} & \mathbf{5} & 6 & 2 & 7 & 3 \end{smallmatrix}\right) = (0,4,6,7,3,5,2,1)$$

$$v' = \text{ba}\mathbf{ba}\text{baba} \qquad \pi_{v'} = \left(\begin{smallmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 4 & 0 & \mathbf{5} & \mathbf{1} & 6 & 2 & 7 & 3 \end{smallmatrix}\right) = (0,4,6,7,3,1)(2,5)$$

This is a generalization of a technique from [Giuliani, L., Masillo, Rizzi, 2021].

Transforming the eBWT of a dB set into the BWT of a dB sequence

v = abababab = $(ab)^4$

a	b	a	b	a	b	a	b
0	4	1	5	2	6	3	7
0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

Transforming . . .

- $v = abababab = (ab)^4$

a	b	a	b	a	b	a	b
0	4	1	5	2	6	3	7
0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

(0)

- v = abababab = $(ab)^4$

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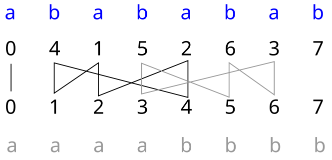
0	4	1	5	2	6	3	7
0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

(0) (1 4 2)

- $v = ababab ab = (ab)^4$



(0) (1 4 2) (3 5 6)

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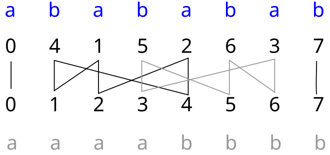

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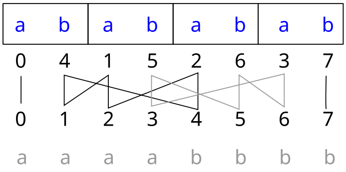

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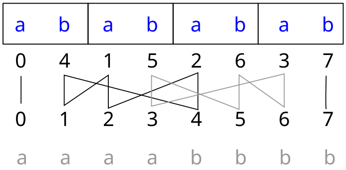

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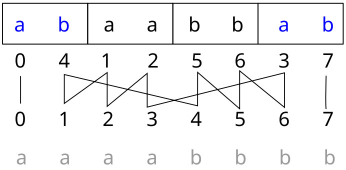
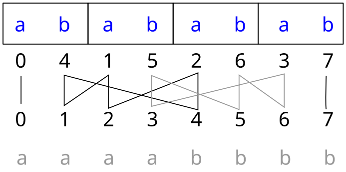


(0) (1 4 5 6 3 2) (7)

If we swap $(3, 4)$ then the resulting string is not in the set $\{ab, ba\}^{2^{k-1}}$. We show that it suffices to swap always within blocks.

Generation of binary de Bruijn sequences of order k

- v = abababab = $(ab)^4$



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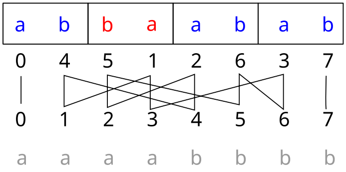


(0) (1 4 2 5 6 3) (7)

We call a block unhappy if its elements are in different cycles. Here we have 4 unhappy blocks, but we need only 3 swaps to get one cycle.

a	b	b	a	a	b	a	b
0	4	5	1	2	6	3	7

0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

(0) (1 4 2 5 6 3) (7)

b	a	b	a	a	b	a	b
4	0	5	1	2	6	3	7
0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

(0 4 2 5 6 3 1) (7)

b	a	b	a	a	b	b	a
4	0	5	1	2	6	3	7
0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

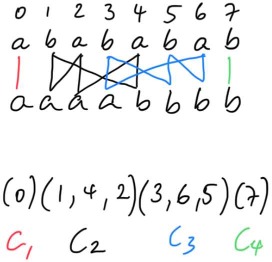
(0 4 2 5 6 7 3 1)

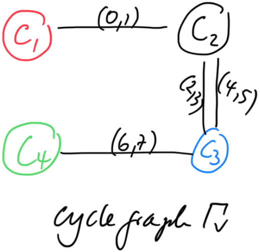
b	a	b	a	a	b	b	a
4	0	5	1	2	6	3	7
0	1	2	3	4	5	6	7
a	a	a	a	b	b	b	b

$$(0\quad 4\quad 2\quad 5\quad 6\quad 7\quad 3\quad 1)$$

- v = babaabba
- $\mathrm{bwt}^{-1}(v)$ = aaabbbab

How to choose the edges





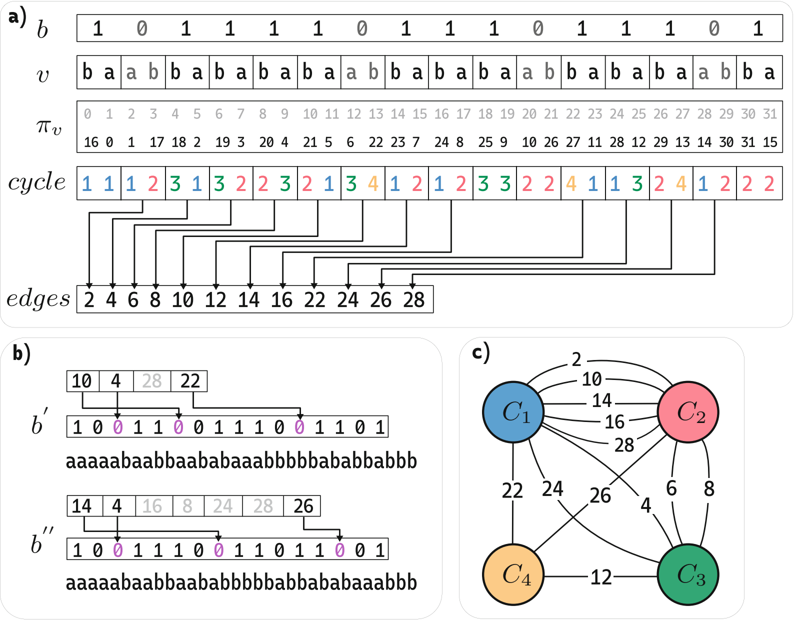
- cycle graph Γ_v: vertices = cycles, edges = unhappy blocks
- Spanning Trees (STs) of Γ_v = (BWTs of) dB sequences
- here: 2 STs = 2 dB seqs (aaabbbab, aaababbb)

Some final details

- The standard permutation can be computed easily: the ith block $\pi_v(\{2i, 2i+1\}) = \{i, n/2 + i\}$,
where $n = 2^k =$ length of dB seq. (no rank-function needed)
- We do not need v or t: replace ab $\mapsto 0$, ba $\mapsto 1$.
- enc(babaabba) $= 1101$, dec(1101) $=$ babaabba

Algorithm overview

1. Choose a random bitstring b of length 2^{k-1}.
2. Compute the standard permutation π_v of $v = dec(b)$.
3. Construct the cycle graph Γ_v.
4. Choose a random spanning tree T of Γ_v.
5. Flip the bits of b corresponding to T, resulting in b'.
6. Invert $s = dec(b')$, resulting in dB seq t.


a)
b
1 0 1 1 1 1 0 1 1 1 0 1 1 1 0 1
v
b a a b b a b a b a b a a b b a b a b a a b b a b a b a a b b a
π_v
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
16 0 1 17 18 2 19 3 20 4 21 5 6 22 23 7 24 8 25 9 10 26 27 11 28 12 29 13 14 30 31 15
cycle
1 1 1 2 3 1 3 2 2 3 2 1 3 4 1 2 1 2 3 3 2 2 4 1 1 3 2 4 1 2 2 2
edges
2 4 6 8 10 12 14 16 22 24 26 28
b)
10 4 28 22
b′
1 0 0 1 1 0 0 1 1 1 0 0 1 1 0 1
aaaaabaabbaababaaabbbbbababbabbb
14 4 16 8 24 28 26
b′′
1 0 0 1 1 1 0 0 1 1 0 1 1 0 0 1
aaaaabaabbaababbbbbabbababaaabbb
c)
C_1
C_2
C_3
C_4
2
10
14
16
28
22
24
26
4
6
8
12

Algorithm implementation and analysis

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   Union-Find data structure, $|\Gamma_v|$ at most $Z_k = \sum_{d|k} Lyn(d)$
   $\alpha(n)$ inverse Ackerman function; $Z_k \sim 2^{k-1}/k = \Theta(n)$ $\mathcal{O}(n\alpha(n))$

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   (We actually do 5 in parallel with 4.)

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   $\alpha(n)$ inverse Ackerman function; $Z_k \sim 2^{k-1}/k = \Theta(n)$ $\mathcal{O}(n\alpha(n))$
5. Flip the bits of b corresponding to T, resulting in b'. $\mathcal{O}(n)$
   (We actually do 5 in parallel with 4.)
6. Invert $s = dec(b')$, resulting in dB sequence t. $\mathcal{O}(n)$

Algorithm implementation and analysis

1. Choose a random bitstring b of length 2^{k-1}. $\mathcal{O}(n)$
2. Compute the standard permutation π_v of $v = dec(b)$.
   Fill in the cycle-array on the fly. $\mathcal{O}(n)$
3. Construct the cycle graph Γ_v.
   Compute the edges array. $\mathcal{O}(n)$
4. Choose a random spanning tree T of Γ_v.
   Union-Find data structure, $|\Gamma_v|$ at most $Z_k = \sum_{d|k} Lyn(d)$
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total running time $\mathcal{O}(n\alpha(n))$
space $\mathcal{O}(n)$

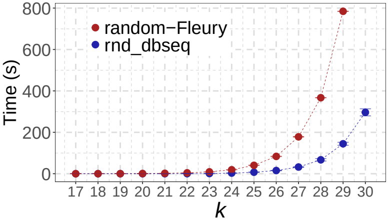
Running time

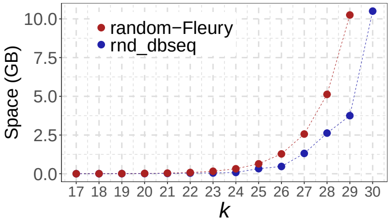
k	17	18	19	20	21	22	23	24	25	26	27	28	29	30
w/o (s)	0.003	0.01	0.02	0.04	0.10	0.29	0.87	2.63	6.07	12.42	27.49	57.19	125.38	247.10
w (s)	0.01	0.02	0.03	0.07	0.16	0.39	0.96	3.11	7.31	15.44	32.32	67.20	144.72	293.49

Average running time in seconds, taken over 100 randomly generated dB sequences, without (w/o) and with (w) the time for outputting the dB sequence, on a laptop with 16 GB of RAM.

Comparison with Fleury's algorithm

- We modified an implementation of Fleury's algorithm from `debruijnsequence.org` → random-Fleury
- random-Fleury cannot construct all possible dB seqs, but serves as the closest available method for comparison





Our algorithm is appr. 10-12 times faster for $17 \leq k \leq 23$, and 5 times faster for $k = 29$, and uses only half the memory.

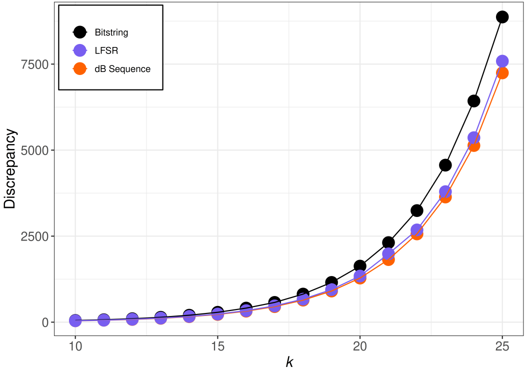
Def. The discrepancy of a binary string is the maximum absolute difference between the number of a's and b's over all (circular) substrings.

- **Low discrepancy is preferable** for certain applications

AAAAAABAAAABBAAABABAAABBBAABAABABBAABBABAABBBBABABABBBABBABBBBBB

|#A - #B| = 17 - 5 = 12

Estimating the average discrepancy of dB sequences



Average discrepancy of LFSRs from (Gabric and Sawada, 2022).

- For studying properties of de Bruijn sequences, not realistic to use random bitstrings or LFSRs as a sample.

Not uniformly at random

Our algorithm does not output all dB sequences according to the uniform probability distribution, for two reasons:

1. the ST of the cycle graph is not chosen uniformly at random
2. even if it was, not every dB sequence would be equally likely to be output

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ad 2 We define the prestige of a dB sequence t as

$$pres(t) = \frac{1}{2^{2^{k-1}}} \sum_{v \in \{\mathrm{ab},\mathrm{ba}\}^{2^{k-1}}} p(t \mid v)$$

Not uniformly at random

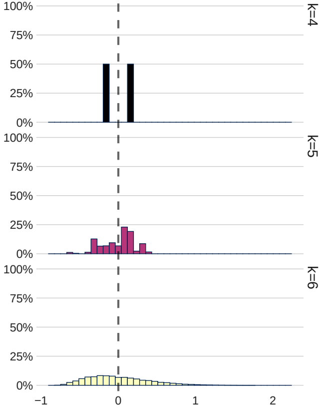

Figure: Comparison of empirical probabilities (left) and prestige (right) to the uniform distribution (vertical line), for $k = 4, 5, 6$. y-axis: % of dB seqs that share the same P_e resp. prestige. x-axes normalized w.r.t. P_u.

Conclusion

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  - time $\mathcal{O}(n\alpha(n))$
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- we improved the estimates for the average discrepancy of binary dB sequences
- our algorithm can be straighforwardly extended to any constant-size alphabet (present on github)

Open problems

- distribution of prestige (for rejection sampling)
- for $\sigma > 2$ a straightforward extension of our algorithm has running time $\mathcal{O}(\sigma n \alpha(n))$, due to up to $\binom{\sigma}{2}$ edges in each block; can this be improved?
- algorithm for uniformly random dB sequences

- paper:
  Proc. of LATIN2024
  (Puerto Varas, Chile,
  18-22 March 2024)

- code at (C++ and python):
  github.com/lucaparmigiani/rnd_dbseq

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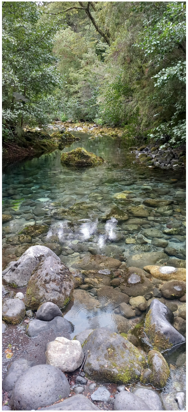

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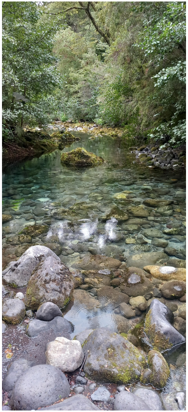

Thank you for your attention!