Dollar or no dollar, that is the question

New combinatorial results on the Burrows-Wheeler-Transform

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Part I:

Introduction

The BWT

The BWT

source: group-media.mercedes-benz.com

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(BWT here stands for: Best Water Technology)

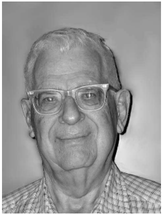
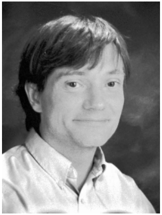
The Burrows-Wheeler-Transform

Ex.: T = banana. The BWT is a permutation of T: nnbaaa

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

Take a string (word) T, list all of its rotations, sort them lexicographically, concatenate last characters: bwt(T).

BWT history

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  as a lossless text compression algorithm
- fully developed and written up together with Michael Burrows in 1994
- appeared as a technical report only, never published
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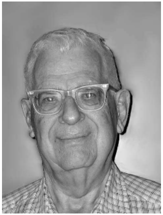

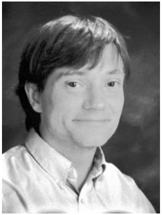

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Why can the BWT be useful in text compression?

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

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

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

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

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4	naban	a
5	nanab	a

- **Obs. 1:** F = all characters of T in lex. order: aaabnn
- **Obs. 2:** for all i: L_i precedes F_i in T:

  $T = \underset{0\,1\,2\,3\,4\,5}{\texttt{banana}}$

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2 occ's of `ana`

```
abanan
anaban
ananab
banana
nabana
nanaba
```

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

2 occ's of `ana`	2 occ's of `na` preceded by `a`
`abanan`	`abanan`
`anaban`	`anaban`
`ananab`	`ananab`
`banana`	`banana`
`nabana`	`nabana`
`nanaba`	`nanaba`

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So: we get a run of `a`'s of length 2, and a run of `n`'s of length 2

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- **Obs. 1:** F = all characters of T in lex. order.
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Ex.: T = banana has 2 occurrences of the pattern ana

2 occ's of ana	2 occ's of na preceded by a	2 occ's of a preceded by n
abanan	abanan	abanan
anaban	anaban	anaban
ananab	ananab	ananab
banana	banana	banana
nabana	nabana	nabana
nanaba	nanaba	nanaba

So: we get a run of a's of length 2, and a run of n's of length 2 (2 = no. occ's).

Of course, things are a bit more complicated:

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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

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

Compression with the BWT

- in original paper: using Move-to-front and Huffman/arithmetic coding

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  - RLE: replace equal-letter-runs by (character, integer)-pair
  - Ex.: bbbbbbbbcaaaaaaaaaaabb $\mapsto$ $(\mathtt{b}, 8), (\mathtt{c}, 1), (\mathtt{a}, 11), (\mathtt{b}, 2)$

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- Def.: $r(T) = \#$ runs of bwt(T)

  Ex.: $r(\texttt{banana}) = 3$ recall: bwt$(\texttt{banana}) = \texttt{nnbaaa}$

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  Ex.: $r(\texttt{banana}) = 3$ recall: bwt$(\texttt{banana}) = \texttt{nnbaaa}$
- for repetitive strings, r is small

BWT magic

The BWT ...

- requires same space as T in bits: $n \log \sigma$ bits $\sigma =$ alphabetsize
  (suffix array: $n \log n$ bits, suffix tree: much more—still $\mathcal{O}(n)$) $n = |T|$
- easier to compress than T, if T repetitive
- very fast (!!!) pattern matching (most basic problem on strings)
- computable in linear time $\mathcal{O}(n)$
- reversible in linear time $\mathcal{O}(n)$ nnbaaa,3 $\mapsto$ banana
- can replace text (suffix array, suffix tree: no)

Compressed data structures for strings

Data structures based on the BWT:

- FM-index [Ferragina and Manzini, FOCS 2000]
- RLFM-index [Mäkinen and Navarro, CPM 2005]
- r-index [Gagie et al, JACM 2020; Bannai et al. TCS 2020]
- some recent developments on r-index [Rossi et al. JCB 2022; Giuliani et al. SEA 2022; Cobas et al. CPM 2021; Boucher et al. SPIRE 2021]

Some tools in bioinformatics (aligners):

- bwa [Durbin and Li, 2009] ca. 41,000 cit.
- bowtie [Langmead and Salzberg, 2010] ca. 36,000 cit.
- soap2 [Li et al., 2009]
- ...

The parameter r

Def. String T, $r =$ number of runs of bwt(T).

- size of data structures $\mathcal{O}(r)$
- algorithms' running time ideally a function of r (not of $n = |T|$)
- increasingly used as a repetitiveness measure of T
- some papers on r:
  - Manzini: "An analysis of the Burrows-Wheeler-Transform" [JACM 2001]
  - Kempa and Kociumaka: "Resolution of the Burrows-Wheeler Transform Conjecture" [FOCS 2020]
  - Navarro: "Indexing Highly Repetitive String Collections, Part I: Repetitiveness Measures" [ACM Comp. Surv., 2021]
  - Mantaci et al.: "Measuring the clustering effect of BWT via RLE" [TCS 2017]

BWT from a combinatorial perspective

- special case of the Gessel-Reutenauer-bijection [Crochemore, Désarménien, Perrin, 2004]
- introduction of the extended BWT (eBWT), a generalization of the BWT to multisets of strings [Mantaci et al. 2007]
- strings T with fully clustering BWTs (e.g. $\text{bwt}(T) = \texttt{bbbbaaccc}$)
  - full characterization for $\sigma = 2$ [Mantaci et al., 2003]
  - partial characterization for $\sigma > 2$ [Puglisi et al., 2008]
  - characterization via interval exchanges [Ferenczi et al., 2013]
- fixpoints of the BWT [Mantaci et al., 2017]
- characterization of BWT images [Likhomanov and Shur, 2011]

Good overview: Rosone and Sciortino: "The Burrows-Wheeler Transform between Data Compression and Combinatorics on Words." [CiE 2013]

- two research communities working on the BWT
- (1) data structures and algorithms on strings and
  (2) combinatorics on words
- little interaction until ...

Dagstuhl workshop "25 years of the Burrows-Wheeler-Transform" (2019)
organized by T. Gagie, G. Manzini, G. Navarro, J. Stoye

But: The two communities use slightly different definitions of the BWT:

- Data Structures and Algorithms on Strings:
  It is assumed that each string terminates with an end-of-string character (denoted \$, smaller than all others)

  $T = \texttt{banana\$}$
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Part II:

Dollar or no dollar, that is the question

1. The transform itself

Different transforms

banana	banana$
abanan	$banana
anaban	a$banan
ananab	ana$ban
banana	anana$b
nabana	banana$
nanaba	na$bana
	nana$ba
nnbaaa	annb$aa

Different transforms

	without dollar (banana)	with dollar (banana$)
the transform	nnbaaa	annb$aa

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the transform	nnbaaa	annb$aa
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remove $	nnbaaa	annbaa
# runs r	3	4

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	without dollar (banana)	with dollar (banana$)
the transform	nnbaaa	annb$aa
remove $	nnbaaa	annbaa
# runs r	3	4

- **Thm.** There exist strings for which the difference in r is $\Theta(\log n)$.
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	without dollar (banana)	with dollar (banana$)
the transform	nnbaaa	annb$aa
remove $	nnbaaa	annbaa
# runs r	3	4

- **Thm.** There exist strings for which the difference in r is $\Theta(\log n)$.
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- This is asymptotically tight: here $r = O(1)$, and upper bound is $\mathcal{O}(\log r \log n)$. [Akagi, Funakoshi, Inenaga, 2021]

Different transforms

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Thm. There exist strings for which the difference in r is $\Theta(\log n)$.

- $r(T\$)$ increases by $\log n$: Fibonacci words of even order $T = Fib(2k), r(T) = 2, r(T\$) = 2k - 1$

  ex.:
  $r(Fib(8)) = 2, r(Fib(8)\$) = 7$
  $r(Fib(12)) = 2, r(Fib(12)\$) = 11$

- $r(T\$)$ decreases by $\log n$: Fibonacci words of odd order without the first character $T = Fib(2k+1)[1:], r(T) = 2k, r(T\$) = 5$

  ex:
  $r(Fib(13)[1:]) = 12, r(Fib(13)[1:]\$) = 5$
  $r(Fib(15)[1:]) = 14, r(Fib(15)[1:]\$) = 5$

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- both additive and multiplicative difference

2. BWT construction

BWT construction

Most BWT construction algorithms first construct the Suffix Array (SA), then construct the BWT from the SA, using: $L_i = T_{SA[i]-1}$ (recall Obs. 2).

ex. $T = \underset{0\,1\,2\,3\,4\,5\,6}{\texttt{banana\$}}$.

SA	
6	$
5	a$
3	ana$
1	anana$
0	banana$
4	na$
2	nana$

BWT construction

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ex. $T = \underset{0123456}{\texttt{banana\$}}$.

SA	
6	$
5	a$
3	ana$
1	anana$
0	banana$
4	na$
2	nana$

SA	L
6	$banana
5	a$banan
3	ana$ban
1	anana$b
0	banana$
4	na$bana
2	nana$ba

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Thus: SA-construction in $\mathcal{O}(n)$ time $\Rightarrow$ BWT-construction in $\mathcal{O}(n)$ time.

BWT construction without dollar

- This works fine if there is a \$.
- What if there is no dollar?

BWT construction without dollar

Problem 1:

banana
0 1 2 3 4 5

SA	
5	a
3	ana
1	anana
0	banana
4	na
2	nana

nnbaaa ✓

BWT construction without dollar

Problem 1:

banana
0 1 2 3 4 5

SA		SA	L
5	a	5	abanan
3	ana	3	anaban
1	anana	1	ananab
0	banana	0	banana
4	na	4	nabana
2	nana	2	nanaba

nnbaaa ✓

BWT construction without dollar

Problem 1:

banana
0 1 2 3 4 5

anaban
0 1 2 3 4 5

SA		SA		L
5	a	5	abanan	n
3	ana	3	anaban	n
1	anana	1	ananab	b
0	banana	0	banana	a
4	na	4	nabana	a
2	nana	2	nanaba	a

nnbaaa ✓

BWT construction without dollar

Problem 1:

banana
0 1 2 3 4 5

SA	
5	a
3	ana
1	anana
0	banana
4	na
2	nana

nnbaaa ✓

SA	L
5	abanan
3	anaban
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4	nabana
2	nanaba

anaban
0 1 2 3 4 5

SA	
2	aban
4	an
0	anaban
3	ban
5	n
1	naban

nbnaaa ✗

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SA		SA	L
5	a	5	abanan
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1	anana	1	ananab
0	banana	0	banana
4	na	4	nabana
2	nana	2	nanaba

nnbaaa ✓

anaban
0 1 2 3 4 5

SA		SA	L
2	aban	2	abanan
4	an	4	ananab
0	anaban	0	anaban
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5	n	5	nabana
1	naban	1	nabana

nbnaaa ✗

BWT construction without dollar

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anaban
0 1 2 3 4 5

SA		SA	L
2	aban	2	abanan
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3	ban	3	banana
5	n	5	nabana
1	naban	1	nabana

nbnaaa ✗

N.B. $suf_i < suf_j \Leftrightarrow conj_i < conj_j$ does not hold in general!

Thus: We need the CA (conjugate array), not the SA!

BWT construction without dollar

Problem 2: If T not primitive, then CA not defined (several identical rotations):

$\underset{0\,1\,2\,3\,4\,5}{\texttt{nanana}} = (\texttt{na})^3$

CA	
1?	anana**n**
3?	anana**n**
5?	anana**n**
0?	nanan**a**
2?	nanan**a**
4?	nanan**a**

Linear-time BWT construction without dollar

- For \$-terminated strings, neither problem exists.
- For Lyndon words (primitive and $<$ all their rotations), neither problem exists.
- All previous BWT-construction algorithms either use \$ or Lyndon rotations.

Our algorithm [Boucher, Cenzato, L., Rossi, Sciortino, SPIRE, 2021]:

- first linear-time BWT-construction algorithm which uses neither \$ nor Lyndon rotations
- adaptation of the SAIS-algorithm for SA-construction [Nong et al., 2011]
- previously, SAIS had been adapted for $T\$$ [Okanohara and Sadakane 2009], and to the bijective BWT [Bannai et al., 2021]

Our algorithm for BWT construction

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

1. assign circular types to positions
2. sort LMS-substrings
3. assign new names to LMS-substrings
4. construct new string, solve recursively
5. induce CA from relative order of LMS-positions

Step 1

0	1	2	3	4	5
b	a	n	a	n	a
L	S	L	S	L	S
	*		*		*

Step 2

	a			*b*	*n*	
S*	1	3	5			
L				0	2	4
S	5	1	3			
	5	1	3	0	2	4

Step 3

5	a	b	a	A
1	a	n	a	B
3	a	n	a	B

Step 4

0	1	2
A	B	B
S	L	L
*		

A	*B*	
0		
	2	1
0	2	1

Step 5

	a			*b*	*n*	
	5	3	1			
				0	4	2
CA	5	3	1	0	4	2
BWT	n	n	b	a	a	a

BWT without dollar

Implementations of SAIS for conjugate array (cais) for

- BWT without $
- eBWT (extended BWT) (see later)
- BBWT (bijective BWT)
- option for including dollar(s)

See `https://github.com/davidecenzato/cais`

3. BWT of string collections

How to compute the BWT of a multiset of strings?

[Cenzato and L., CPM 2022]

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

It turns out that there are several non-equivalent methods in use:

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

The different BWT variants

1. eBWT($\mathcal{M}$): the extended BWT of Mantaci et al. (2007)
   uses omega-order instead of lexicographical order: e.g. `aba` $<_\omega$ `ab`

The different BWT variants

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5. colexBWT($\mathcal{M}$) $=$ multidol($\mathcal{M}, \gamma$), where γ is the permutation corresponding to the colexicographic ('reverse lexicographic').

Interesting intervals

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

BWT variant	example
non-sep.based	
eBWT($\mathcal{M}$)	CGGGATGTACGTTAAAAA
separator-based	
dollarEBWT($\mathcal{M}$)	GGAAACGG$$$TTACTGTAAA
multidolBWT($\mathcal{M}$)	GAGAAGCG$$$TTATCTGAAA
concatBWT($\mathcal{M}$)	AAGAGGGC$$$TTACTGTAAA
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in color: **interesting intervals**

Interesting intervals

An interval $[i, j]$ is **interesting** if it is the SA-interval of a left-maximal shared suffix U. Then and only then can two separator-based BWTs differ in $[i, j]$.

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

A$#	G
A$. . .	G
A$. . .	C

U = A$

concBWT

$\texttt{A\$}_2\texttt{...TG}$	G
$\texttt{A\$}_4\texttt{...ATC}$	C
$\texttt{A\$}_5\texttt{...GG}$	G

U = A$

mdolBWT

$\texttt{A\$}_1\texttt{ATC}$	C
$\texttt{A\$}_2\texttt{GG}$	G
$\texttt{A\$}_3\texttt{TG}$	G

U = A$

dolEBWT

Order of shared suffixes

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BWT variant	example	order of shared suffixes
eBWT($\mathcal{M}$)	the extended BWT CGGGATGTACGTTAAAAA	omega-order of strings (mixed in with substrings)
dollarEBWT($\mathcal{M}$)	eBWT($\{T_i\$: T_i \in \mathcal{M}\}$) GGAAACGG$$$TTACTGTAAA	lexicographic order of strings
multidolBWT($\mathcal{M}$)	bwt($T_1\$_1 T_2\$_2 \cdots T_k\$_k$) GAGAAGCG$$$TTATCTGAAA	input order of strings
concatBWT($\mathcal{M}$)	bwt($T_1\$ T_2\$ \cdots T_k\$\#$) AAGAGGGC$$$TTACTGTAAA	lexicographic order of subsequent strings in input
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In the k-prefix (shared suffix: \$) of the BWT we see the output order.

Input order dependence

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

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

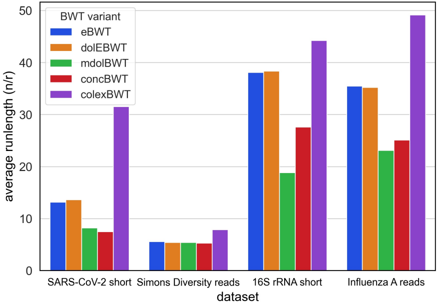
$\mathcal{M}_2$ = [ACG,ATATG,GGA,TGA,ATCA] mdolBWT($\mathcal{M}_2$) = GGAAAGGC$$$TTACTGTAAA

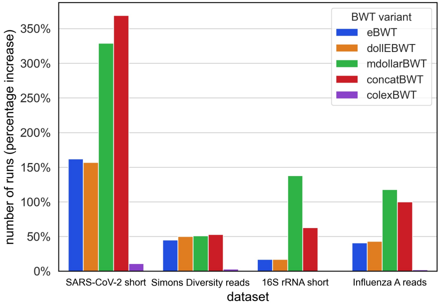
$\mathcal{M}_1$ = [ATATG,TGA,ACG,ATCA,GGA] concBWT($\mathcal{M}_1$) = AAGAGGGC$$$TTACTGTAAA

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

The parameter r

Results regarding r on four short sequence datasets, of all BWT variants.





Left: average runlength (n/r). Right: number of runs r (percentage increase with respect to the optimal BWT of [Bentley et al., ESA 2020]).
(In each experiment: 500,000 seq.s of length between 50 and 301.)

The different BWT variants

- BWT variants differ significantly among each other ($>$ 11% Hamming distance on some data sets)
- we theoretically explained these differences ("interesting intervals")
- differences especially high on large sets of short sequences
- multidolBWT and concatBWT depend on the input order
- differences extend to parameter r (number of runs of the BWT) (up to a factor of 4.2 in our experiments)

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We suggest

- to standardize the definition of r (colexBWT or optBWT)
- optBWT now implemented (see Cenzato and L., WCTA 2022; Cenzato, Guerrini, L., Rosone, forthcoming)

4. A side question

What is the output order of the concatBWT?

ex. ~~$\mathcal{M} = \{\texttt{ATATG}, \texttt{TGA}, \texttt{ACG}, \texttt{ATCA}, \texttt{GGA}\}$~~ $\mathcal{M} = [\texttt{ATATG}, \texttt{TGA}, \texttt{ACG}, \texttt{ATCA}, \texttt{GGA}]$

concatBWT$(\mathcal{M}) = \text{BWT}(\texttt{ATATG\$TGA\$ACG\$ATCA\$GGA\$}\#)$

Map strings to their lexicographic rank:

$$\begin{array}{lcl} \texttt{ACG} & \mapsto & \texttt{a} \\ \texttt{ATATG} & \mapsto & \texttt{b} \\ \texttt{ATCA} & \mapsto & \texttt{c} \\ \texttt{GGA} & \mapsto & \texttt{d} \\ \texttt{TGA} & \mapsto & \texttt{e} \end{array}$$

$$\mathcal{M} = \underbrace{\texttt{ATATG}}_{\texttt{b}}\$\underbrace{\texttt{TGA}}_{\texttt{e}}\$\underbrace{\texttt{ACG}}_{\texttt{a}}\$\underbrace{\texttt{ATCA}}_{\texttt{c}}\$\underbrace{\texttt{GGA}}_{\texttt{d}}\$\# \quad \mapsto \quad \texttt{beacd\#}.$$

What is the output order of the concatBWT?

$\mathcal{M} = [\texttt{ATATG}, \texttt{TGA}, \texttt{ACG}, \texttt{ATCA}, \texttt{GGA}]$

index	concatBWT	rotation
23	A	$#ATATG$TGAACGATCA$GGA
10	A	ACGATCAGGA#ATATG$TGA
14	G	$ATCA$GGA$#ATATG$TGA$ACG
19	A	GGA#ATATGTGAACG$ATCA
6	G	TGAACG$ATCA$GGA$#ATATG

input: b e a c d #   **output:** d e a c b

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input: b e a c d # **output:** d e a c b

BWT(beacd#) = de#acb ⇝ deacb

output = BWT(**input#**) (remove the # from the output)

Part III:

Conclusion

Dollar or no dollar, that is the question.

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Conclusion

The two definitions of the BWT (with and without dollar) are non-equivalent. In particular,

1. differences in the transform itself: $r(T)$ vs. $r(T\$)$
2. BWT construction: cannot use SA when no dollar is present
3. BWT of string collections: several non-equivalent methods in use

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Thank you for your attention!

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