Computing the optimal BWT of very large string collections

Davide Cenzato[1], Veronica Guerrini[2], Zsuzsanna Lipták[3], Giovanna Rosone[2]

[1]Ca' Foscari University of Venice, Department of Environmental Sciences, Informatics and Statistics

[2]University of Pisa, Department of Computer Science

[3]University of Verona, Department of Computer Science

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The Burrows-Wheeler-Transform (BWT)

- **sorting** the rotations of the input text

text: BANANA

↓

rotations of the text

ABANAN
ANABAN
ANANAB
BANANA
NANABA
NABANA

→

BWT

NNBAAA

String collections availability

The focus has shifted from individual sequences to collections of strings

- strings collections are abundant in bioinformatics
- BWT plays a **central role** in processing such large and repetitive datasets
- pattern matching while keeping data compressed (**run-length encoding**)

The Burrows-Wheeler-Transform for string collections

- basis of several **compressed data structures** for strings
- originally defined for **single sequences**
- several tools in literature computing **different BWT variants**

text		BWT
ATATGTGAACGATCAGGA	→	GGACAGTTATGCATAAGA
string collection		
{ATATG,TGA,ACG,ATCA,GGA}	→	?

The effect on the r parameter

There are **different methods** to compute the BWT of string collections

- systematically analyzed the different methods [Cenzato and Lipták, CPM 2022]

These differences extend to the **number of runs** of the BWT ($\boldsymbol{r}$)

- $r(\mathrm{w})$ = number of equal-letter runs of BWT(w)
- depend on the **input order** of the sequences

The **most used** BWT variant is the "multidollar-BWT"

The multidollar BWT

$$\mathrm{mdolBWT}(\mathcal{M}) = \mathrm{BWT}(T_1\$_1 T_2\$_2 \ldots T_k\$_k)$$

ATATG $\$_1$TGA $\$_2$ACG $\$_3$ATCA $\$_4$GGA $\$_5$ →

$\$_1$ … ATATG	G
$\$_2$ … TGA	A
$\$_3$ … ACG	G
$\$_4$ … ATCA	A
$\$_5$ … GGA	A
A$\$_2$ … TG	G
A$\$_4$ … ATC	C
A$\$_5$ … GG	G
ACG$\$_3$ … $\$_2$	\$
ATATG$\$_1$ … $\$_5$	\$
ATCA$\$_4$ … $\$_3$	\$
ATG$\$_1$ … AT	T
CA$\$_4$ … AT	T
CG$\$_3$ … A	A
G$\$_1$ … ATAT	T
G$\$_3$ … AC	C
GA$\$_2$ … T	T
GA$\$_5$ … G	G
GGA$\$_5$ … $\$_4$	\$
TATG$\$_1$ … A	A
TCA$\$_4$ … A	A
TG$\$_1$ … ATA	A
TGA$\$_2$ … $\$_1$	\$

$\$_1$ … ATATG	G
$\$_2$ … TGA	A
$\$_3$ … ACG	G
$\$_4$ … ATCA	A
$\$_5$ … GGA	A

A$\$_2$ … TG	G
A$\$_4$ … ATC	C
A$\$_5$ … GG	G

- **traditionally** used for generating the suffix tree and suffix array of multiple strings
- append (implicitly) **different** dollars
- shared suffixes: **input order**

The effect on the r parameter

- different input orders generate **different outputs**

SAP-intervals

$r = 17$

$ATATG\,\$_1 TGA\,\$_2 ACG\,\$_3 ATCA\,\$_4 GGA\,\$_5$ → G A G A A | G C G | \$ \$ \$ T T A | T C | T G | \$ A A A \$

$r = 15$

$GGA\,\$_1 ATATG\,\$_2 ACG\,\$_3 TGA\,\$_4 ATCA\,\$_5$ → A G G A A | G G C | \$ \$ \$ T T A | T C | G T | \$ A A A \$

$r = 14$

$ATCA\,\$_1 GGA\,\$_2 TGA\,\$_3 ACG\,\$_4 ATATG\,\$_5$ → A A A G G | C G G | \$ \$ \$ T T A | C T | G T | \$ A A A \$

Colexicographic order (aka reverse lexicographic order RLO) [Cox et al., Bioinformatics, 2012]

- Is **colexicographic order** optimal?

Computing the Optimal BWT

Bentley et al. [ESA 2020] introduced a linear-time algorithm for computing the **optimal permutation** of the input collection, which yields the minimum number of runs of the resulting multidollarBWT.

- we refer to this transform as **optimal BWT (optBWT)**

Here, we give the **first tool** **("optimalBWT")** to compute the optBWT:

- use the BWT, the SAP-array, and the algorithm by Bentley et al.
- **reduce the number of runs** up to a 31 factor
- **negligible** time and space overhead

The SAP-array

The SAP-array is a **bitvector** storing the positions of the BWT blocks containing rotations starting with a shared suffix.

- the 0s define the starting points of the SAP-intervals
- the 1s define the extensions of the SAP-intervals

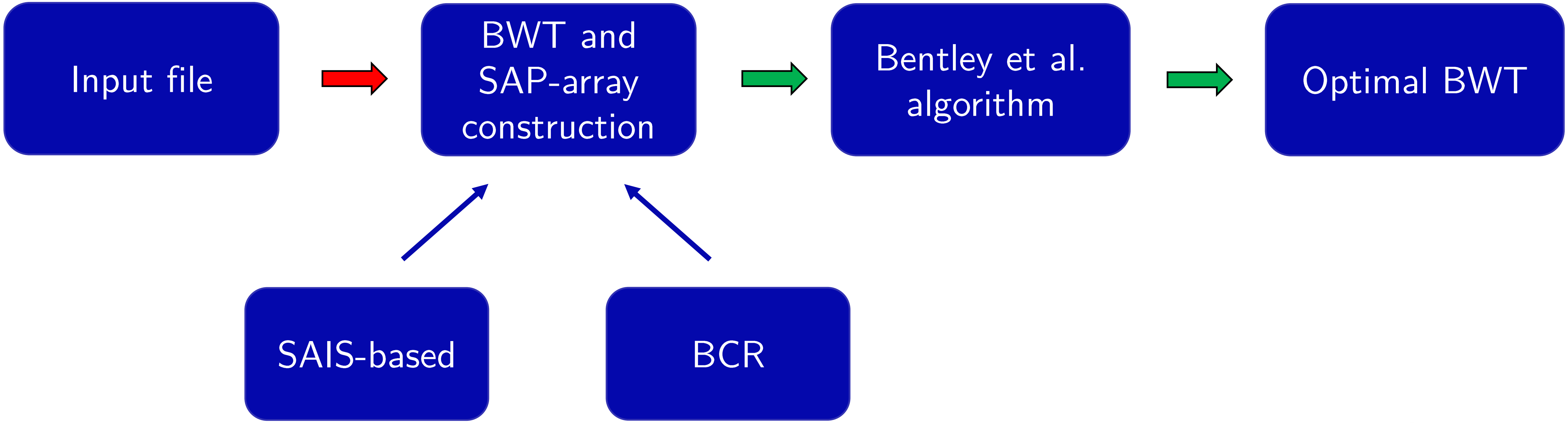
all rotations starting with \$ → 0 1 1 1 1 | 0 1 1 | 0 0 …

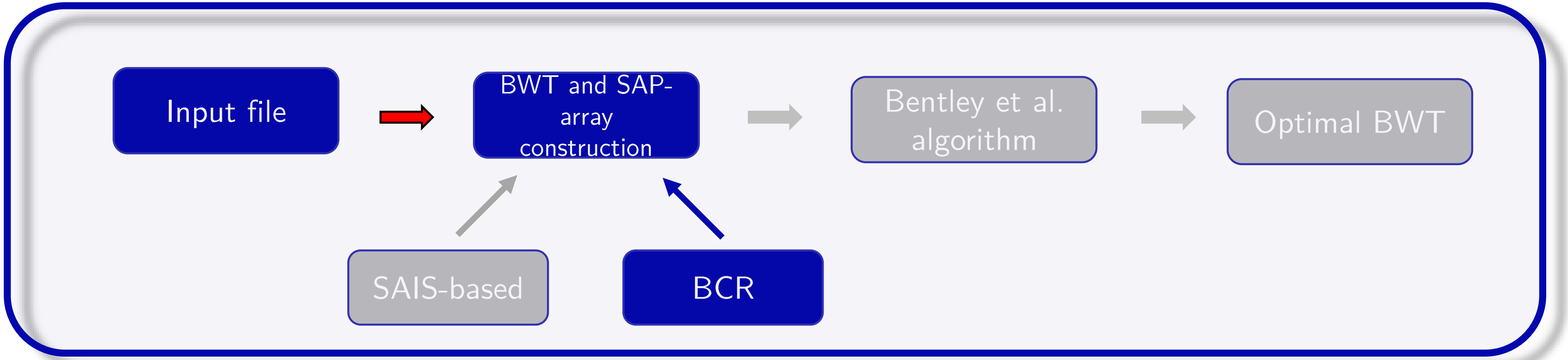
↑ all rotations starting with A\$

$\$_1$ … ATATG	G	0
$\$_2$ … TGA	A	1
$\$_3$ … ACG	G	1
$\$_4$ … ATCA	A	1
$\$_5$ … GGA	A	1
A$\$_2$ … TG	G	0
A$\$_4$ … ATC	C	1
A$\$_5$ … GG	G	1
ACG$\$_3$ … $\$_2$	\$	0
ATATG$\$_1$ … $\$_5$	\$	0
ATCA$\$_4$ … $\$_3$	\$	0
ATG$\$_1$ … AT	T	0
CA$\$_4$ … AT	T	0
CG$\$_3$ … A	A	0
G$\$_1$ … ATAT	T	0
G$\$_3$ … AC	C	1
GA$\$_2$ … T	T	0
GA$\$_5$ … G	G	1
GGA$\$_5$ … $\$_4$	\$	0
TATG$\$_1$ … A	A	0
TCA$\$_4$ … A	A	0
TG$\$_1$ … ATA	A	0
TGA$\$_2$ … $\$_1$	\$	0

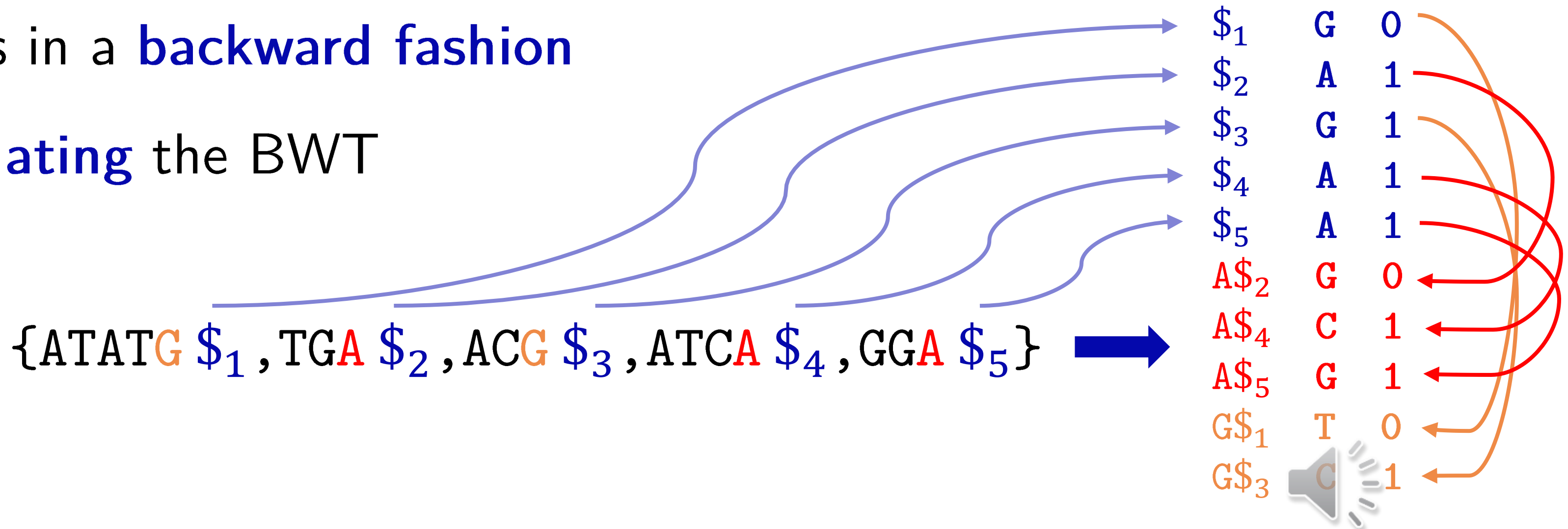
The Workflow

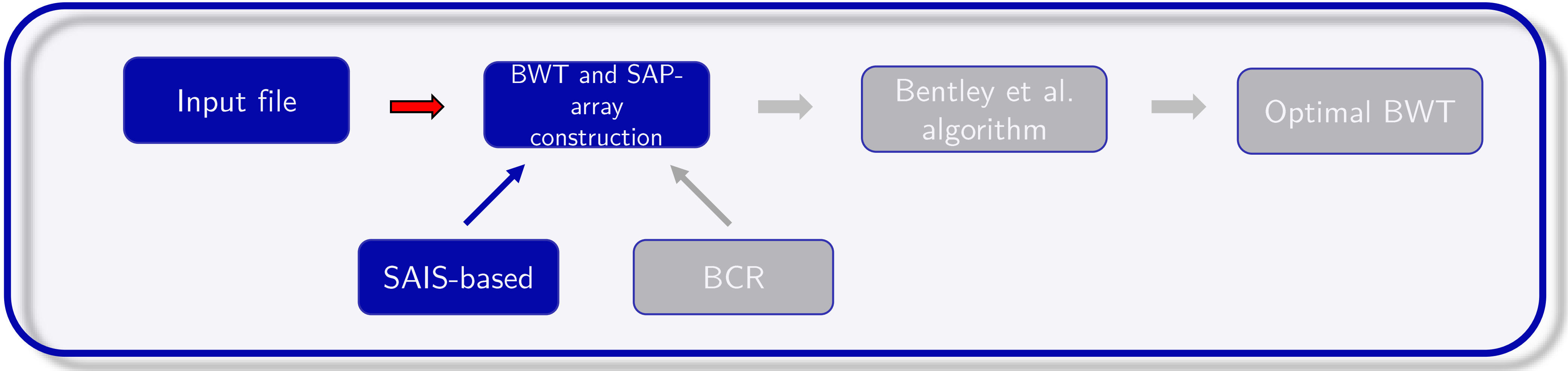
Our method is divided in two steps, first (→), we compute the BWT, and second (→), we compute the optimal permutation of the BWT characters.



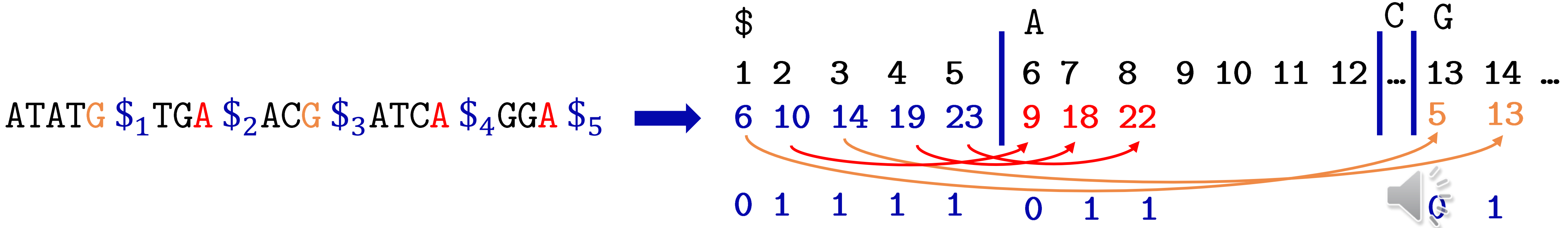


- BCR inserts BWT characters in a **backward fashion**
- update SAP-array **while updating** the BWT





- SAIS sort suffixes by **induced sorting**
- **update** SAP-array while inducing types



Bentley et al. reduced the problem of finding an optimal input permutation to the **Tuple Ordering** (TO) problem.

```
0 1 1 1 1 1 1 | 0 1 1 1 1 | 0 1 | 0 0 | 0 1 | 0 0 0 0 0 0 | 0 1 | 0 1 | 0 1 | 0 0 0
A A T A T A A | G A A C T | C T | C $ | G G | C A $ $ $ T | A C | A A | G G | $ $ $
```

(A,T) (A,C,G,T) (C,T)(C)($) (G) (C)(A)($)($)($)(T)(A,C) (A) (G) ($)($)($)

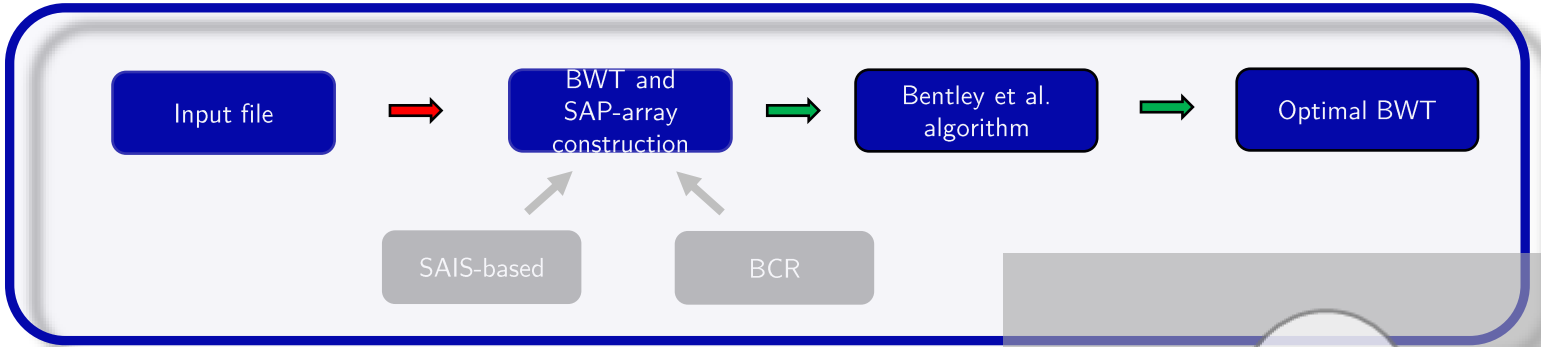
(A,T)(A,C,G,T)(C,T)(C)($)(G)(C)(A)($)($)($)(T)(A,C)(A)(G)($)($)($)

(T,A)(A,C,G,T)(T,C)(C)($)(G)(C)(A)($)($)($)(T)(C,A)(A)(G)($)($)($)

- we implemented this algorithm using a **stack** data structure containing the Parikh vectors of the SAP-intervals
- we keep inserting the Parikh vectors in the stack until we find either a fixed position or a tuple containing one character

(A,T)(A,C,G,T)(C,T)(C)($)(G)(C)(A)($)($)($)(T)(A,C)(A)(G)($)($)($)

$ A C G T
(0,5,0,0,2)

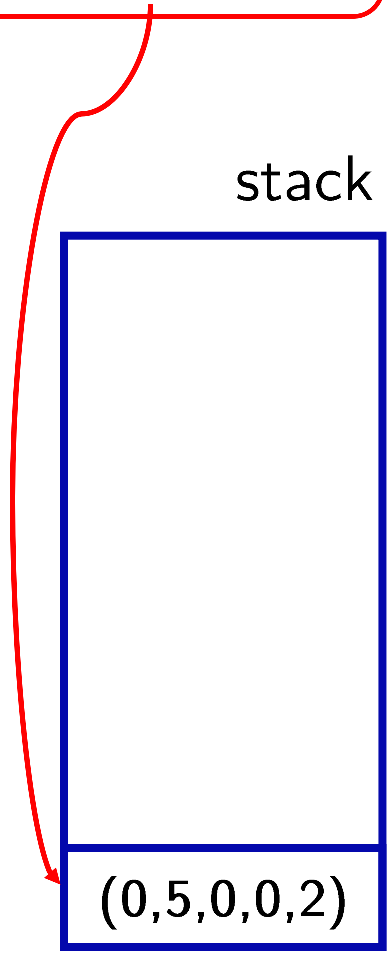


- we output the optimal BWT **permuting** different blocks separately

Computing the optimal BWT

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

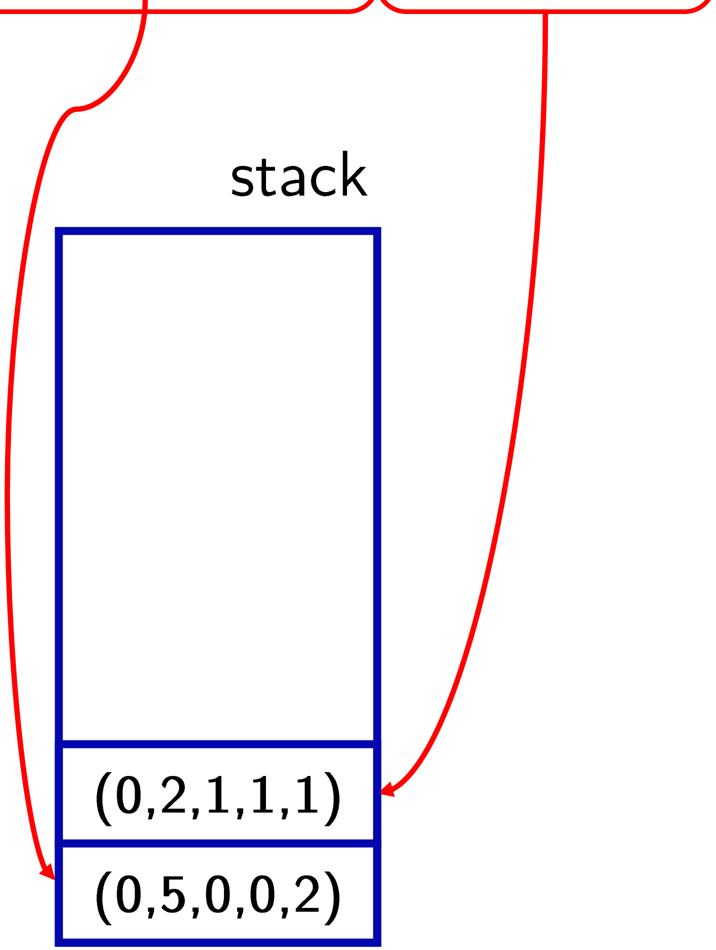
A A T A T A A G A A C T C T C $ G G C A $ $ $ T A C A A G G $ $ $



Algorithm 1 Procedure to process a Parikh vector P

```
if Stack is empty then
    if there is exactly one j such that P[j] > 0 then   // interval not interesting
        write P[j] copies of character j
    else
        if P[x] > 0 where x is the last character inserted in the BWT then
            write P[x] copies of the character x, P[x] ← 0
        end if
        Stack ← pushTop(P)                 // push a new Parikh vector on the stack
    end if
else
    T ← Stack.top()                              // first element of the stack
    if there are at least two j s.t. T[j] > 0 and P[j] > 0 then
        Stack ← pushTop(P)
    else
        write corresponding characters for each T in Stack   // see text for details
    end if
end if
```

```
0 1 1 1 1 1 1 0 1 1 1 1 0 1 0 0 0 1 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0
A A T A T A A G A A C T C T C $ G G C A $ $ $ T A C A A G G $ $ $
```



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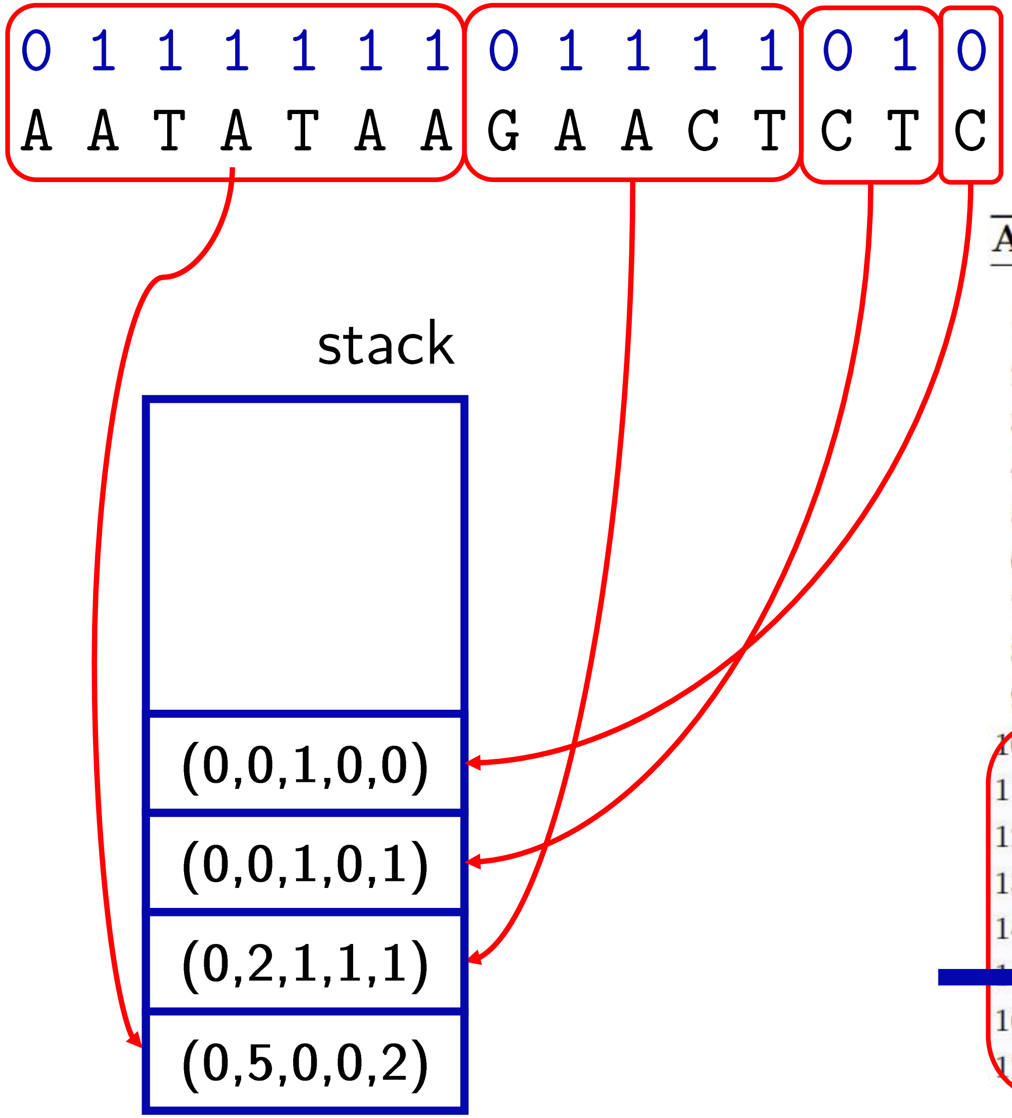
```

Computing the optimal BWT



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```
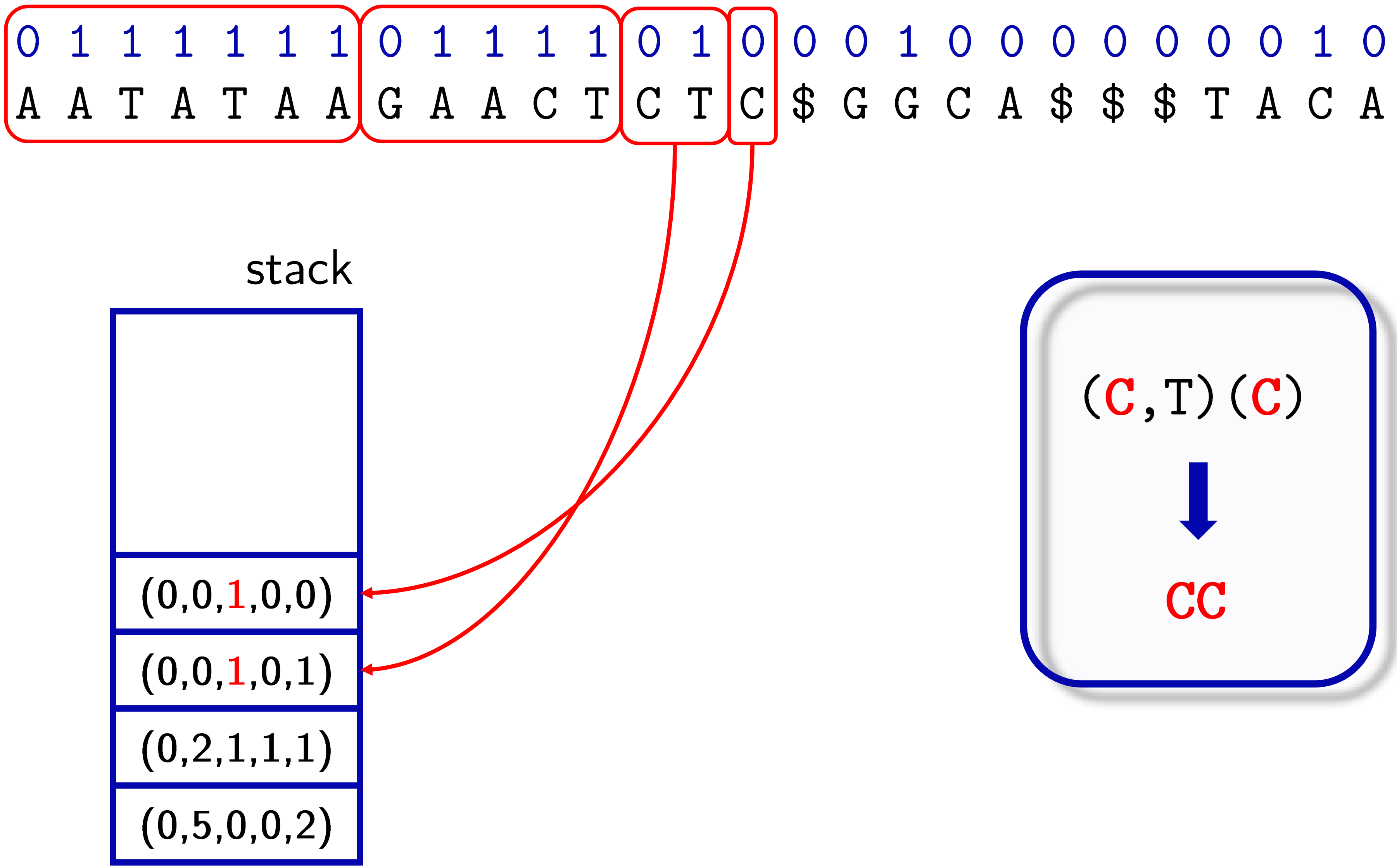
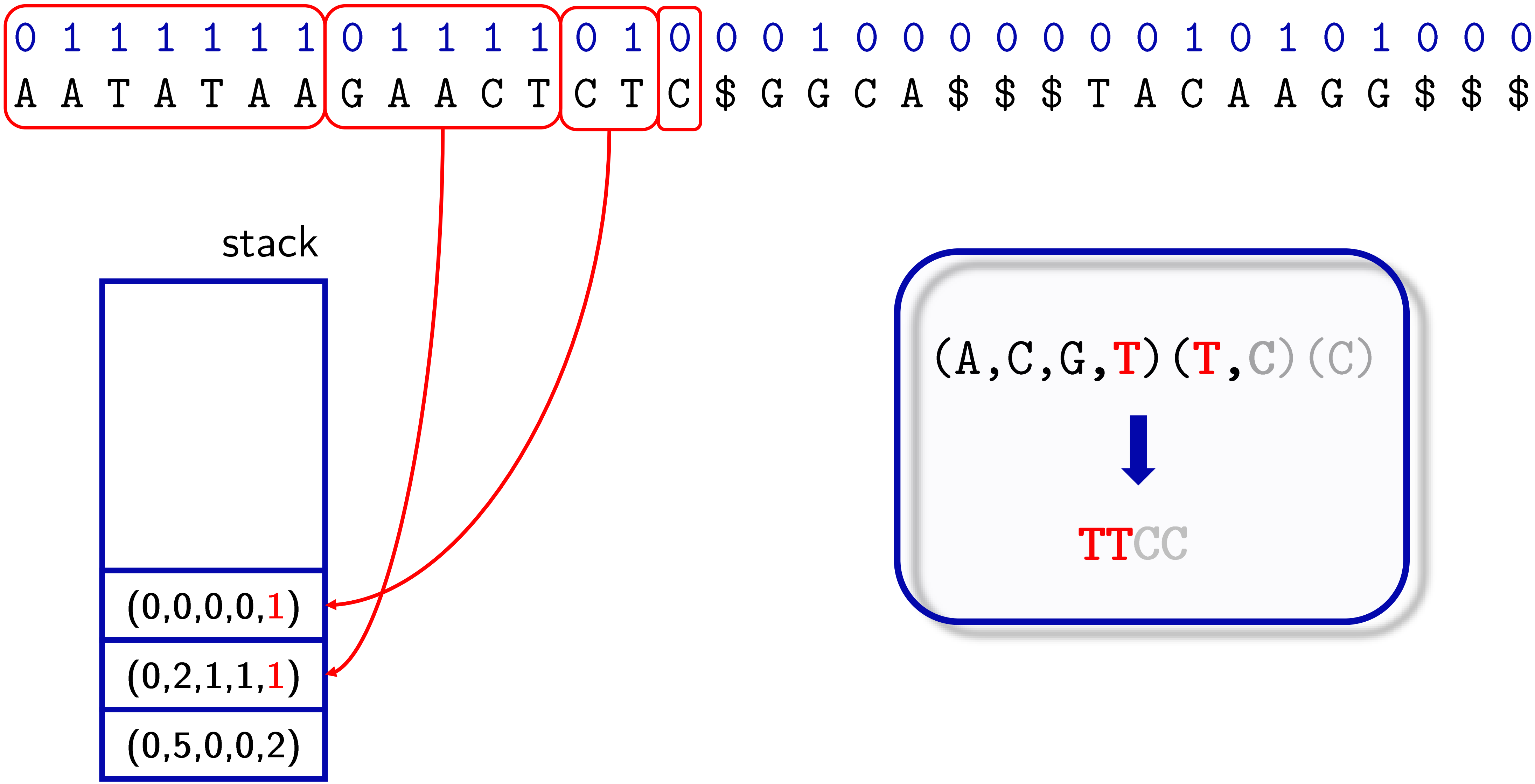
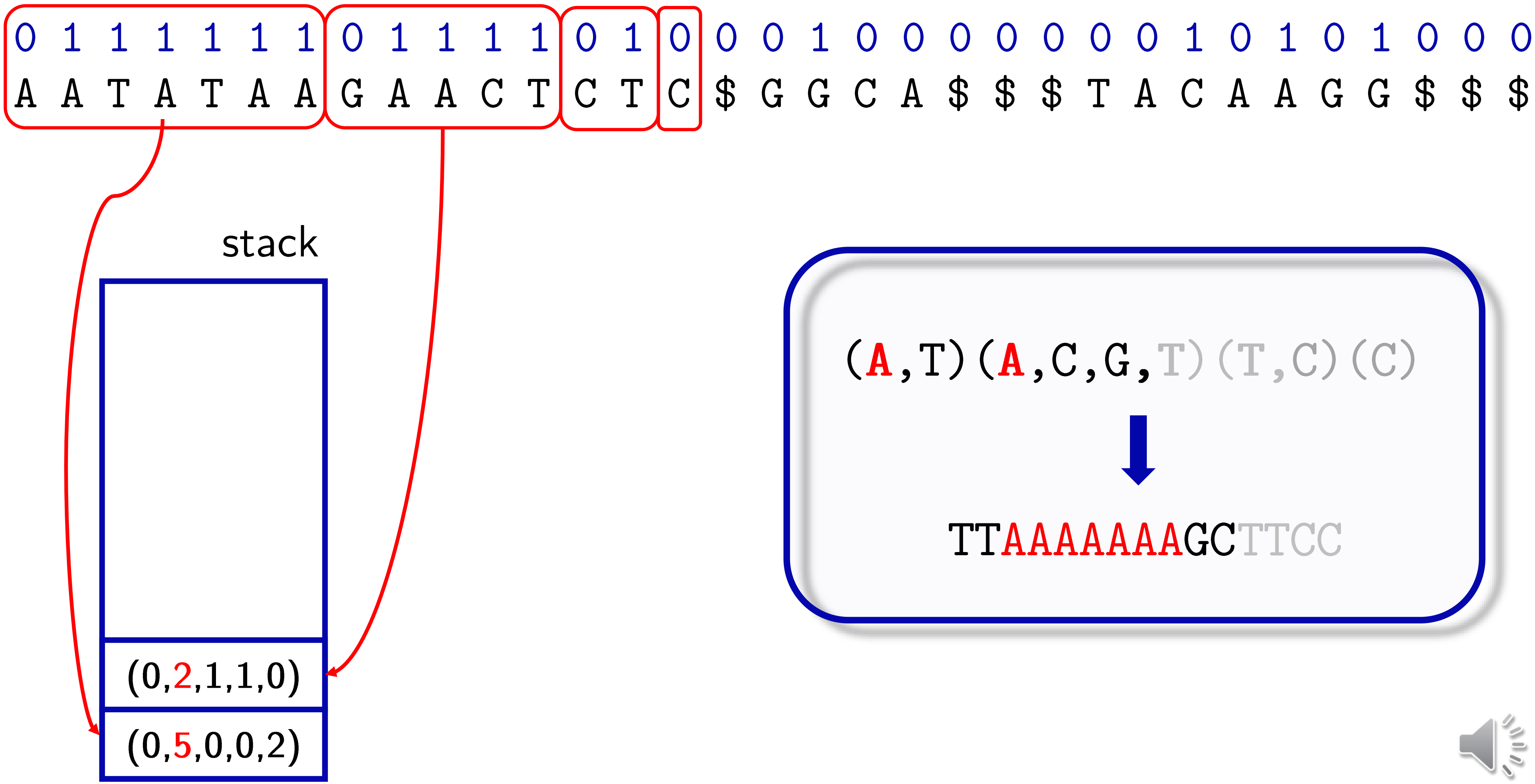

Computing the optimal BWT

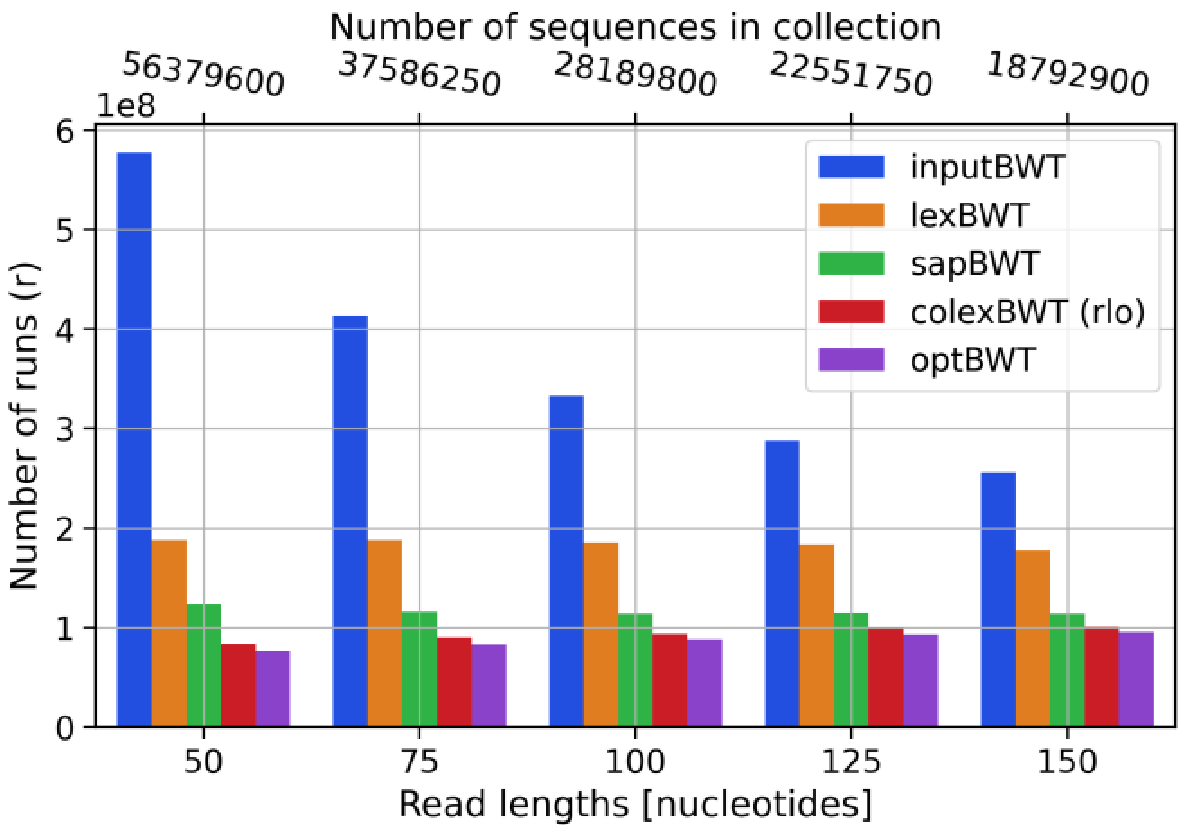


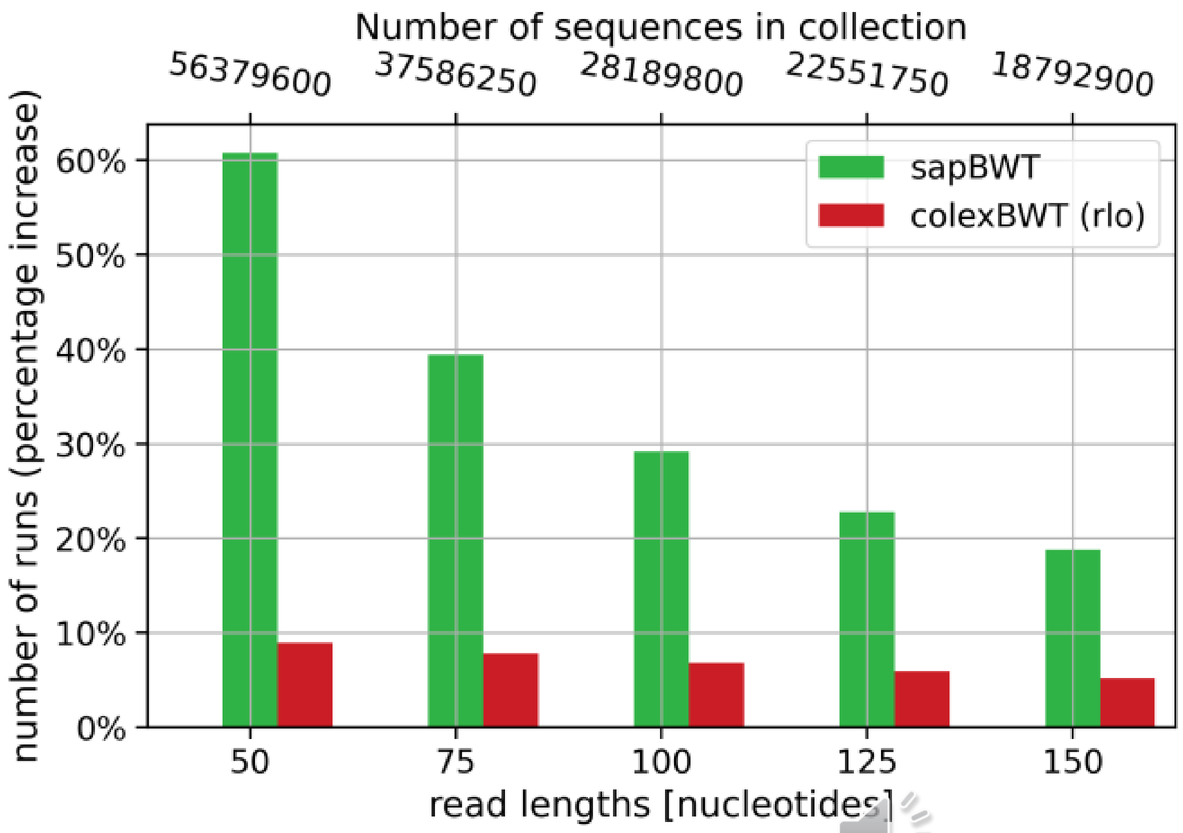
Computing the optimal BWT




0 1 1 1 1 1 1 0 1 1 1 1 0 1 0 0 0 1 0 0 0 0 0 0 0 1 0 1 0 1 0 0 0
A A T A T A A G A A C T C T C $ G G C A $ $ $ T A C A A G G $ $ $
stack
(0,2,1,1,0)
(0,5,0,0,2)
(A,T)(A,C,G,T)(T,C)(C)
TTAAAAAAAGCTTCC

- Pseudomonas **aeruginosa**





Real data

- we tested our method on 7 **real-life** datasets
- **different features**: read length, dataset size, n/r

dataset		description	length BWT n	len.	no. seq	r_{opt}	n/r_{opt}	n/r
1	ERR732065–70	*HIV-virus*	1,345,713,812	150	8,912,012	11,539,661	116.62	27.62
2	SRR12038540	*SARS-CoV-2 RBD*	1,690,229,250	50	33,141,750	14,864,523	113.71	8.08
3	ERR022075_1	*E. Coli str. K-12*	2,294,730,100	100	22,720,100	71,203,469	32.23	8.83
4	SRR059298	*Deformed wing virus*	2,455,299,082	72	33,634,234	48,376,632	50.75	9.83
5	SRR065389–90	*C. Elegans*	14,095,870,474	100	139,563,074	921,561,895	15.30	6.26
6	SRR2990914_1	*Sindibis virus*	15,957,722,119	36	431,289,787	105,250,120	151.62	4.81
7	ERR1019034	*H. Sapiens*	123,506,926,658	100	1,222,840,858	10,860,229,434	11.37	5.35

Real data

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data set	number of runs increase compared to optimal BWT (factor and perc.)				resource usage (optBWT)	
	inputBWT	colexBWT (rlo)	sapBWT	lexBWT	RAM (GB)	Time (hh:mm:ss)
1	**4.22** (322.26%)	1.03 (3.48%)	1.53 (53.06%)	1.30 (30.13%)	6.45 (1.02×)	7:18 (1.12×)
2	**14.07** (1306.95%)	1.15 (14.54%)	1.21 (20.75%)	3.52 (252.39%)	8.08 (1.03×)	6:32 (1.15×)
3	**3.65** (264.90%)	1.07 (6.52%)	1.30 (29.63%)	2.07 (107.01%)	11.15 (1.04×)	18:29 (1.26×)
4	**5.17** (416.52%)	1.04 (4.38%)	1.55 (55.33%)	1.55 (54.87%)	21.03 (1.02×)	22:08 (1.08×)
5	**2.44** (144.36%)	1.05 (5.05%)	1.16 (15.73%)	2.03 (103.35%)	4.31 (1.04×)	2:25:46 (1.28×)
6	**31.49** (3048.66%)	1.04 (4.30%)	1.79 (79.40%)	1.89 (89.17%)	8.86 (1.05×)	1:59:46 (1.39×)
7	**2.13** (112.56%)	1.04 (4.17%)	1.12 (11.89%)	1.96 (96.04%)	34.42 (1.03×)	26:24:18 (1.48×)

Conclusions

We presented the first tool for computing the BWT of a string collection that guarantees the **fewest** possible runs.

- number of runs reduction is **significant for all read lengths**
- on real-data, the optBWT can reduce r by up to a **31 factor**
- the space and time **overhead** to compute the optimal BWT is small
- can compute the optimal BWT of **very large** string collections
- implementation **available** on GitHub

Thank you for your attention

contact: davide.cenzato@unive.it

github: https://github.com/davidecenzato/optimalBWT