On the Burrows-Wheeler Transform of string collections

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A (non-efficient) algorithm: List all of rotations of string T, sort them lexicographically, concatenate last characters: bwt(banana) = nnbaaa

AWARDS & RECOGNITION

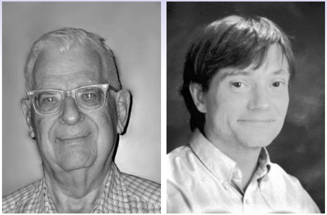
Inventors of BW-transform and the FM-index Receive Kanellakis Award

2022

Michael Burrows, Google; **Paolo Ferragina**, University of Pisa; and **Giovanni Manzini**, University of Pisa, receive the **ACM Paris Kanellakis Theory and Practice Award** for inventing the BW-transform and the FM-index that opened and influenced the field of Compressed Data Structures with fundamental impact on Data Compression and Computational Biology. In 1994, Burrows and his late coauthor David Wheeler published their paper describing revolutionary data compression algorithm based on a reversible transformation of the input—the "Burrows-Wheeler Transform" (BWT). A few years later, Ferragina and Manzini showed that, by orchestrating the BWT with a new set of mathematical techniques and algorithmic tools, it became possible to build a "compressed index," later called the FM-index. The introduction of the BW Transform and the development of the FM-index have had a profound impact on the theory of algorithms and data structures with fundamental advancements.

source: `https://awards.acm.org/kanellakis`

The BWT



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- recent: *r*-index [Gagie et al, JACM 2020; Bannai et al. TCS 2020]

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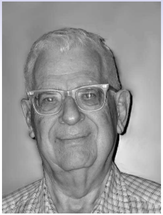
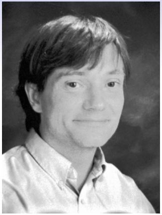

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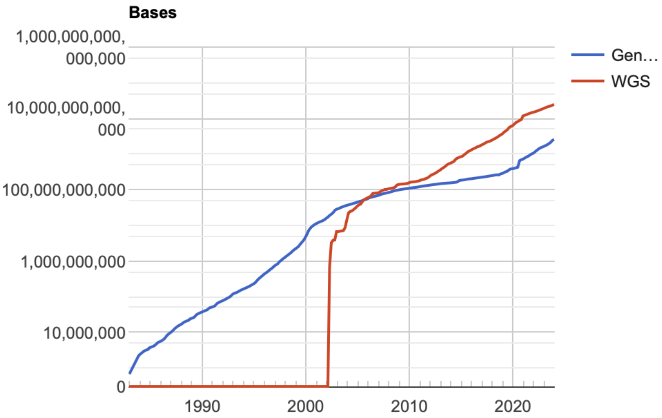
Some properties of the BWT:

- computable in linear time $\mathcal{O}(n)$ $\qquad n = |T|$
- reversible in linear time $\mathcal{O}(n)$
- uncompressed: same space as text
- if T repetitive, good for compression (see later)

GenBank and WGS Statistics



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- SARS-CoV-2 viral sequences

From strings to string collections

Our data is

- growing rapidly, and
- changing: **from individual strings to string collections**
- many of these consist of **many similar copies** of the same string

Outline of talk

- The Burrows-Wheeler Transform (BWT)
- The extended BWT (eBWT)
- Other variants of the BWT for string collections
- Why does it matter?
- Conclusions

The Burrows-Wheeler Transform

The Burrows-Wheeler Transform (BWT)

Recall: $T =$ `banana`. The BWT is a permutation of T: `nnbaaa`

all rotations (conjugates)		all rotations, sorted
`banana`		`abanan`
`ananab`	$\longrightarrow$	`anaban`
`nanaba`	lexicographic order	`ananab`
`anaban`		`banana`
`nabana`		`nabana`
`abanan`		`nanaba`

Why is the BWT useful in text compression?

BWT-matrix (F = first column, L = last column)

	F		L
1	a	bana	n
2	a	naba	n
3	a	nana	b
4	b	anan	a
5	n	aban	a
6	n	anab	a

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- **Obs. 1:** F = all characters of T in lex-order: `aaabnn`
- **Obs. 2:** for all i: L_i precedes F_i in T (cyclically): $T = \underset{1\,2\,3\,4\,5\,6}{\texttt{banana}}$

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  $T = \underset{1}{\mathtt{b}}\underset{2}{\mathtt{a}}\underset{3}{\mathtt{n}}\underset{4}{\mathtt{a}}\underset{5}{\mathtt{n}}\underset{6}{\mathtt{a}}$
- **Obs. 3:** all occurrences of a substring appear in consecutive rows as prefix

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Ex.: $T =$ `banana` has 2 occurrences of the substring `ana`

2 occ's of `ana`

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abanan
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banana
nabana
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rotation	BWT
`...`	
`he caverns measureless to man, And sank in tumult to a ...`	t
`he caves. It was a miracle of rare device, A sunny pleasure-...`	t
`he dome of pleasure Floated midway on the waves; Where was ...`	t
`he fountain and the caves. It was a miracle of rare device,...`	t
`he green hill athwart a cedarn cover! A savage place! as ...`	t
`he hills, Enfolding sunny spots of greenery. But oh! that ...`	t
`he milk of Paradise.`	t
`he mingled measure From the fountain and the caves. It was a ...`	t
`he on honey-dew hath fed, And drunk the milk of Paradise.  ...`	␣
`he played, Singing of Mount Abora. Could I revive within me ...`	s
`he sacred river ran, Then reached the caverns measureless ...`	t
`he sacred river, ran Through caverns measureless to man ...`	t
`he sacred river. Five miles meandering with a mazy motion ...`	t
`he shadow of the dome of pleasure Floated midway on the waves ...`	T
`he thresher's flail: And mid these dancing rocks at once and ...`	t
`he waves; Where was heard the mingled measure From the ...`	t

Kubla Kahn by Samuel Coleridge (1998 characters)

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many `the`'s, some `he`, `she`, `The`

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  Compression: $T \mapsto \underbrace{\text{RLE(bwt}(T))}_{\text{storage space: } O(r)}$

  Ex.: `banana` $\mapsto$ `n2b1a3`

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- good if r is much smaller than $n = |T|$
(i.e. if few runs)
- for **repetitive strings**, r is small
(repetitive: many repeated substrings)

Reversing the BWT (lossless compression)

input: nnbaaa, 4 — bwt(T), i: where $1 \leq i \leq n$

output: (wanted) banana. — T: i'th rotation lex.ly

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	F					L
1	a	b	a	n	a	n
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3	a	n	a	n	a	b
4	b	a	n	a	n	a
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	F	L
1	abana	n
2	anaba	n
3	anana	b
4	banan	a
5	naban	a
6	nanab	a

$T = \underset{1\,2\,3\,4\,5\,6}{\texttt{banana}}$

Recall:

Obs. 1: F = all characters of T in lex-order:

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input: nnbaaa, 4

	L
1	n
2	n
3	b
4	a
5	a
6	a

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input: `nnbaaa`, 4

	F	L
1	a	n
2	a	n
3	a	b
4	b	a
5	n	a
6	n	a

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3	a	b	a
4	b	a	
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6	n	a	

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4	b	a
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1	a	n
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2	a	n
3	a	b
4	b	a
5	n	a
6	n	a

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input: `nnbaaa`, 4

	F	L
1	a	n
2	a	n
3	a	b
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5	n	a
6	n	a

b a n a n a

The BWT of string collections

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- Our string collections are highly repetitive:
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- But: how do we compute the BWT of a multiset?

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Generalization of the BWT to multisets:
the extended BWT (eBWT) (next)

The extended BWT

The extended BWT

[Mantaci, Restivo, Rosone, Sciortino, TCS, 2007]

Ex. $\mathcal{M} = \{\texttt{bana}, \texttt{an}\}$. The eBWT is a permutation of the characters of $\mathcal{M}$: eBWT$(\mathcal{M}) = \texttt{nbnaaa}$.

all rotations (conjugates)		all rotations, sorted	
bana		aban	n
anab	$\longrightarrow$	anab	b
naba	omega order	an	n
aban		bana	a
an		naba	a
na		na	a

N.B. anab $<_\omega$ an, since $\texttt{anab} \cdot \texttt{anab} \cdots <_{\text{lex}} \texttt{an} \cdot \texttt{an} \cdot \texttt{an} \cdot \texttt{an} \cdots$

The extended BWT

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

$\mathcal{M} = \{\texttt{bana}, \texttt{an}\}$

omega-order		lex-order	
aban	n	aban	n
anab	b	an	n
an	n	anab	b
bana	a	bana	a
naba	a	na	a
na	a	naba	a

N.B. With the lex-order, the LF-property would not hold!

The extended BWT

- omega-order instead of lex-order
- same as lex-order if neither string is prefix of the other
- omega-order necessary for the LF-property
- the eBWT inherits BWT properties: clustering effect, reversibility, useful for lossless text compression, efficient pattern matching, ...
- However, until recently no linear-time algorithm known.

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- However, until recently no linear-time algorithm known.

2021:

- linear-time algorithm [Bannai, Kärkkäinen, Köppl, Piatkowski, CPM 2021]
- We simplified this algorithm, and
- gave first efficient implementations of the eBWT: tools `pfpebwt,cais`

  [Boucher, Cenzato, L., Rossi, Sciortino, SPIRE 2021]

Other BWT variants for string collections

The BWT of string collections

[Cenzato and L., CPM 2022, Arxiv 2023]

Question: How do dedicated tools compute the BWT of a string collection? (string collection: multiset of strings)

- We studied 18 publicly available tools.
- Only ours compute the eBWT (`pfpebwt,cais`).
- We identified 4 more non-equivalent approaches: the resulting BWTs are all different.
- Often the method is not explicitly stated.
- **Underlying assumption: they are all the same.**
- But they differ a lot (Hamming distance, number of runs).
- **N.B.:** all BWT variants are correct (LF-property, . . .)

The other BWT variants for string collections

The different approaches are:

1. extended BWT of strings with terminator symbol \$ (dollarEBWT)
2. concatenate strings, separating them with different dollars (multidolBWT)
3. first sort colexicographically, then do 2. (colexBWT)
4. concatenate strings, separating them with same dollar (concatBWT)

All use terminator / separator symbols ('dollars'). So we call them separator-based BWT variants.

The BWT variants for string collections

Ex. $\mathcal{M} = \{\mathtt{ATATG}, \mathtt{TGA}, \mathtt{ACG}, \mathtt{ATCA}, \mathtt{GGA}\}$

variant (our terminology)	result on example	tools
eBWT	CGGGATGTACGTTAAAAA	pfpebwt,cais
dollarEBWT	GGAAACGG$$$TTACTGTAAA	G2BWT, msbwt
multidolBWT	GAGAAGCG$$$TTATCTGAAA	gsufsort, ropebwt2, eGSA, Merge-BWT, eGAP, nvSetBWT, BCR-LCP-GSA, grlBWT, BEETL, bwt-lcp-parallel
colexBWT	AAAGGCGG$$$TTACTGTAAA	ropebwt2, BCR-LCP-GSA
concatBWT	$AAGAGGGC$#$TTACTGT$AAA$	BigBWT, r-pfbwt, CMS-BWT tools for single strings

The dollar-eBWT

1. dollarEBWT($\mathcal{M}$) = eBWT($\{T_i\$: T_i \in \mathcal{M}\}$), $\quad \$ < c$ for all char's c

Now no string is prefix of another $\implies$ omega-order same as lex-order.

$\mathcal{M} = \{\mathtt{bana\$}, \mathtt{an\$}\}$

dollarEBWT

\$an	n
\$bana	a
a\$ban	n
an\$	\$
ana\$b	b
bana\$	\$
n\$a	a
na\$ba	a

nan\$b\$aa

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nan\$b\$aa

eBWT of $\{\mathtt{bana}, \mathtt{an}\}$

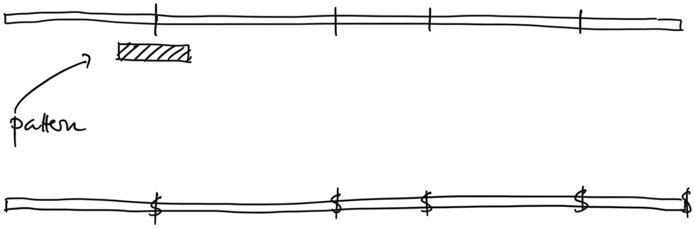
aban	n
anab	b
an	n
bana	a
naba	a
na	a

nbnaaa

The different BWT variants

The other 3 methods concatenate the input strings, and then apply the classical BWT.

The main issue here is to avoid spurious substrings:



The multidollar BWT

2. multidolBWT($\mathcal{M}$) $=$ bwt($T_1\$_1 T_2\$_2 \cdots T_k\$_k$), where dollars are smaller than characters from Σ, and $\$_1 < \$_2 < \ldots < \$_k$

Ex. $\mathcal{M} = \{\texttt{ATATG}, \texttt{TGA}, \texttt{ACG}, \texttt{ATCA}, \texttt{GGA}\} \rightsquigarrow$

bwt($\texttt{ATATG}\$_1\texttt{TGA}\$_2\texttt{ACG}\$_3\texttt{ATCA}\$_4\texttt{GGA}\$_5$) $=$ GAGAAGCG\$\$TTATCTG\$AAA\$

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bwt($\mathtt{ATATG\$_1TGA\$_2ACG\$_3ATCA\$_4GGA\$_5}$) = $\mathtt{GAGAAGCG\$\$\$TTATCTG\$AAA\$}$

- most commonly used method
- analogous to Generalized Suffix Tree and Generalized Suffix Array
- dollars are different only conceptually (break ties by index)
- equivalent: concatenate without separators, use bitstring marking string beginnings

The colex BWT

3. colexBWT($\mathcal{M}$): multidolBWT of the strings in colexicographic order

colex order $=$ lexicographic order of the reverse strings

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colex order: ATCA, GGA, TGA, ACG, ATATG $\rightsquigarrow$

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colex order: ATCA,GGA,TGA,ACG,ATATG $\rightsquigarrow$

bwt($\mathtt{ATCA\$_1GGA\$_2TGA\$_3ACG\$_4ATATG\$_5}$) = AAAGGCGG$$TTACTGTAAA

- reduces number of runs (see later)
- implemented as an option in ropebwt2,BCR-LCP-GSA

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(for easier comparison, we simplify to `AAGAGGGC$$$TTACTGT$AAA$`)

- very easy to implement
- used e.g. in `BigBWT`,`CMS-BWT`.

Interesting intervals

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BWT variant	example
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multidolBWT($\mathcal{M}$)	GAGAAGCG$$$TTATCTGAAA
colexBWT($\mathcal{M}$)	AAAGGCGG$$$TTACTGTAAA
concatBWT($\mathcal{M}$)	AAGAGGGC$$$TTACTGTAAA

in color: **interesting intervals**

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Lemma: If two separator-based BWTs differ in position i then $i \in [b, e]$ for some interesting interval $[b, e]$.

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Def. U is called **a left-maximal shared suffix** if there exist two strings $S_1, S_2 \in \mathcal{M}$ such that U is a suffix of $S_1\$$ and $S_2\$$ and is preceded by different characters in S_1 and S_2. An interval $[b, e]$ is **interesting** if it corresponds to all occurrences of some left-maximal shared suffix U (i.e., its SA-interval).

Ex. $\mathcal{M} = \{\mathtt{ATATG}, \mathtt{TG\underline{A}}, \mathtt{ACG}, \mathtt{ATC\underline{A}}, \mathtt{GG\underline{A}}\}$, $U = \mathtt{A\$}$.

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```
A$ATC   C
A$GG    G
A$TG    G
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dollarEBWT

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A\$GG	G	$\mathtt{A\$_4}\cdots$	C
A\$TG	G	$\mathtt{A\$_5}\cdots$	G
dollarEBWT		multidolBWT	

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A\$GG	G	$\mathtt{A\$_4}\cdots$	C	$\mathtt{A\$_2}\cdots$	G
A\$TG	G	$\mathtt{A\$_5}\cdots$	G	$\mathtt{A\$_3}\cdots$	G
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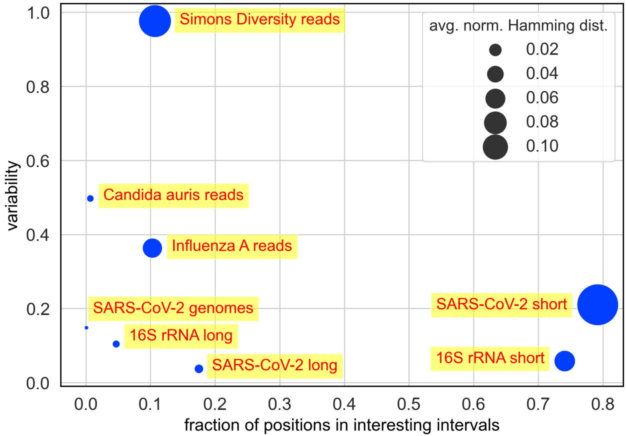
A\$GG	G	$\mathtt{A\$}_4 \cdots$	C	$\mathtt{A\$}_2 \cdots$	G	A\$A $\cdots$	G
A\$TG	G	$\mathtt{A\$}_5 \cdots$	G	$\mathtt{A\$}_3 \cdots$	G	A\$G $\cdots$	C
dollarEBWT		multidolBWT		colexBWT		concatBWT	

Hamming distance between separator-based BWTs



Variability

$$var(\mathcal{M}) = \frac{\sum_{[b,e] \text{ interesting int.}} var([b,e])}{\sum_{[b,e] \text{ interesting int.}} (e-b+1)}, \text{ where } var([b,e]) = \text{max no. runs in } [b,e]$$

(depends on Parikh vector)

Why does it matter?

Theoretician: You are all using different methods to compute the BWT of string collections, and the results are pretty different!

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Theoretician: But it's not nice that your tool computes a different thing from your competitor's.

Programmer: I am never going to use her tool anyway!

Why you should care

1. number of runs
2. the parameter r is not well-defined
3. input order dependence

1. Number of runs

r = number of runs of the BWT.

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BWT variant	example	r	r w/o \$'s
non-sep. based			
eBWT($\mathcal{M}$)	CGGGATGTACGTTAAAAA	11	11
separator-based			
dollarEBWT($\mathcal{M}$)	GGAAACGG\$\$\$TTACTGT\$AAA\$	14	11
multidolBWT($\mathcal{M}$)	GAGAAGCG\$\$\$TTATCTG\$AAA\$	17	14
colexBWT($\mathcal{M}$)	AAAGGCGG\$\$\$TTACTGT\$AAA\$	14	11
concatBWT($\mathcal{M}$)	AAGAGGGC\$\$\$TTACTGT\$AAA\$	15	12

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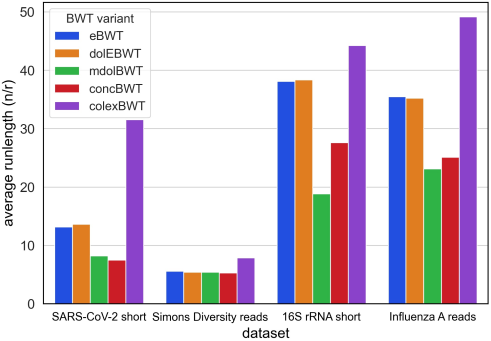

Average runlength (n/r) on four short sequence datasets, of all BWT variants. (500,000 sequences each, of length between 50 and 301.)

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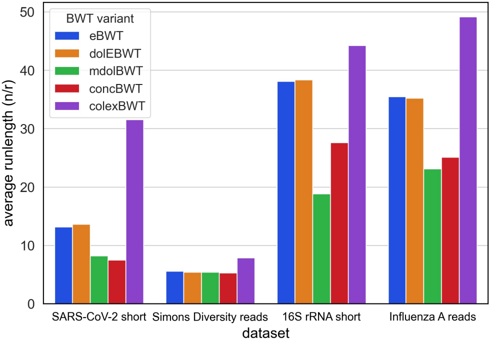

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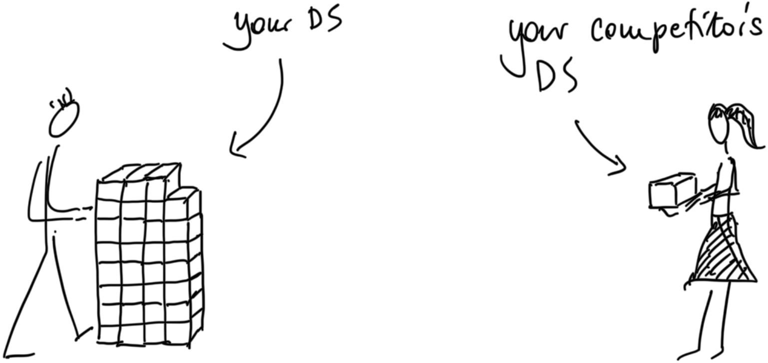
(500,000 sequences each, of length between 50 and 301.)

- On these datasets, difference of a factor of up to 4.2.
- In a separate work, difference of a factor of up to 31.
  [Cenzato, Guerrini, L., Rosone, DCC 2023]

size of data structures $\mathcal{O}(r)$



So maybe you should care...

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- size of data structures $\mathcal{O}(r)$ (r-index) Gagie et al. [JACM 2020], Bannai et al. [TCS 2020]

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- increasingly used as a repetitiveness measure of T, similar to z (number of Lempel-Ziv phrases)
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  - in theoretical work on repetitiveness measures — Kempa and Kociumaka [FOCS 2020], Navarro [ACM Comp. Surv., 2021], Akagi et al. [Inf. Comp. 2023]

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N.B. multidolBWT and concatBWT depend on the input order!

$\mathcal{M}_1$ = [ATATG,TGA,ACG,ATCA,GGA]   mdolBWT($\mathcal{M}_1$) = GAGAAGCG$$$TTATCTGAAA

$\mathcal{M}_2$ = [ACG,ATATG,GGA,TGA,ATCA]   mdolBWT($\mathcal{M}_2$) = GGAAAGGC$$$TTACTGTAAA

$\mathcal{M}_1$ = [ATATG,TGA,ACG,ATCA,GGA]   concBWT($\mathcal{M}_1$) = AAGAGGGC$$$TTACTGTAAA

$\mathcal{M}_2$ = [ACG,ATATG,GGA,TGA,ATCA]   concBWT($\mathcal{M}_2$) = AGAGACGG$$$TTACTTGAAA

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$\mathcal{M}_1$ = [ATATG,TGA,ACG,ATCA,GGA] concBWT($\mathcal{M}_1$) = AAGAGGGC$$$TTACTGTAAA

$\mathcal{M}_2$ = [ACG,ATATG,GGA,TGA,ATCA] concBWT($\mathcal{M}_2$) = AGAGACGG$$$TTACTTGAAA

Thus, giving the same dataset to the same tool but in different order can produce very different results! (incl. the number of runs)

The multidollar BWT can simulate all others

Prop. Let $\mathcal{M}$ be given, and L some separator-based BWT on $\mathcal{M}$. Then there exists an input permutation π such that $\text{multidol}(\pi(\mathcal{M})) = L$.

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- We implemented this algorithm in our tool `optimalBWT` [Cenzato, Guerrini, L., Rosone, DCC 2023]

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- optBWT minimizes r, and has been implemented
- definition of r should be standardized (optBWT or colexBWT)

Open Problems

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- characterize string collections for which differences highest
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My personal conclusion:

Definitions matter!

Acknowledgements

- Davide Cenzato and Zsuzsanna Lipták: *A survey of BWT variants for string collections*, `arXiv:2202.13235` (conf. version: CPM 2022)
  `github.com/davidecenzato/BWT-variants-for-string-collections`
- Davide Cenzato, Veronica Guerrini, Zsuzsanna Lipták, and Giovanna Rosone: *Computing the optimal BWT for very large string collections*, DCC 2023.
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Thank you for your attention!