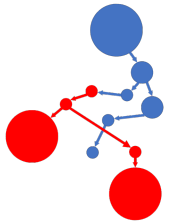
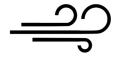


WGT
Wheeler Graph Toolkit



WGT: Tools and algorithms for recognizing, visualizing and generating Wheeler graphs

2023.04.14

@KuanHaoChao

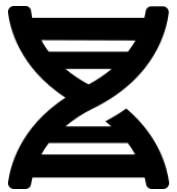
Presenter : Kuan-Hao Chao (khchao.com)

Kuan-Hao Chao†, Pei-Wei Chen†, Sanjit A. Seshia, Ben Langmead

Berkeley
UNIVERSITY OF CALIFORNIA

JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

Department of Computer Science



RECOMB-SEQ

Why is Wheeler graph interesting?: XBW *2005*

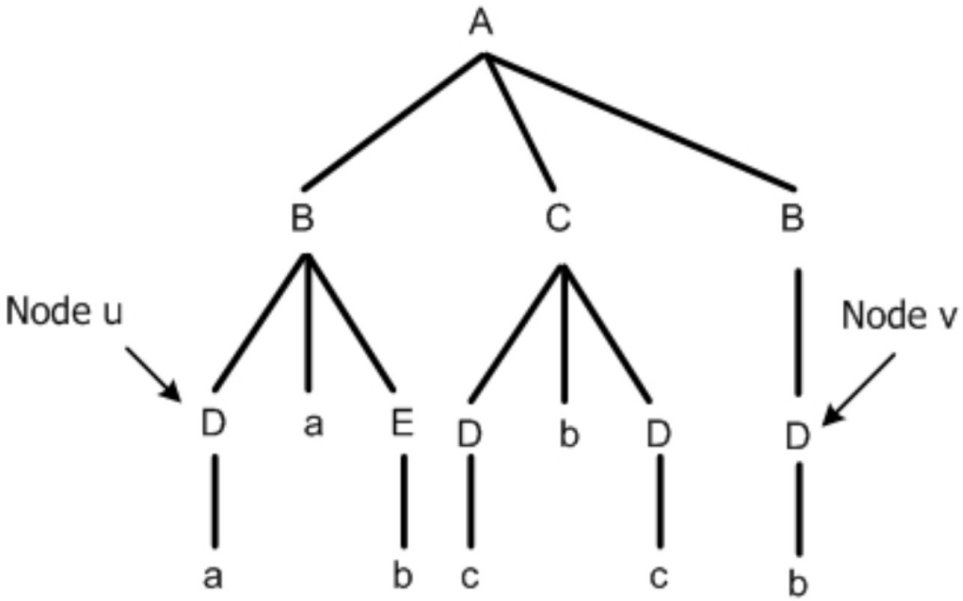
Browse Conferences > Annual IEEE Symposium on Found... > 46th Annual IEEE Symposium on ...

Annual IEEE Symposium on Foundations of Computer Science

Structuring labeled trees for optimal succinctness, and beyond

Publisher: IEEE | Cite This | PDF

P. Ferragina ; F. Luccio ; G. Manzini ; S. Muthukrishnan



(a)

S_{last}	S_α	S_π
0	A	*empty string*
0	B	A
0	D	BA
1	a	DBA
0	a	BA
1	E	BA
1	b	EBA
0	C	A
0	D	CA
1	c	DCA
0	b	CA
1	D	CA
1	c	DCA
1	B	A
1	D	BA
1	b	DBA

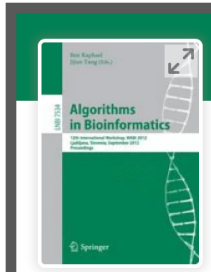
(b)

stable sort

	S_{last}	S_α	S_π	
1	0	A	*empty string*	
2	0	B	A	p(u)
3	0	C	A	
4	1	B	A	p(v)
5	0	D	BA	u
6	0	a	BA	u's siblings
7	1	E	BA	
8	1	D	BA	v
9	0	D	CA	
10	0	b	CA	
11	1	D	CA	
12	1	a	DBA	
13	1	b	DBA	
14	1	c	DCA	
15	1	c	DCA	
16	1	b	EBA	

(c)

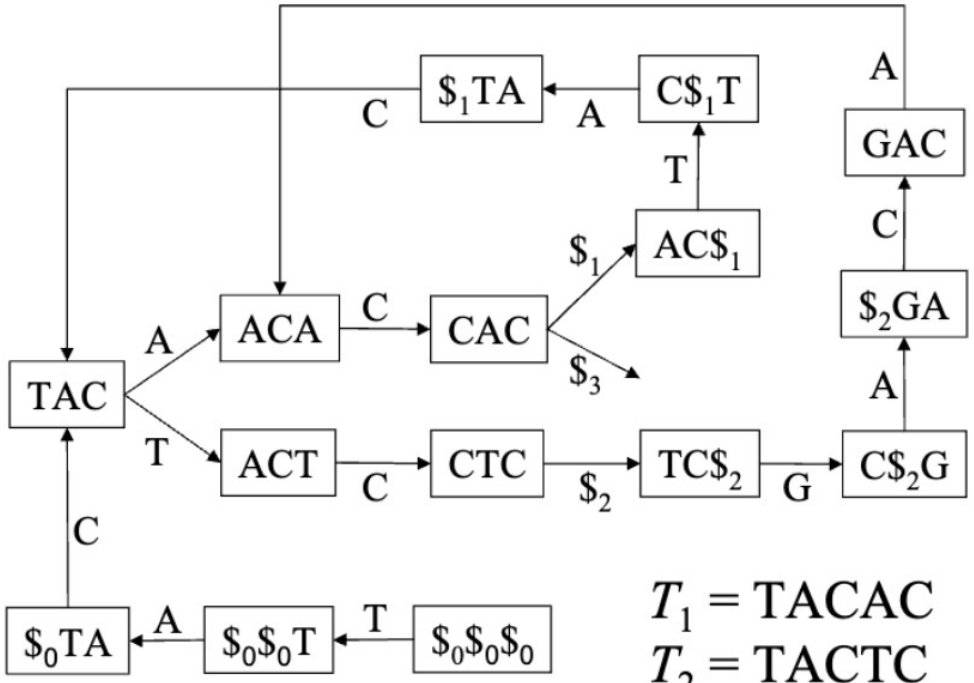
Why is Wheeler graph interesting?: BOSS *2012*



Succinct de Bruijn Graphs

Alexander Bowe, Taku Onodera, Kunihiko Sadakane & Tetsuo Shibuya

Conference paper 2012



$T_1 = \text{TACAC}$
$T_2 = \text{TACTC}$
$T_3 = \text{GACTC}$

F	
$\$_i$	0
A	3
C	7
G	13
T	14

Incoming edge label **Outgoing edge label**

	last	Node	*W*
$\$_i$	1	$\$_0\$_0\$_0$	T
	1	AC$\$_1$	T
	1	TC$\$_2$	G
A	1	ACA	C
	1	$\$_2$GA	C
	1	$\$_0$TA	C
	1	$\$_1$TA	C-
C	0	CAC	$\$_3$
	1	CAC	$\$_1$
	1	GAC	A
	0	TAC	T
	1	TAC	A-
	1	CTC	$\$_2$
G	1	C$\$_2$G	A
T	1	$\$_0\$_0$T	A
	1	C$\$_1$T	A
	1	ACT	C

Why is Wheeler graph interesting?: GCSA *2014*

IEEE/ACM TRANSACTIONS ON COMPUTATIONAL BIOLOGY AND BIOINFORMATICS, VOL. 11, NO. 2, MARCH/APRIL 2014 375

Indexing Graphs for Path Queries with Applications in Genome Research

Jouni Sirén, Niko Välimäki, and Veli Mäkinen

2014

```
G A C G T A - C T G
G A C G T A - - - G
G A T G T A - C T G
G A C - T A C C T G
```

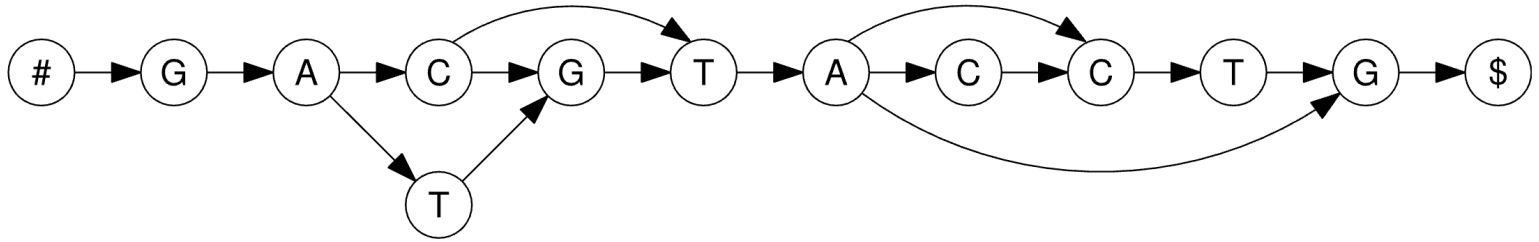


Fig. 4. A reverse deterministic automaton corresponding to the first 10 positions of the multiple alignment in Fig. 1.

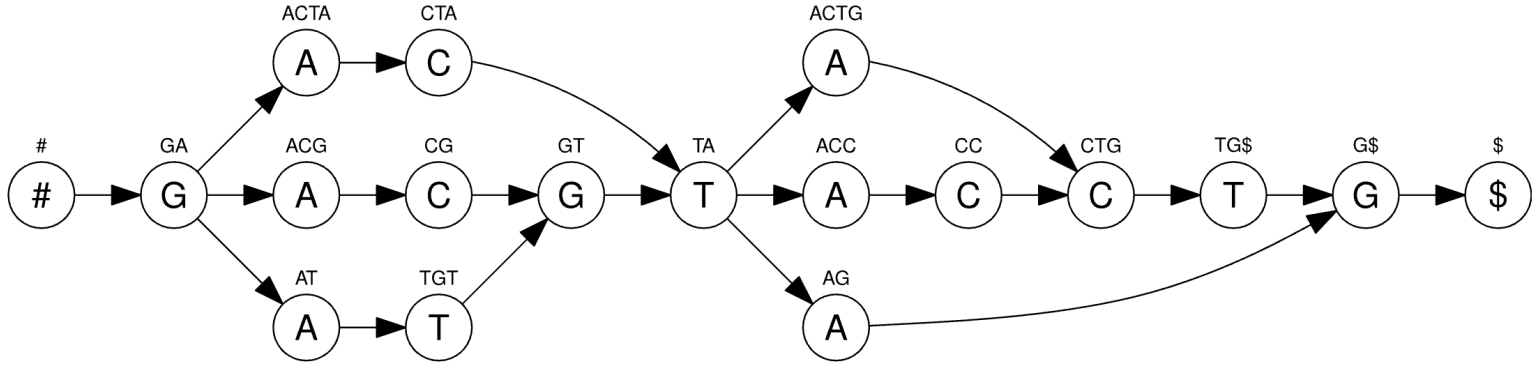


Fig. 5. A prefix-sorted automaton built for the automaton in Fig. 4. The strings above nodes are prefixes $p(v)$.

Why is Wheeler graph interesting?: VG *2017-18*

OPEN ACCESS

Indexing Variation Graphs

Author: Jouni Sirén | AUTHORS INFO & AFFILIATIONS

https://doi.org/10.1137/1.9781611974768.2

2017

Published: 01 October 2018

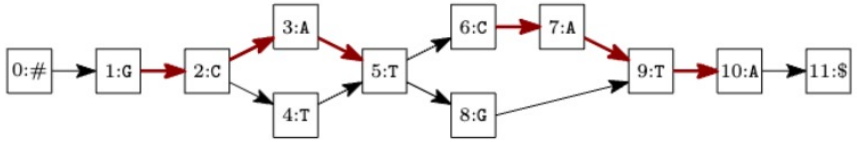
Variation graph toolkit improves read mapping by representing genetic variation in the reference

Erik Garrison, Jouni Sirén, Adam M Novak, Glenn Hickey, Jordan M Eizenga, Eric T Dawson, William Jones, Shilpa Garg, Charles Markello, Michael F Lin, Benedict Paten & Richard Durbin

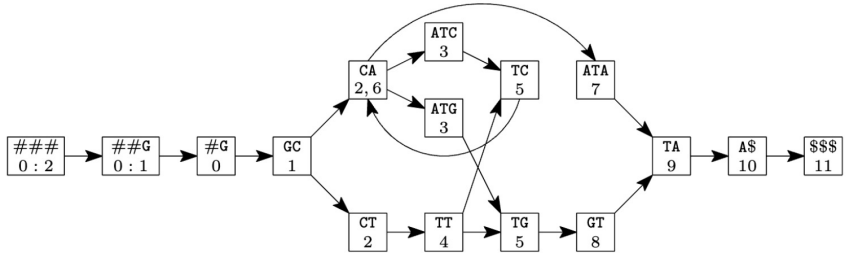
Nature Biotechnology **36**, 875–879 (2018) | Cite this article

2018

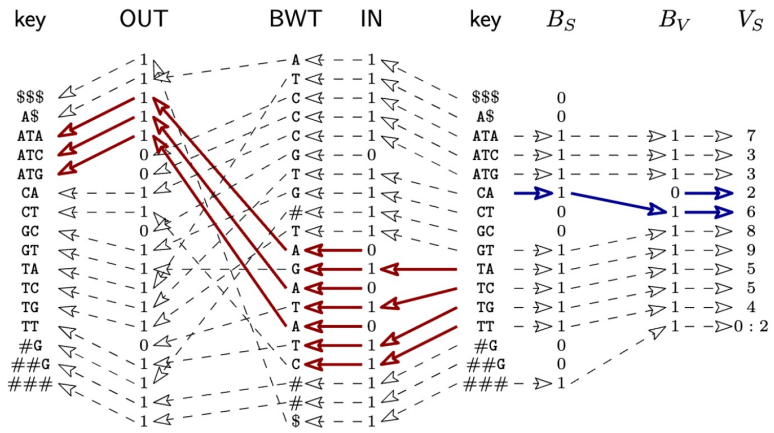
***G*: Input graph**

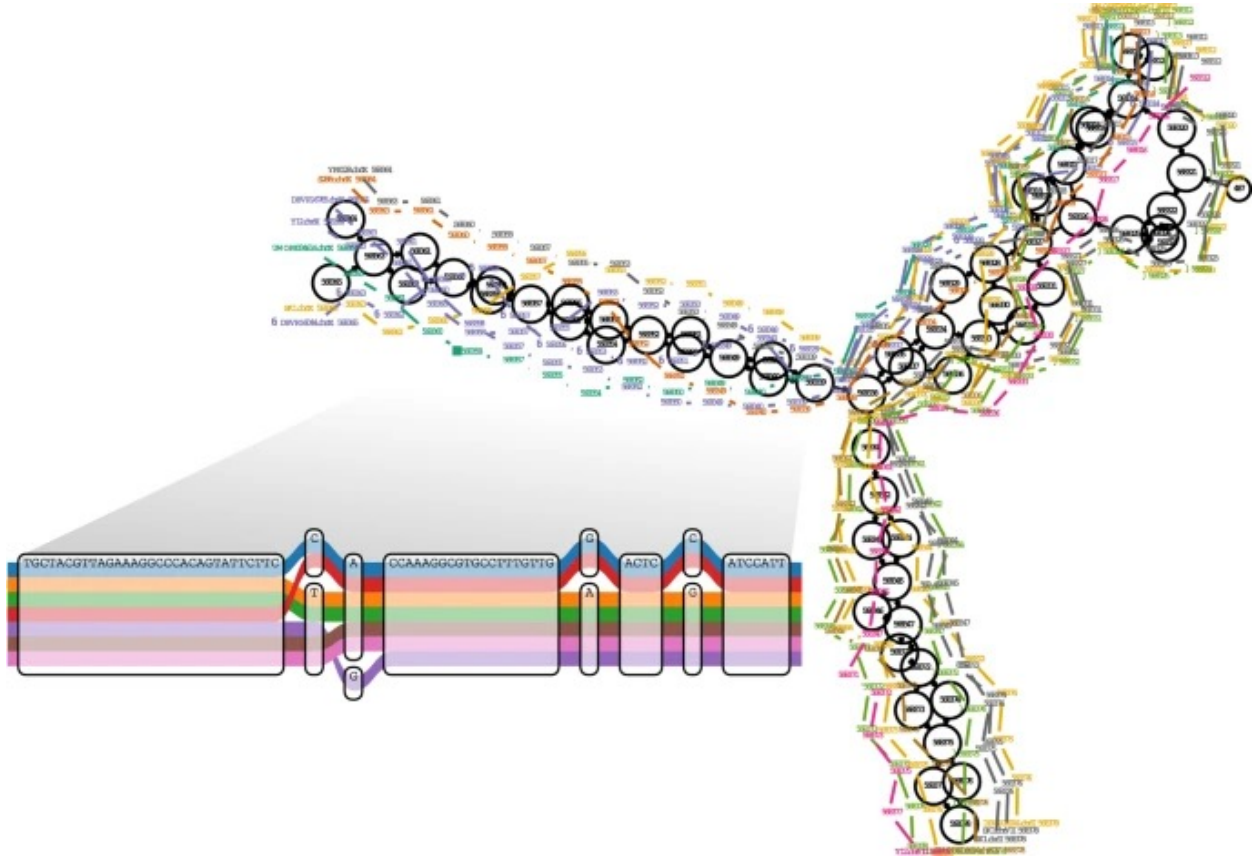


***G′*: Order-3 de Bruijn graph**



GCSA* for graph *G″





Why is Wheeler graph interesting?: HISAT2 *2019*

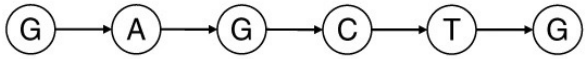
Graph-based genome alignment and genotyping with HISAT2 and HISAT-genotype

nature biotechnology

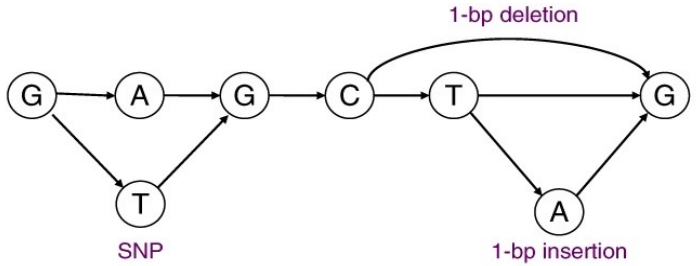
Daehwan Kim[1*], Joseph M. Paggi[2], Chanhee Park[1], Christopher Bennett[1] and Steven L. Salzberg[3,4]

2019

1. Reference sequence (6 bp long)

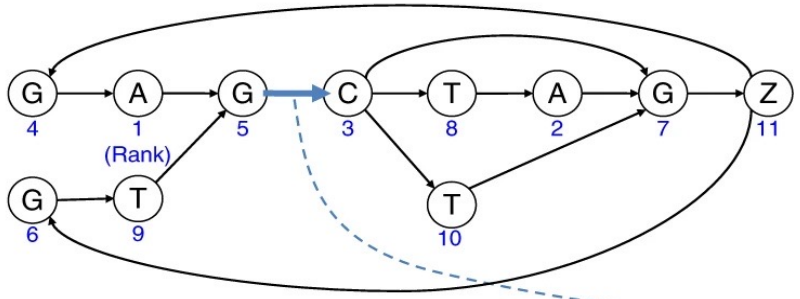


2. Graphical representation (original graph)



Prefix doubling and pruning

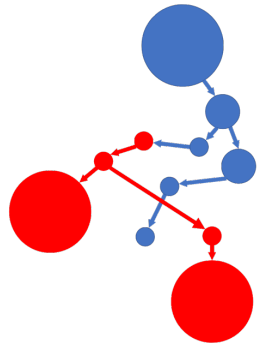
3. Prefix-sorted graph



4. Tabular representation of the prefix-sorted graph

Outgoing edge(s)			Incoming edge(s)	
Node rank	First		Last	Node rank
1	A		G	1
2	A		T	2
3	C		G	3
	C		Z	4
	C		A	5
4	G		T	
5	G		Z	6
6	G		A	7
7	G		C	
8	T		T	
9	T		C	8
10	T		G	9
11	Z		C	10
	Z		G	11

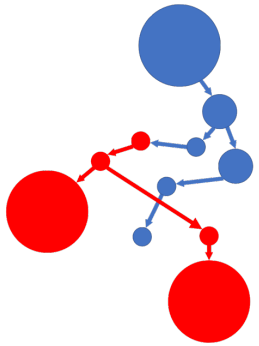
Our Contribution



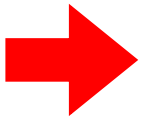
WGT
Wheeler Graph Toolkit

- A Wheeler graph visualizer: bipartite representation
- Implemented the first Wheeler graph *recognizer*
- Wheeler graph *generators*: Random WG / Trie / DBG / RDG

Our Contribution



WGT
Wheeler Graph Toolkit



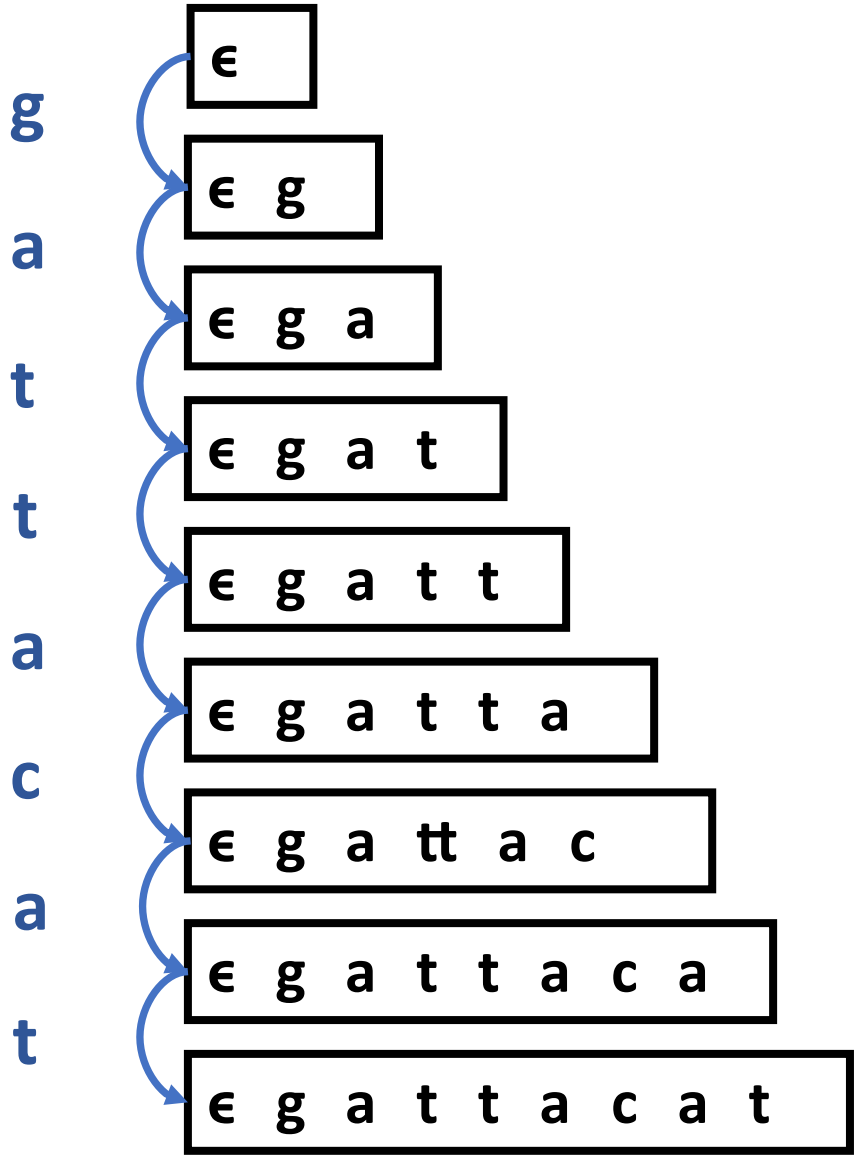
- ***A Wheeler graph visualizer: bipartite representation***

- Implemented the first Wheeler graph *recognizer*

- Wheeler graph *generators*: Random WG / Trie / DBG / RDG

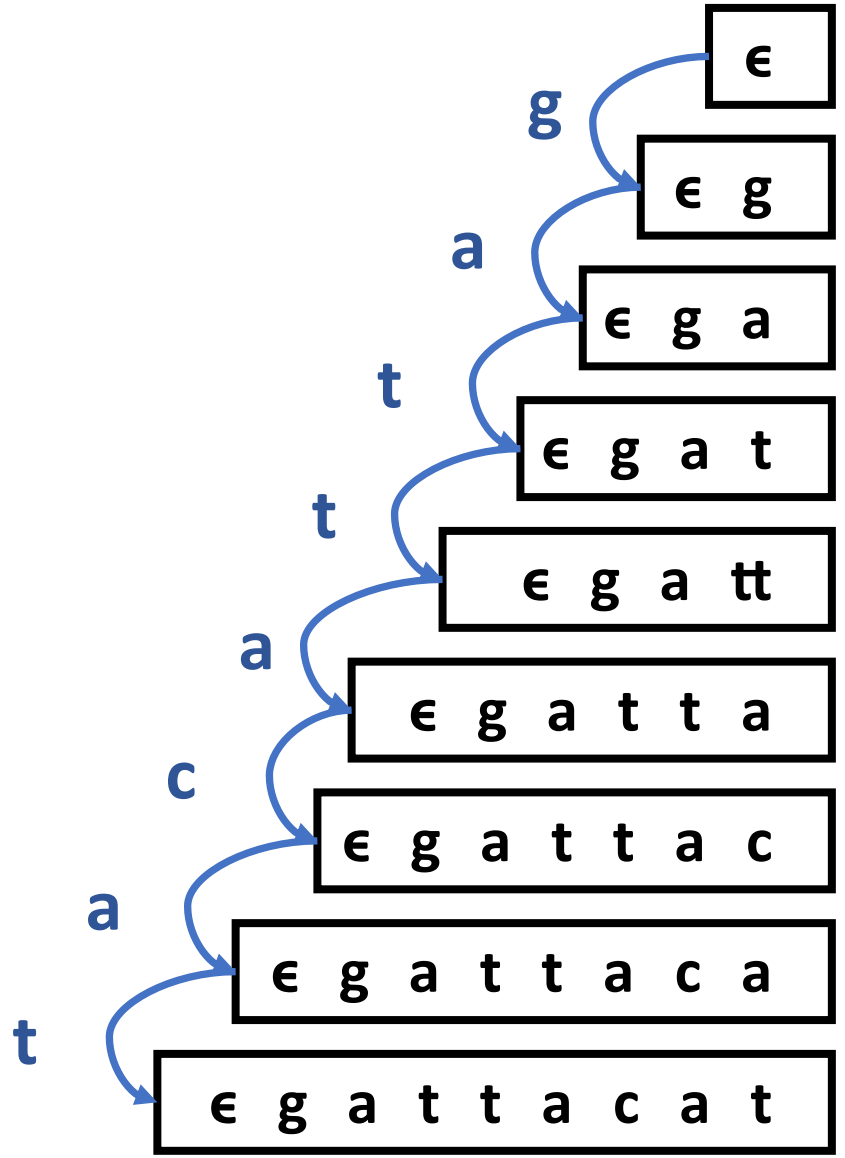
Representing a Sequence in Wheeler Graph

T: ϵgattacat



Representing a Sequence in Wheeler Graph

T: ϵgattacat



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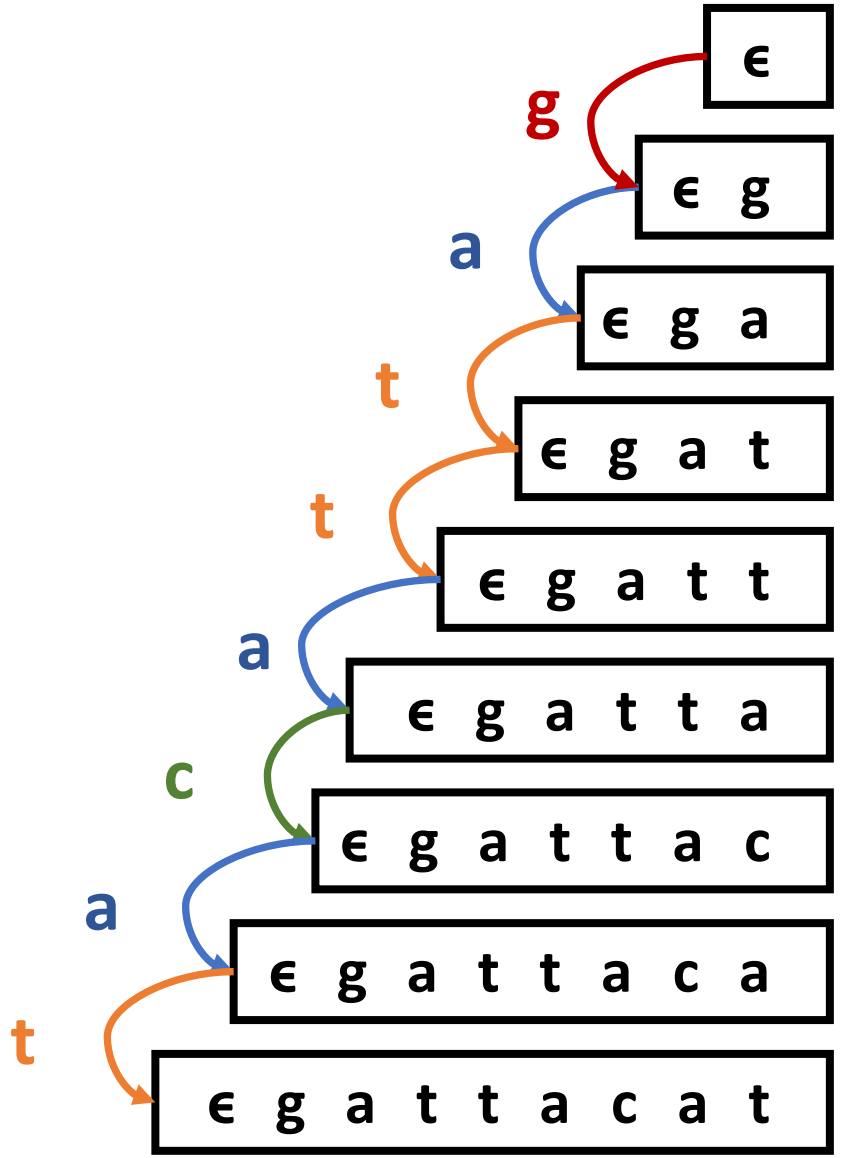

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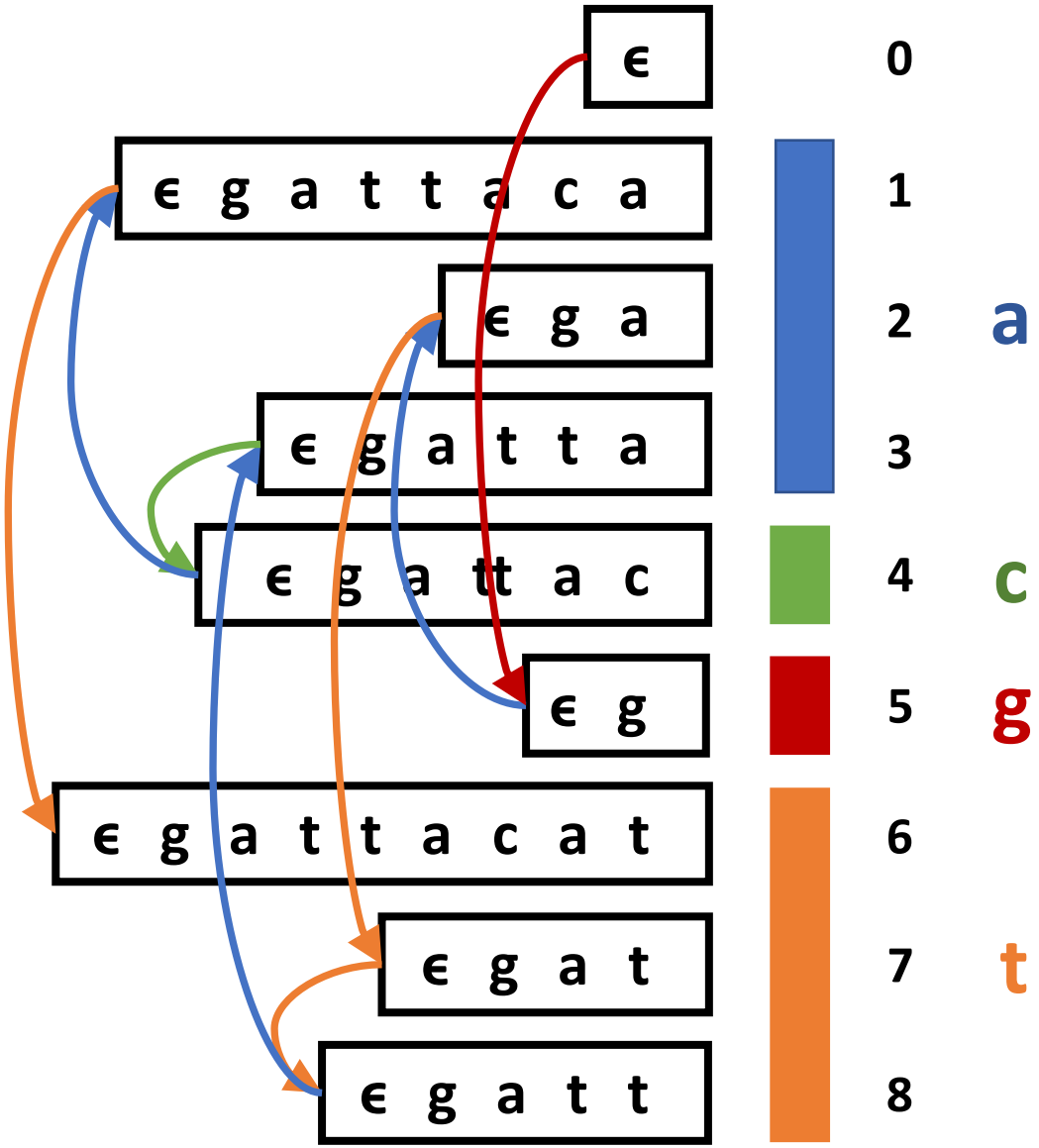

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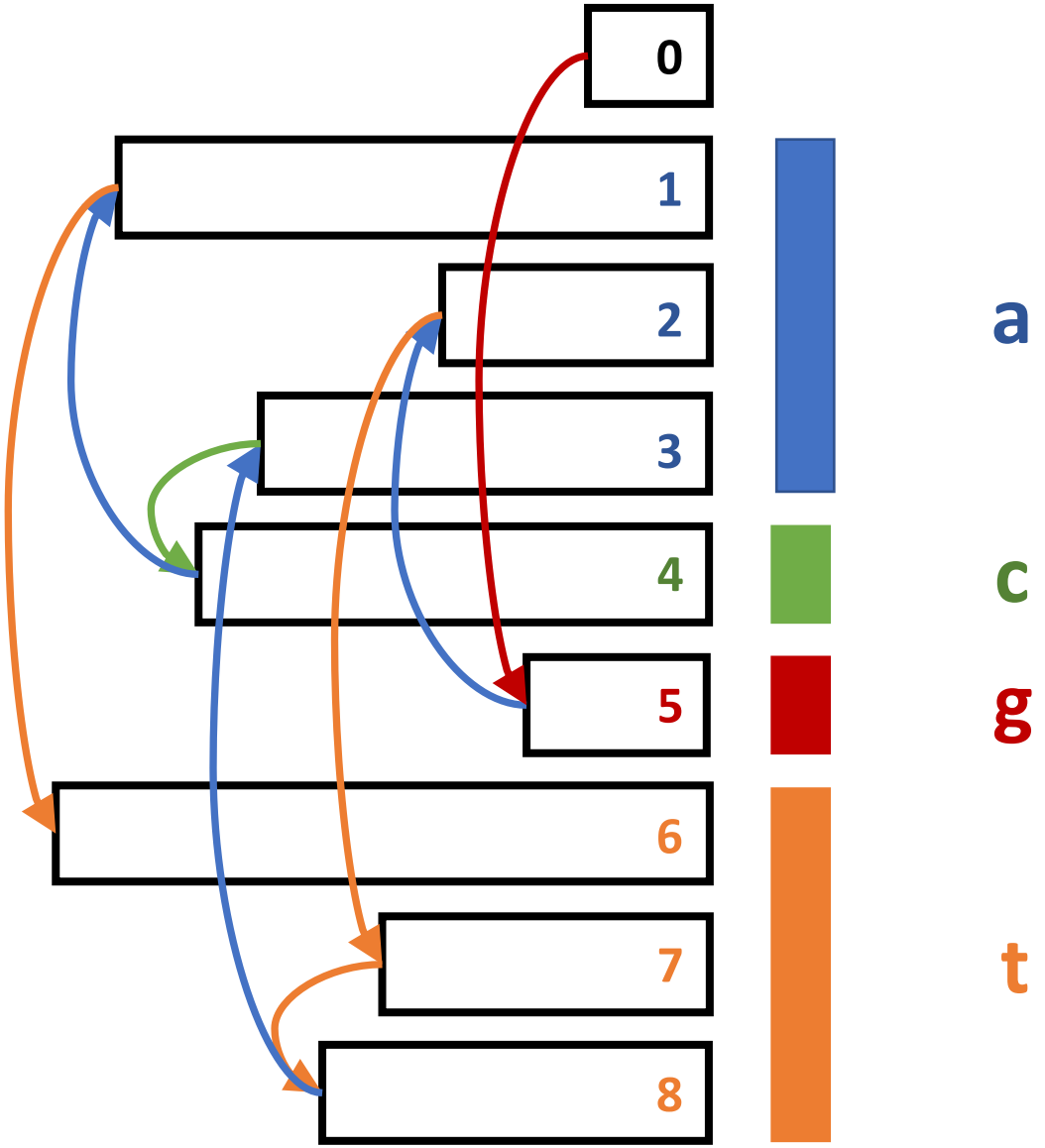

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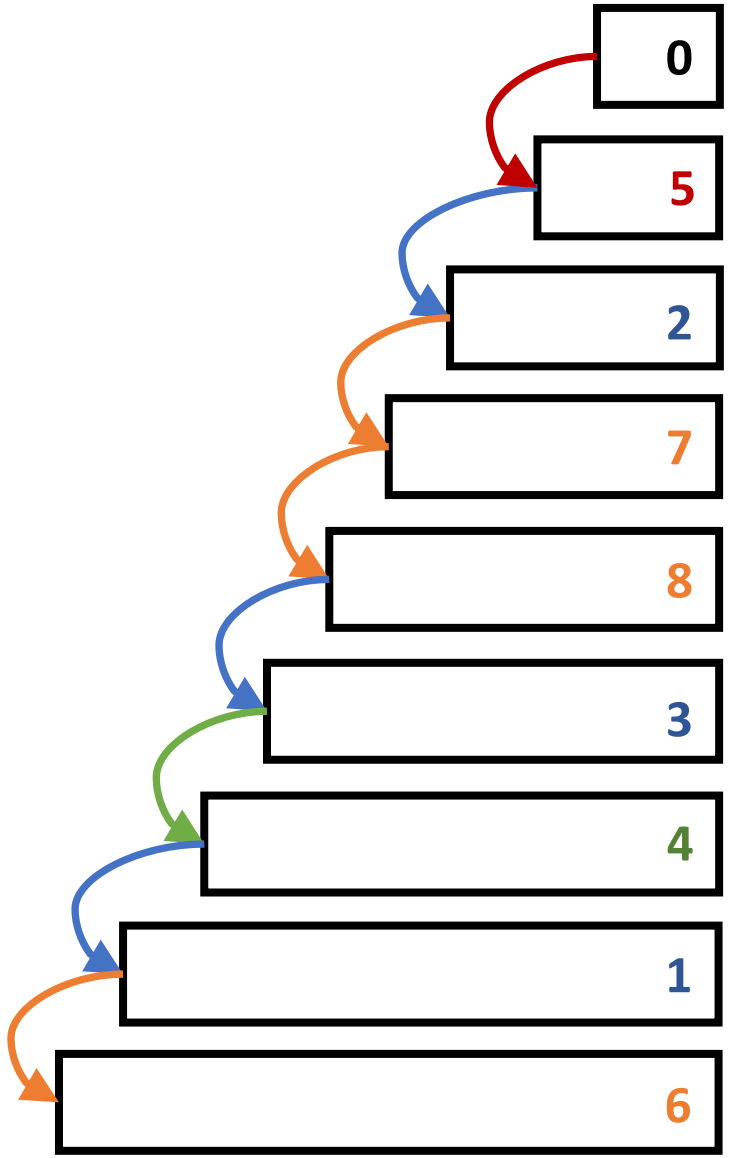

Representing a Sequence in Wheeler Graph

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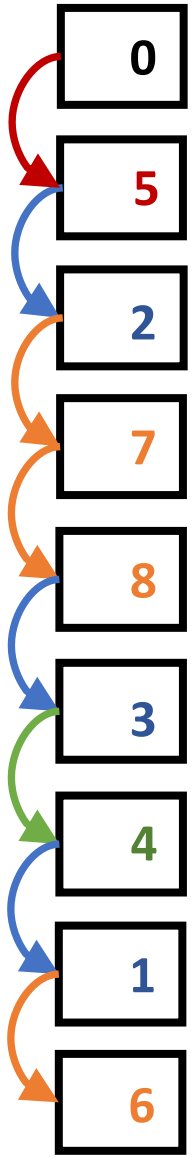
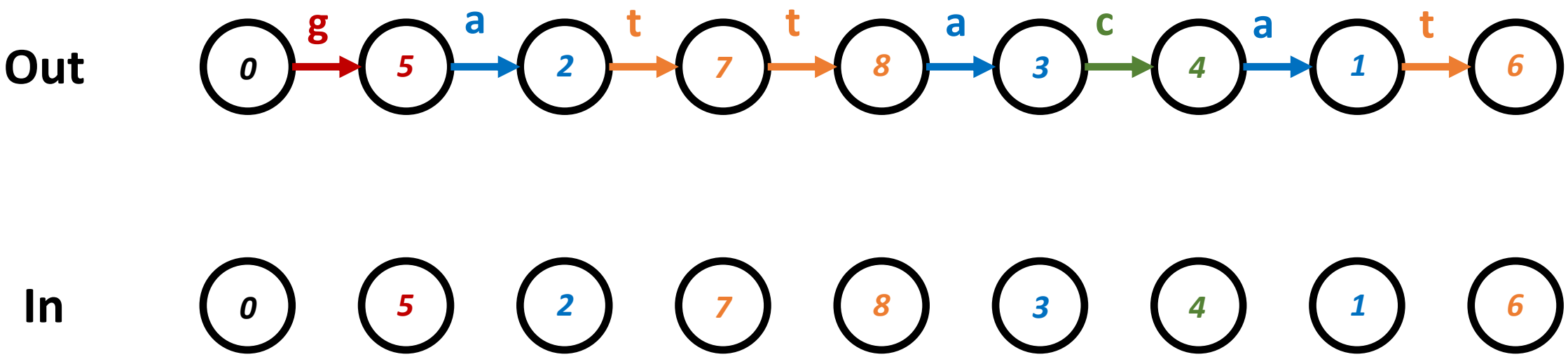


Visualizer: Bipartite WG Representation

T: ∈gattacat



Visualizer: Bipartite WG Representation

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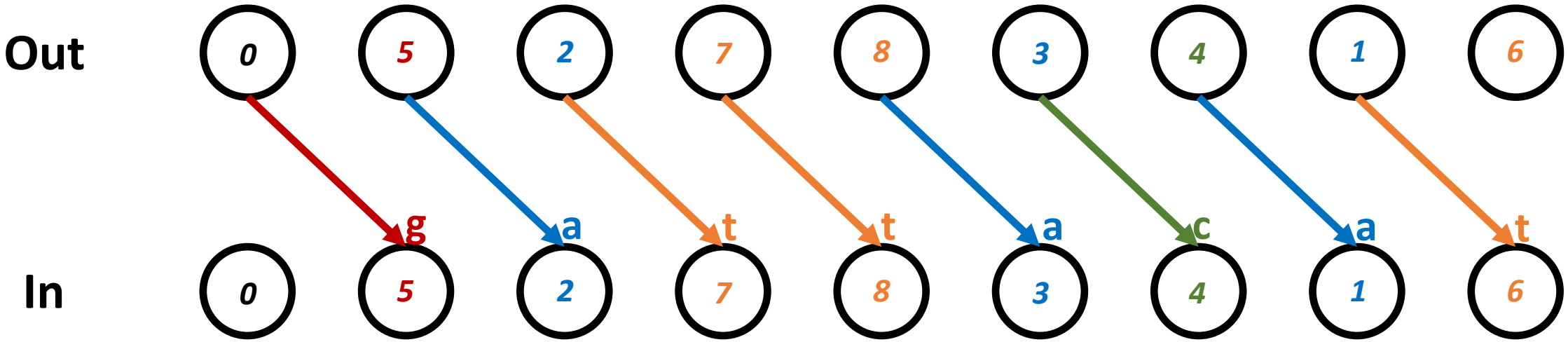

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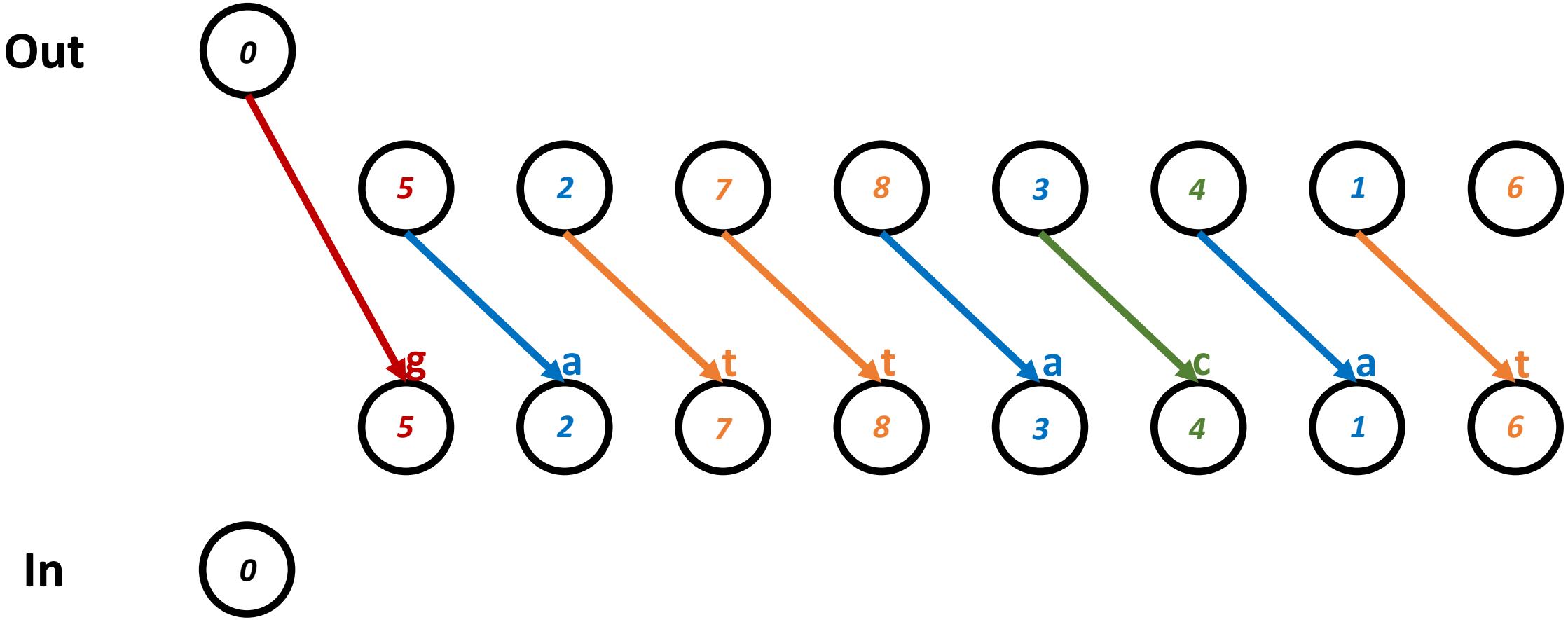

Visualizer: Bipartite WG Representation

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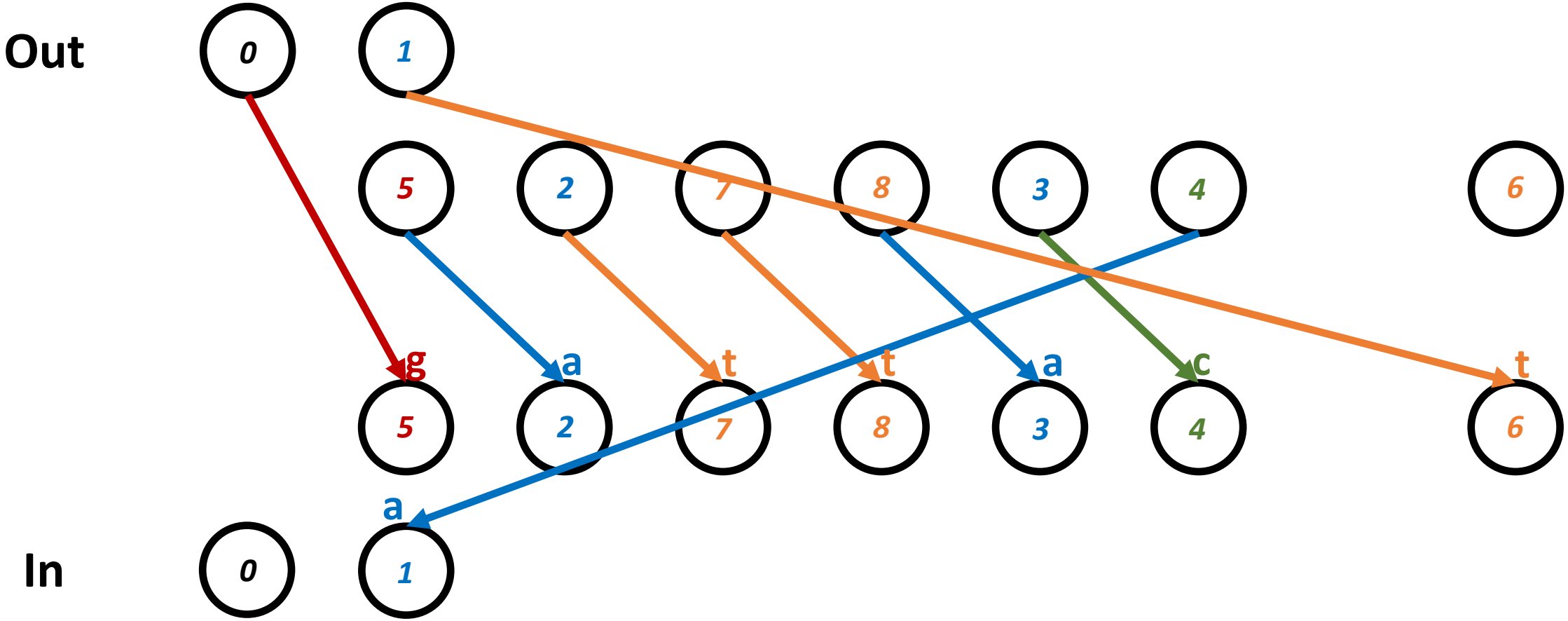

Visualizer: Bipartite WG Representation

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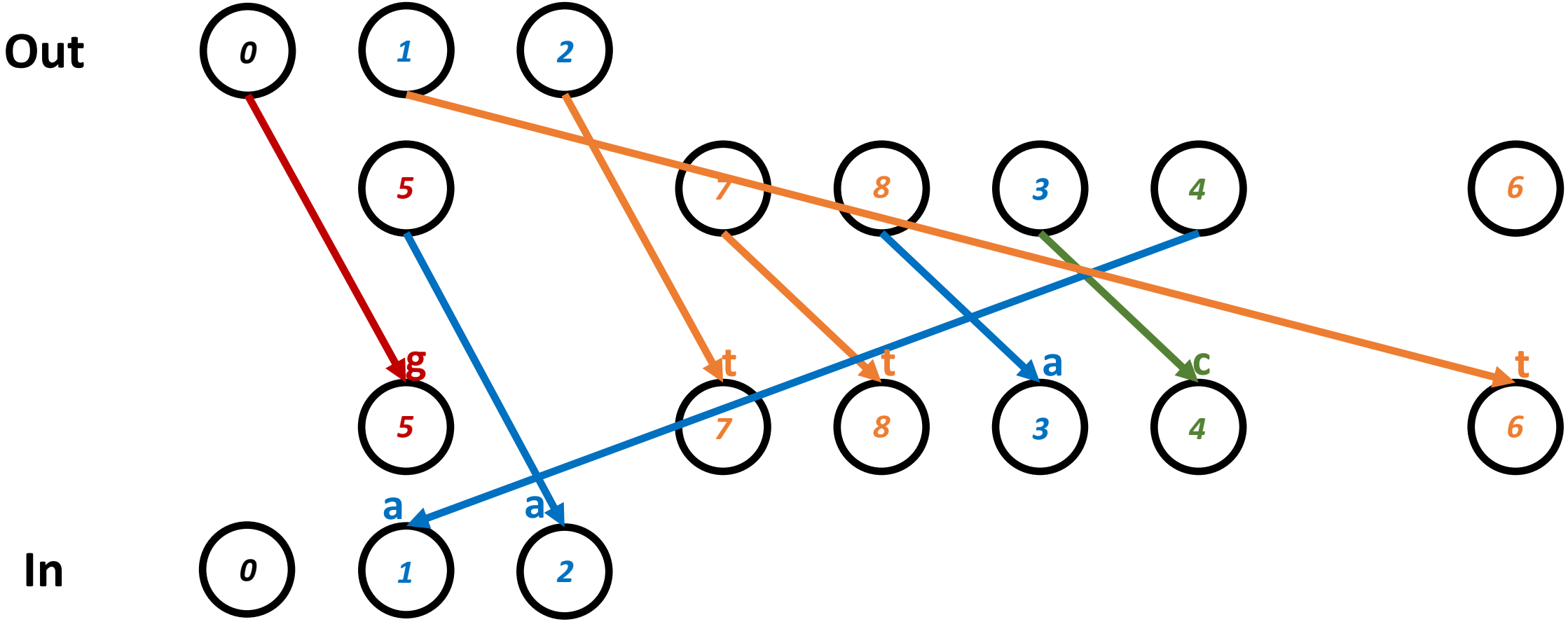

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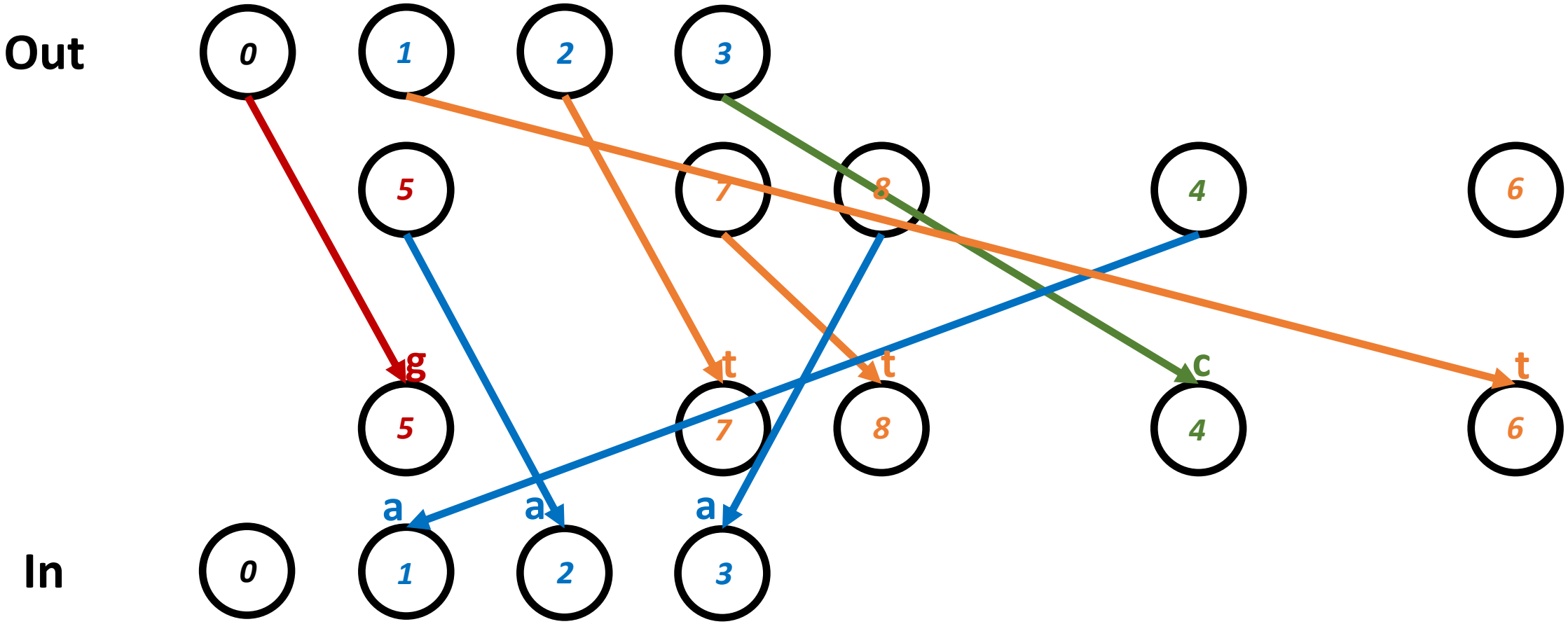

Visualizer: Bipartite WG Representation

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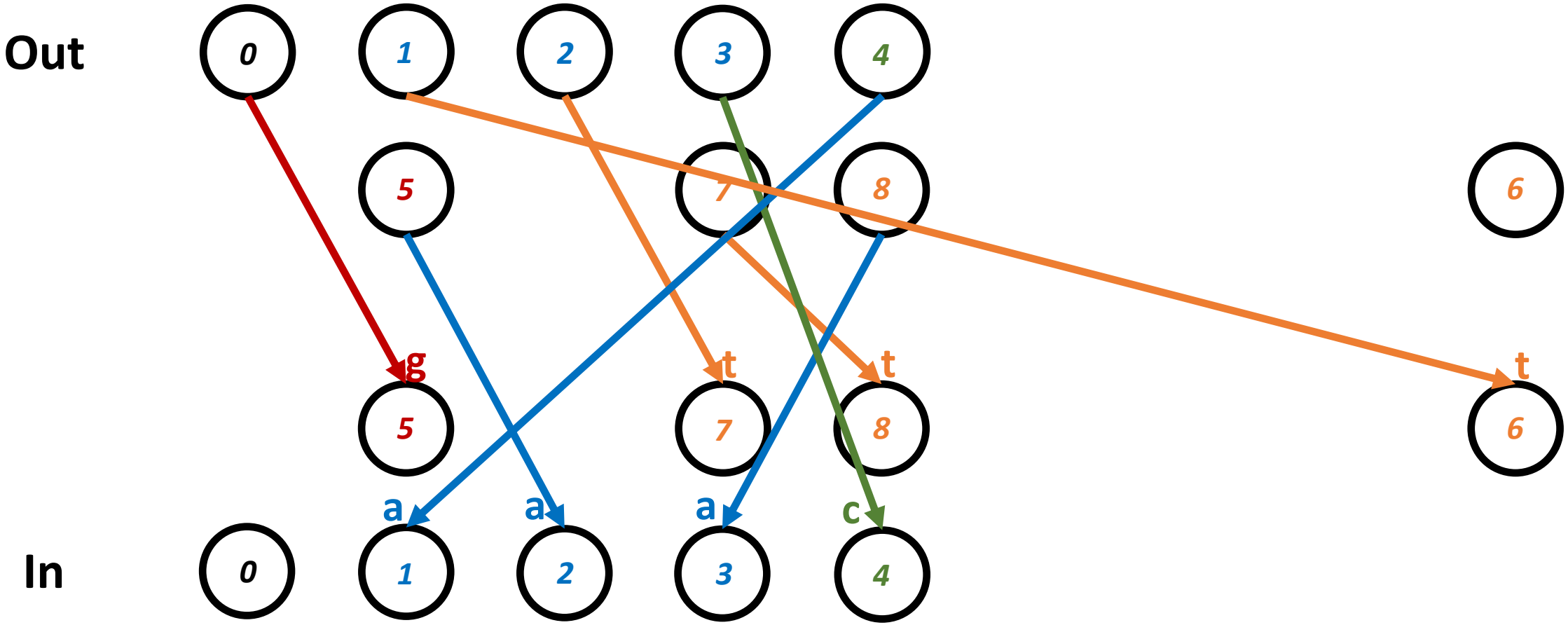
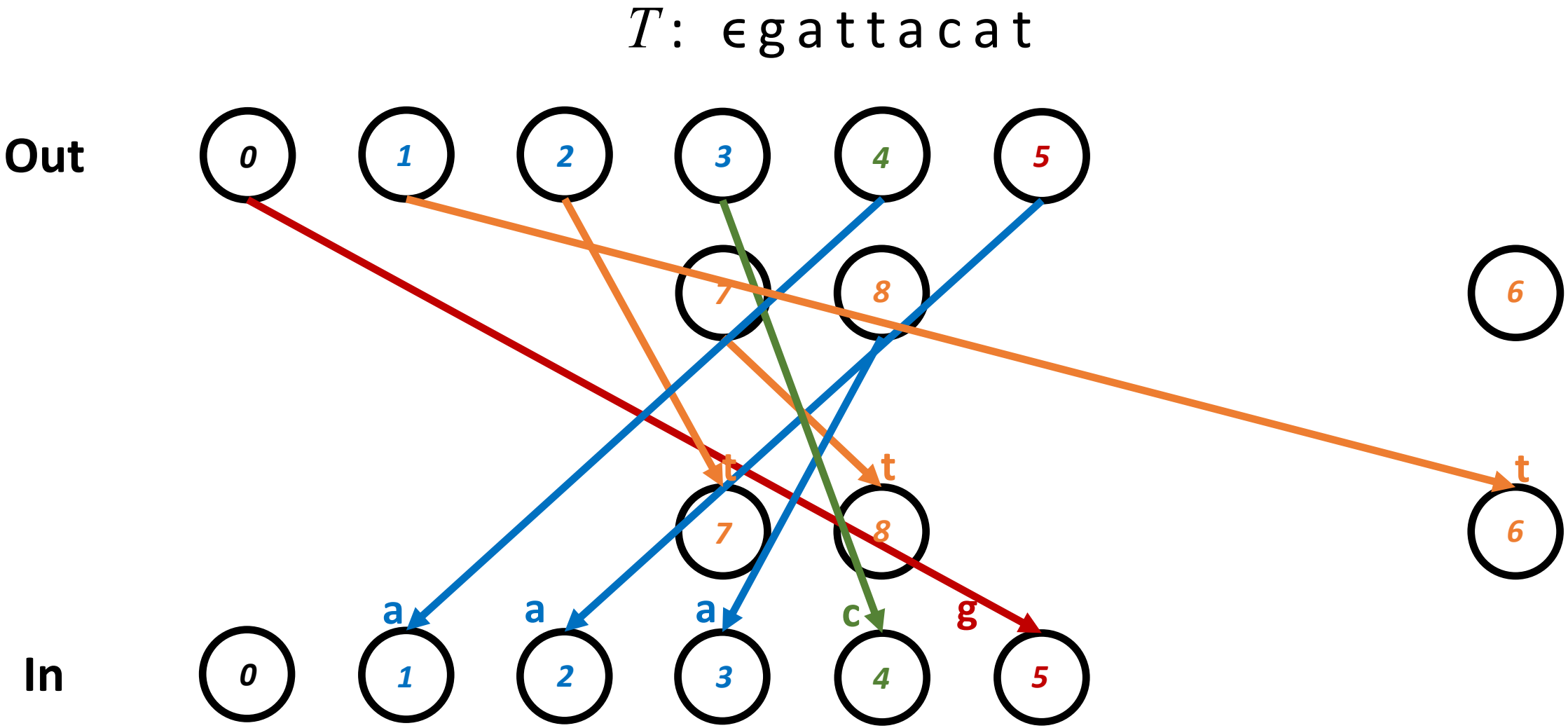
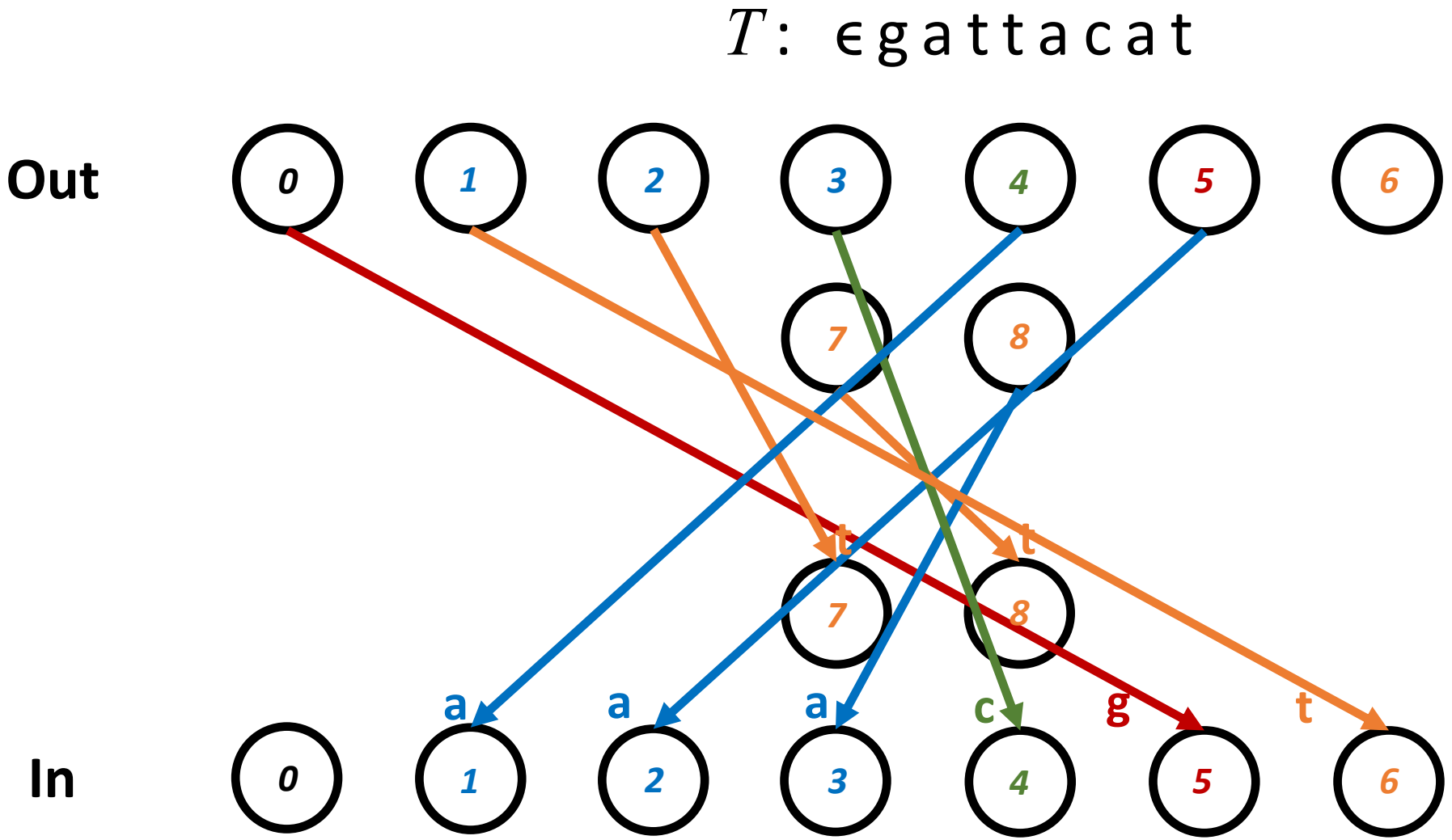


Visualizer: Bipartite WG Representation

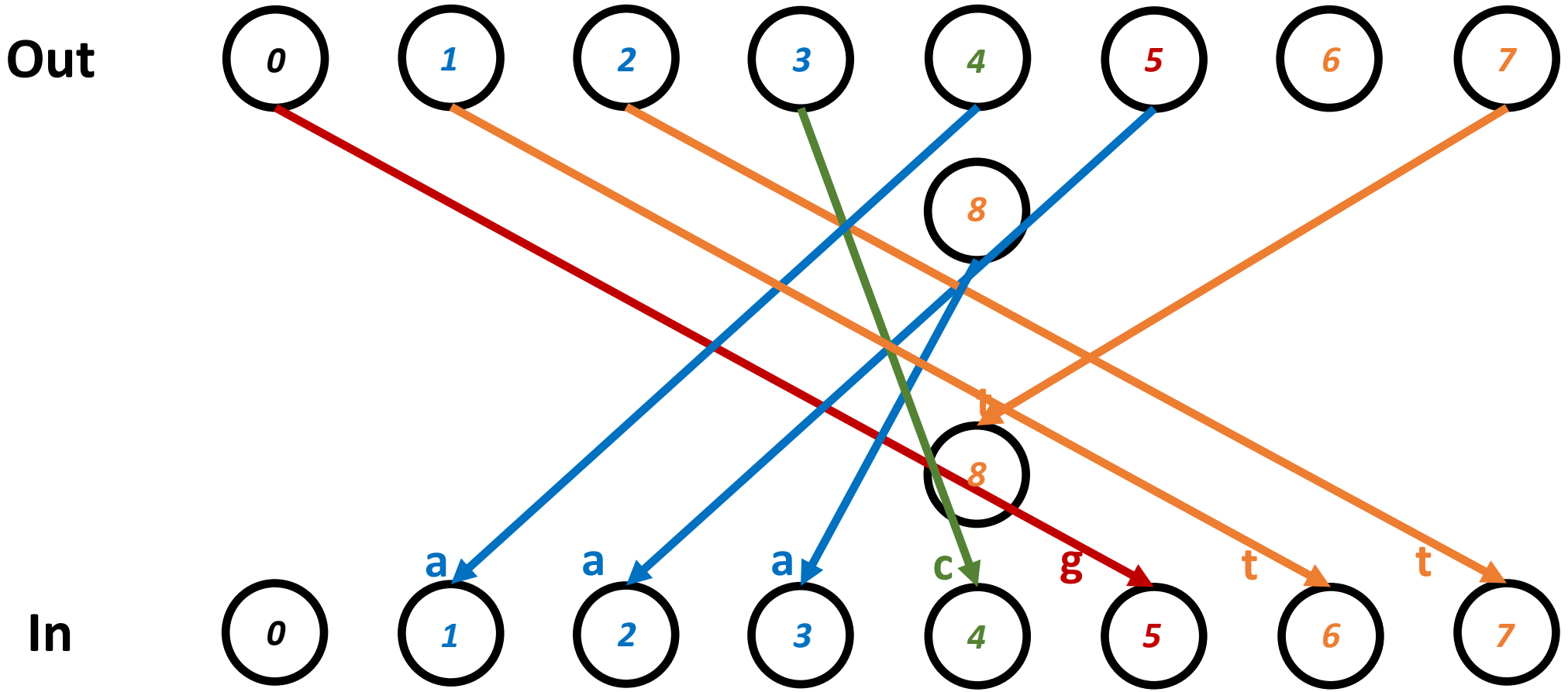


Visualizer: Bipartite WG Representation



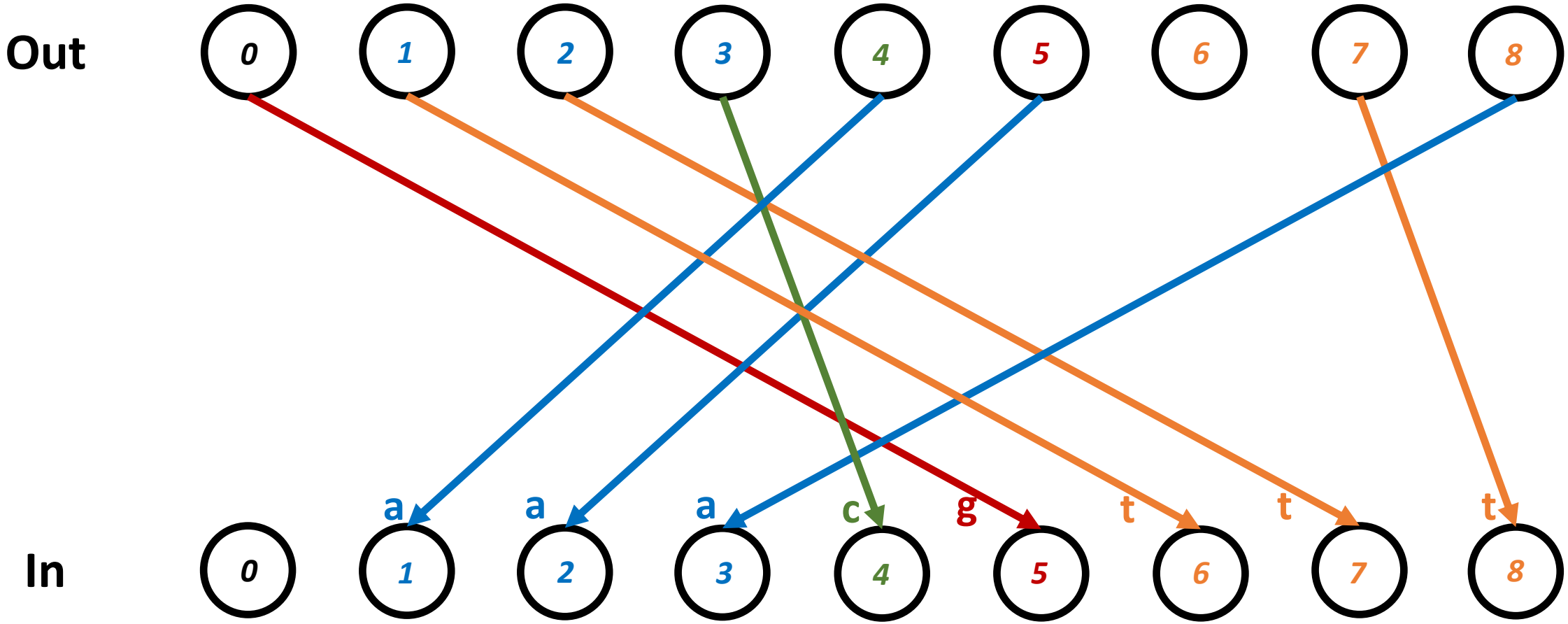
Visualizer: Bipartite WG Representation

T: ϵgattacat

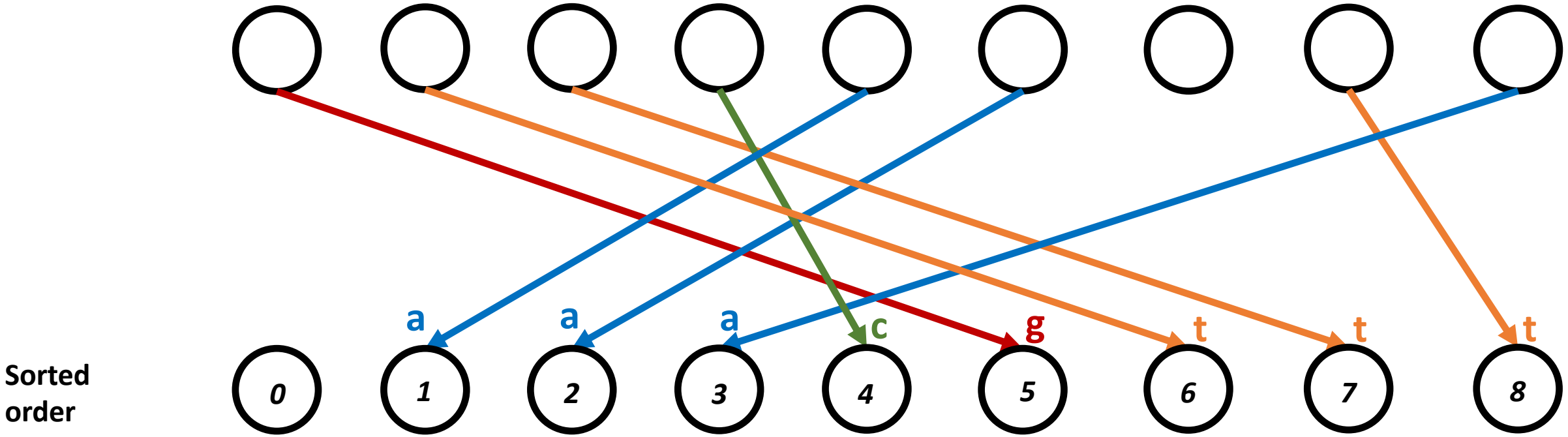


Visualizer: Bipartite WG Representation

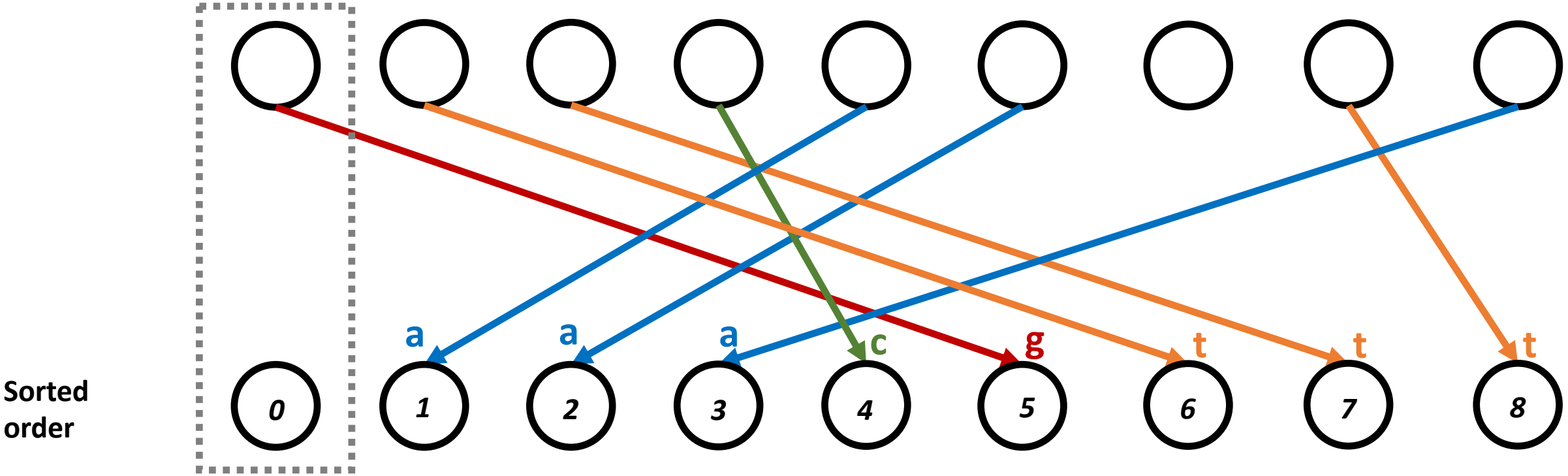
T: ϵ g a t t a c a t



Wheeler Graph Definition

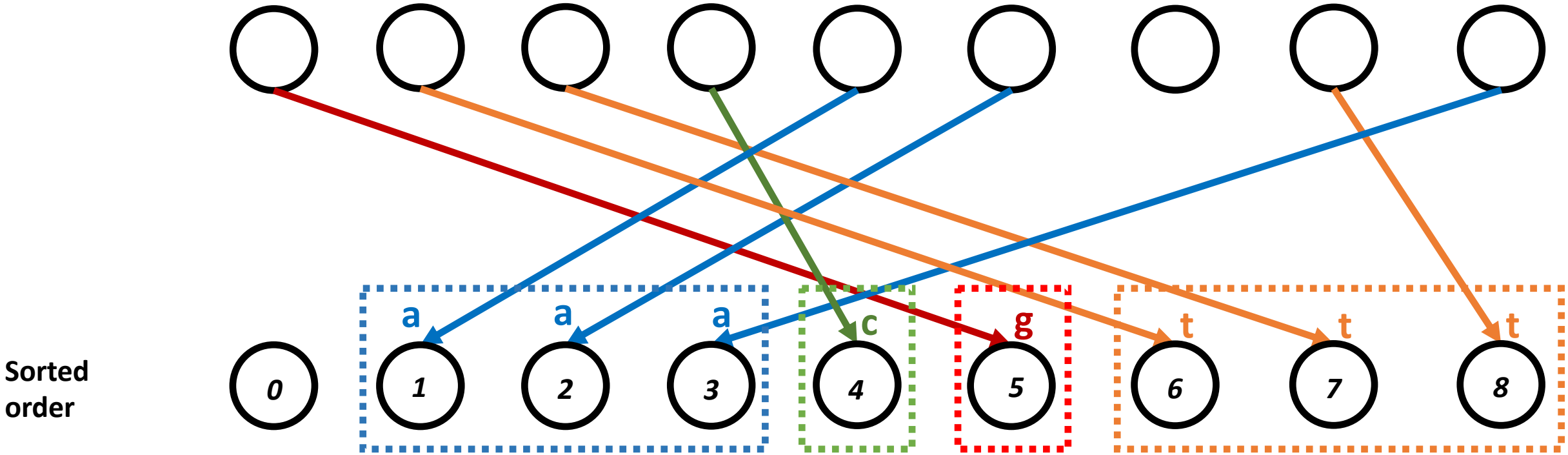


Wheeler Graph Definition

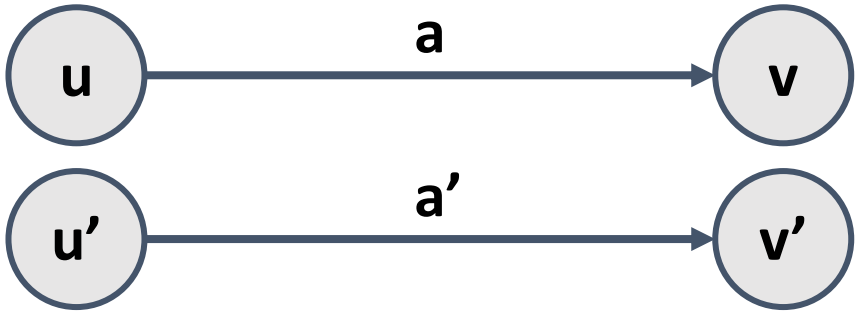


- 1. Node with indegree 0 comes before every other nodes.

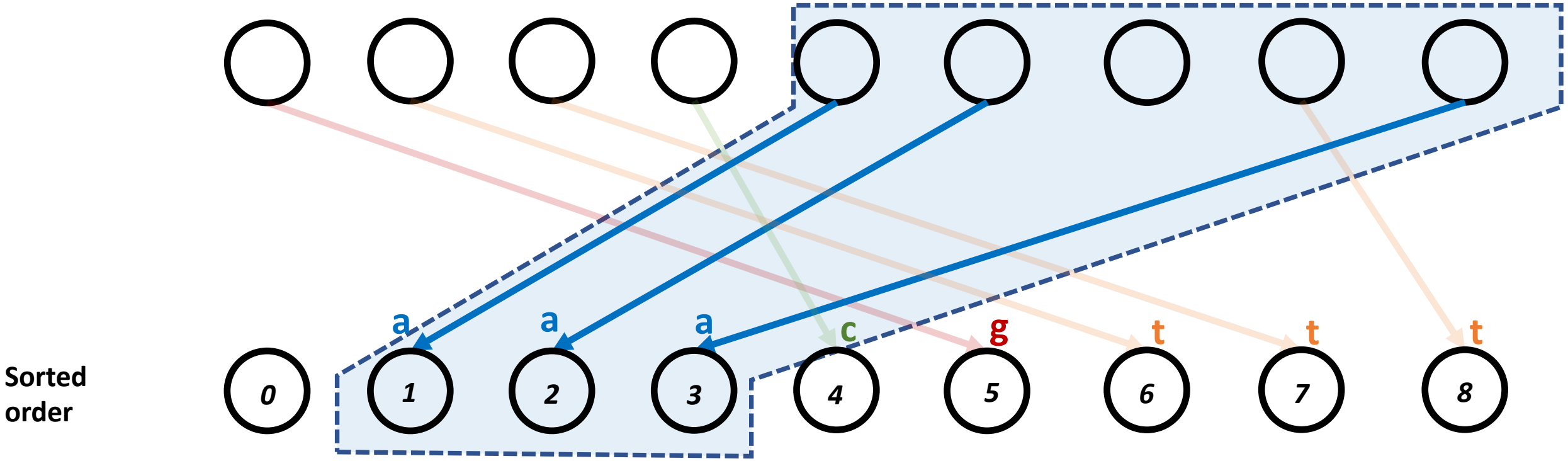
Wheeler Graph Definition



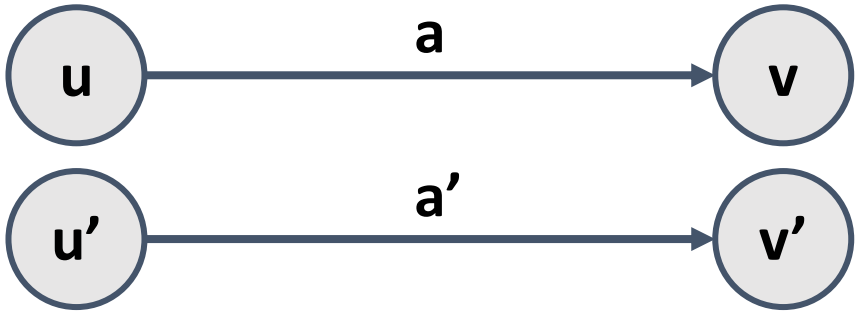
1. Node with indegree 0 comes before every other nodes.
2. $a \prec a' \implies v < v'$



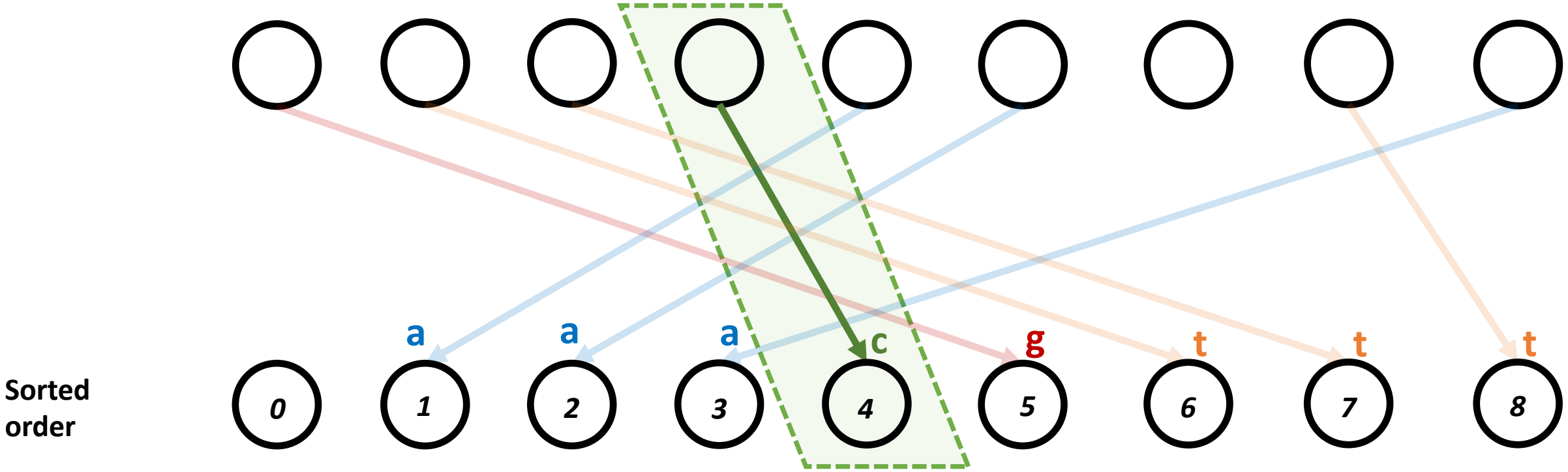
Wheeler Graph Definition



1. Node with indegree 0 comes before every other nodes.
2. $a \prec a' \implies v < v'$
3. $(a = a') \wedge (u < u') \implies v \leq v'$



Wheeler Graph Definition



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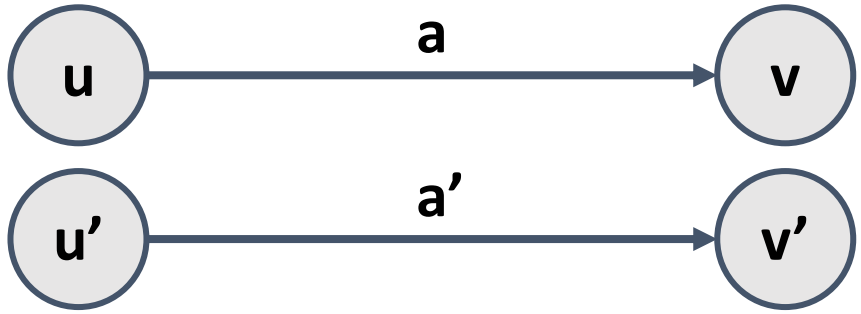
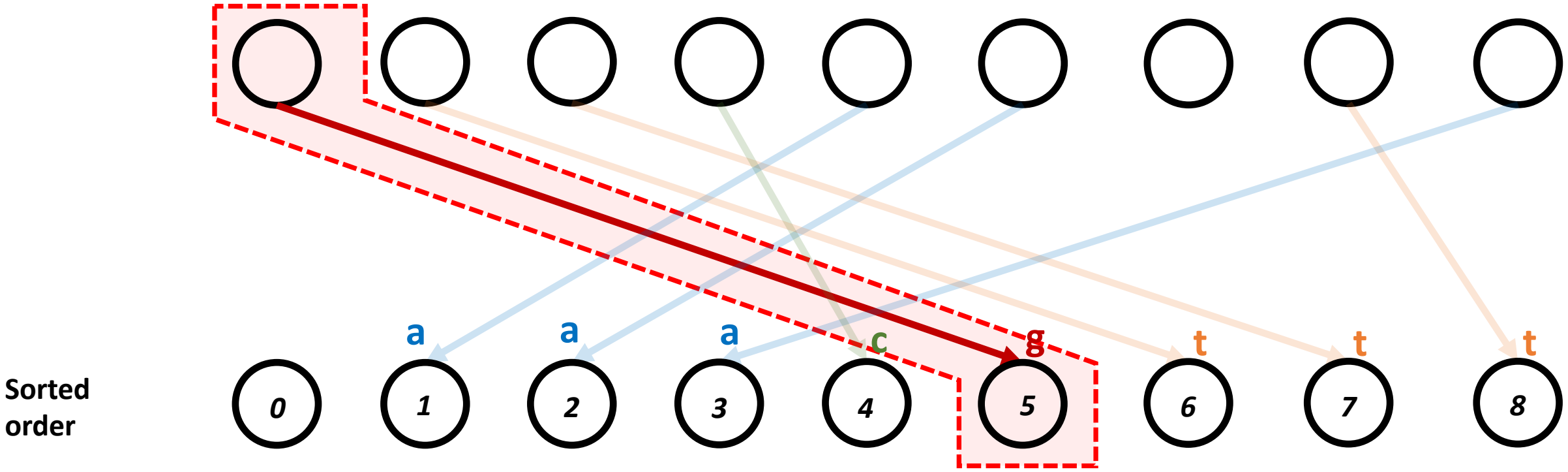


Wheeler Graph Definition



1. Node with indegree 0 comes before every other nodes.
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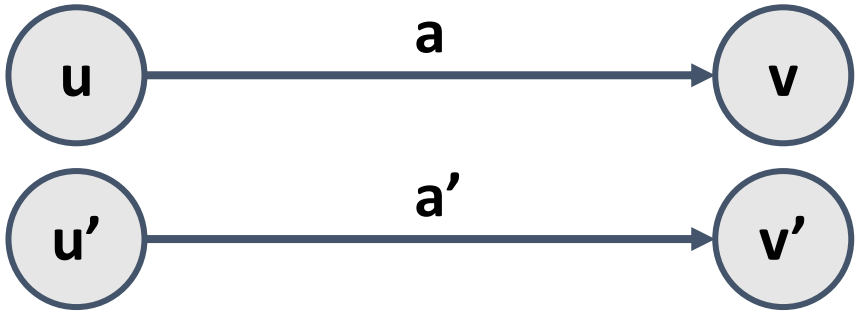

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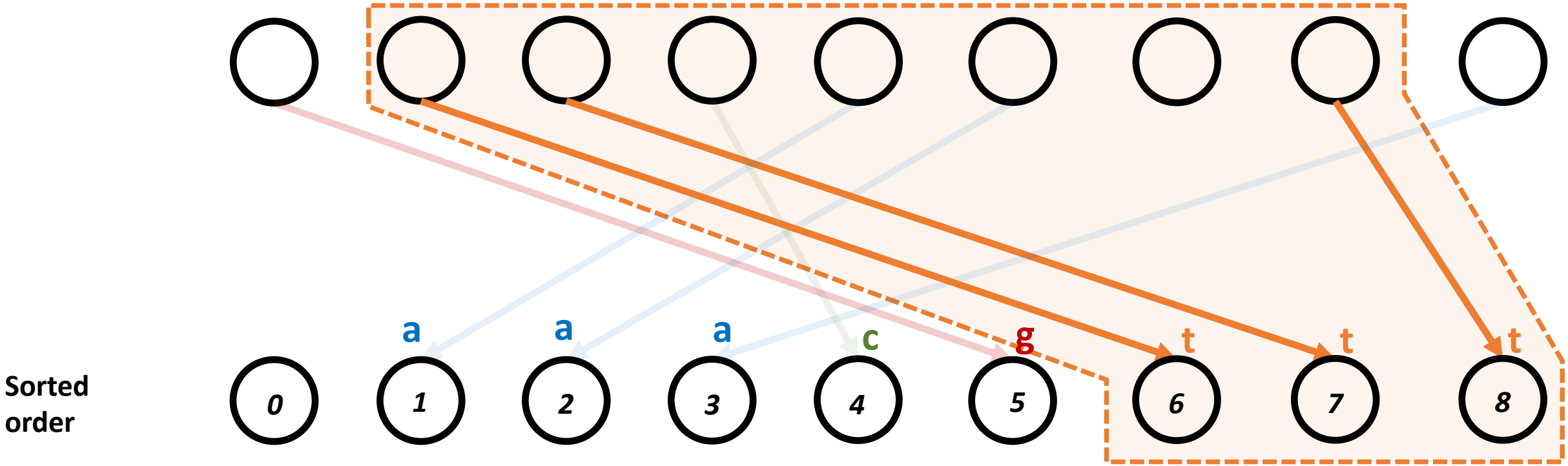

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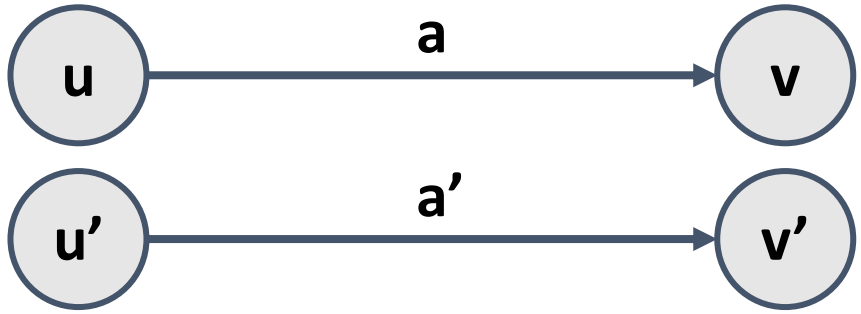

Wheeler Graph: beyond Definition

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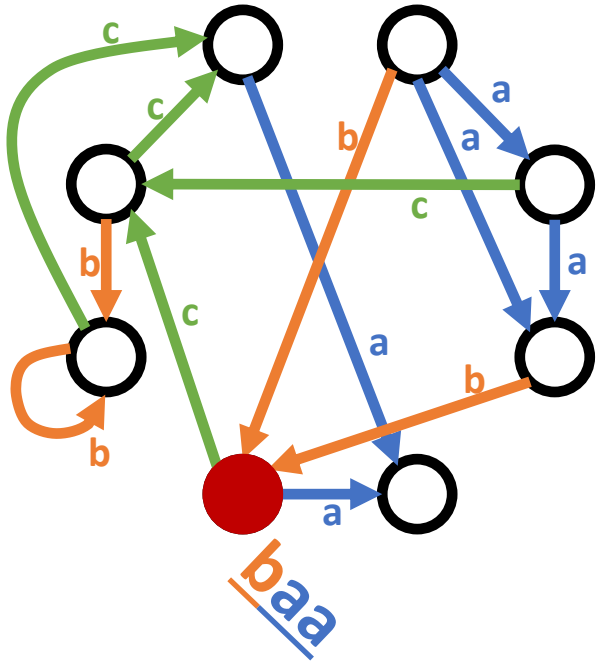

- Mathematical rules of
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Wheeler graphs: A framework for BWT-based data structures ☆

Travis Gagie [a], Giovanni Manzini [b,c,*], Jouni Sirén [d]

2017

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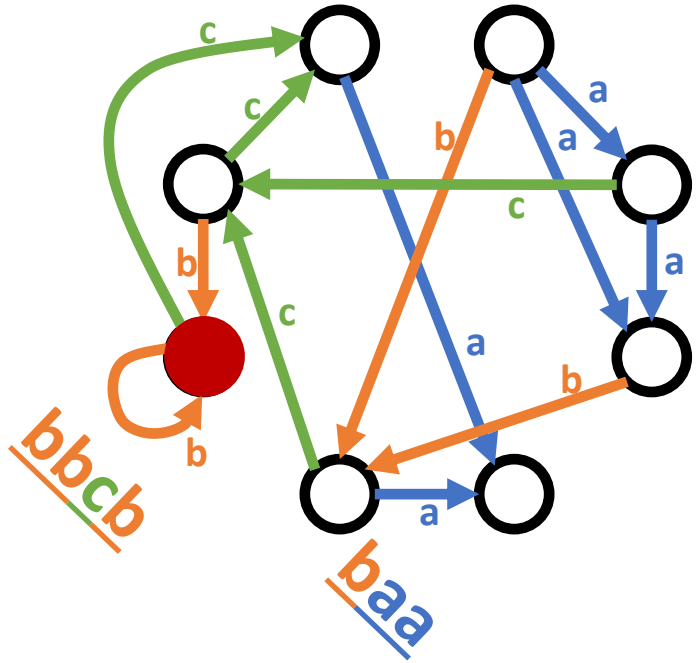

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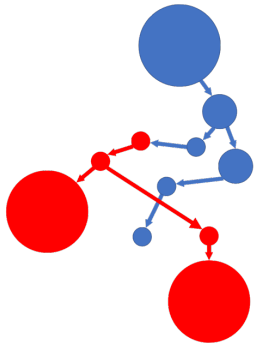
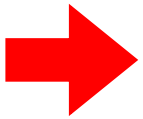
Our Contribution



WGT
Wheeler Graph Toolkit



- ***A Wheeler graph visualizer: bipartite representation***

- Implemented the first Wheeler graph *recognizer*

- Wheeler graph *generators*: Random WG / Trie / DBG / RDG

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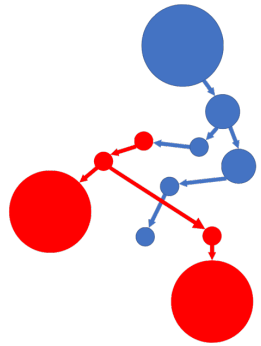

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IEEE/ACM TRANSACTIONS ON COMPUTATIONAL BIOLOGY AND BIOINFORMATICS, VOL. 11, NO. 2, MARCH/APRIL 2014

Indexing Graphs for Path Queries with Applications in Genome Research

Jouni Sirén, Niko Välimäki, and Veli Mäkinen 2014

De Bruijn Graph

=> All are WG ✅

GCSA Reverse deterministic graph

=> Not always WG ⛔

(1) genome coordinates are collapsed.

De Bruijn Graph

K = 4

GACGTA-CTG

GACGTA---G

GATGTA-CTG

GAC-TACCTG

De Bruijn Graph

K = 4

```
GACGTA-CTG
GACGTA---G
GATGTA-CTG
GAC-TACCTG
```

Remove gap &
append $
at the end of the alignment

K = 4

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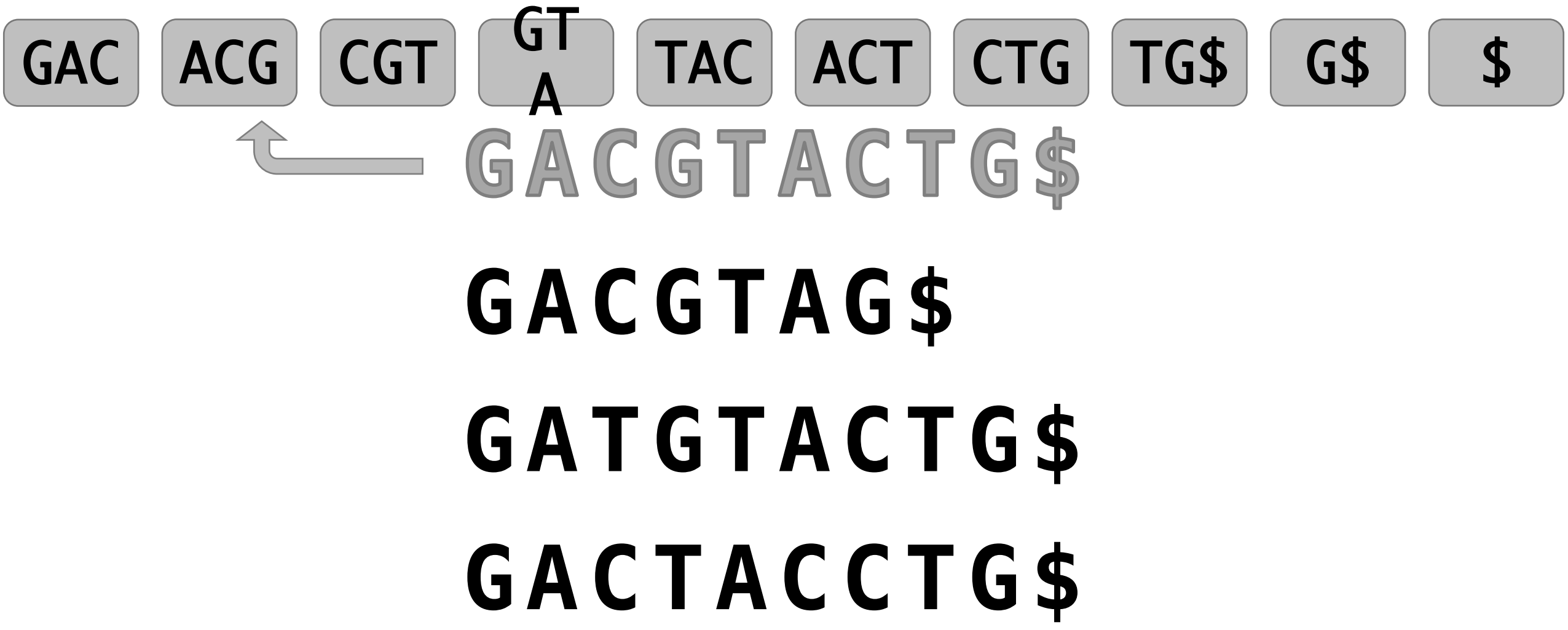

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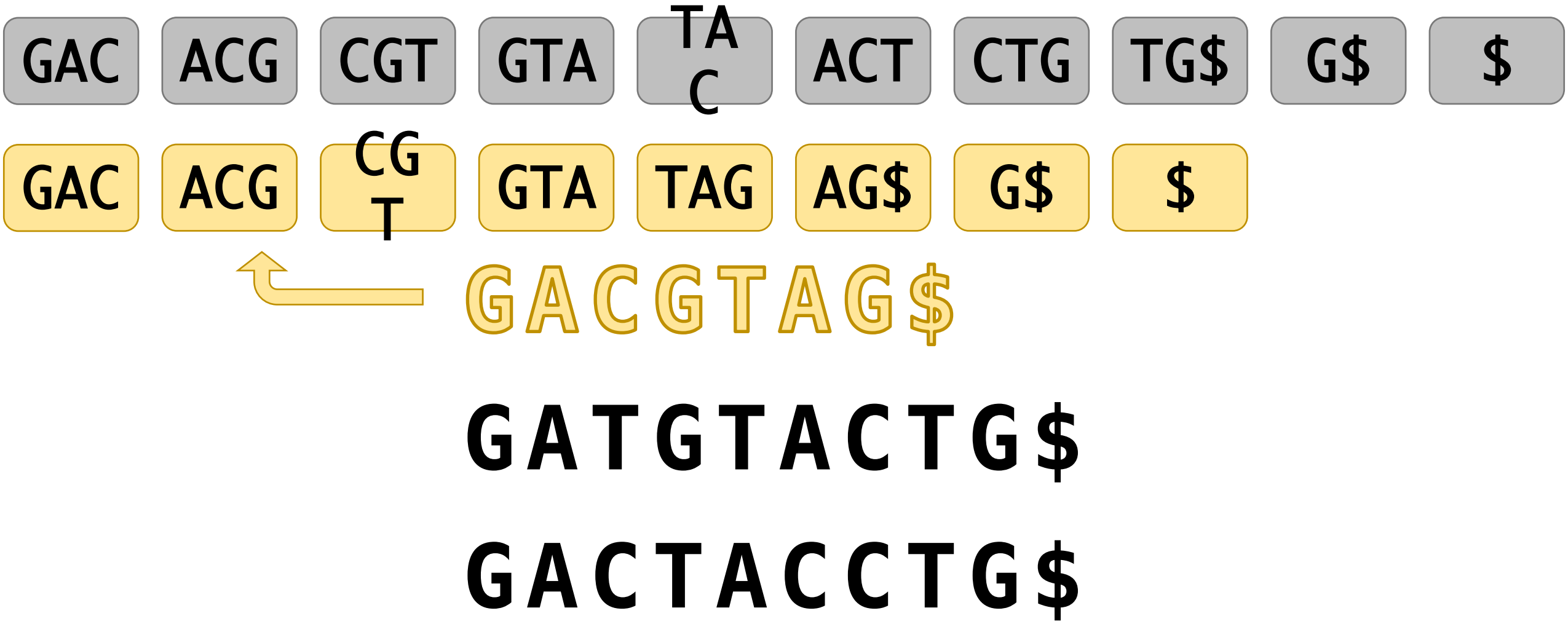

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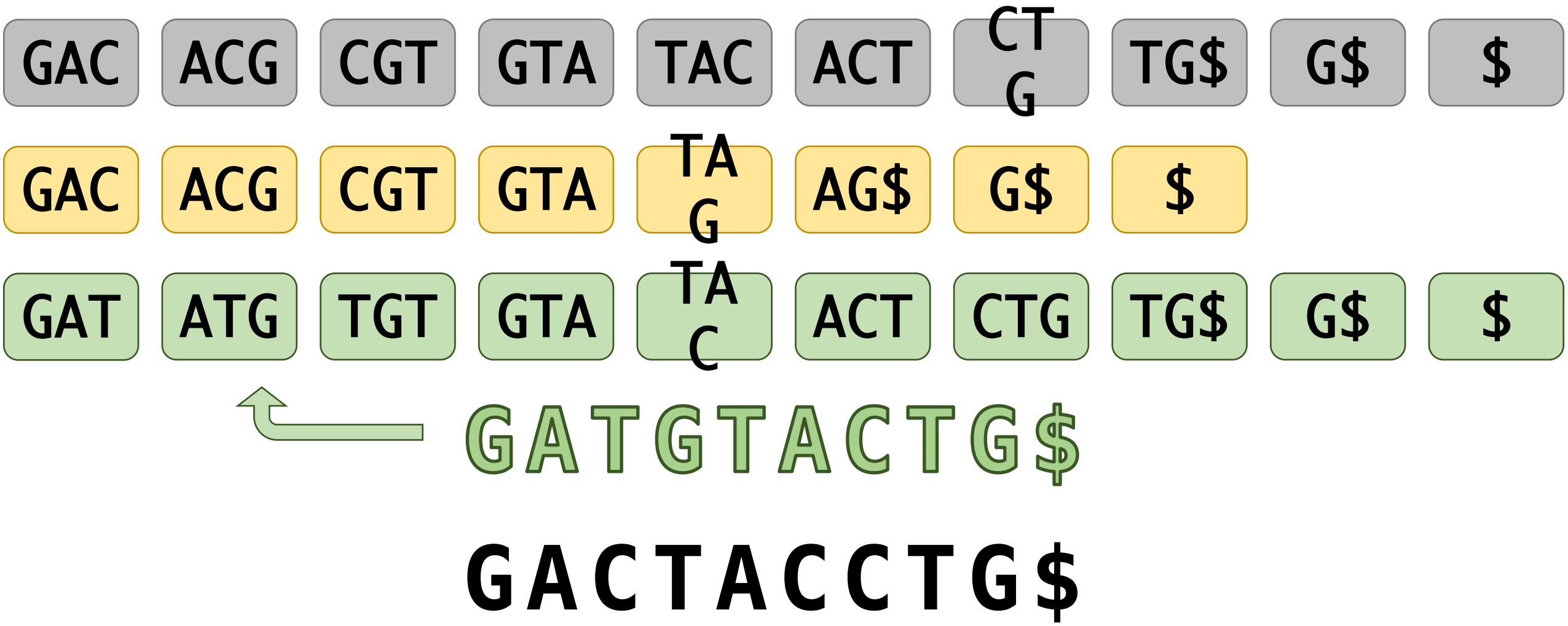

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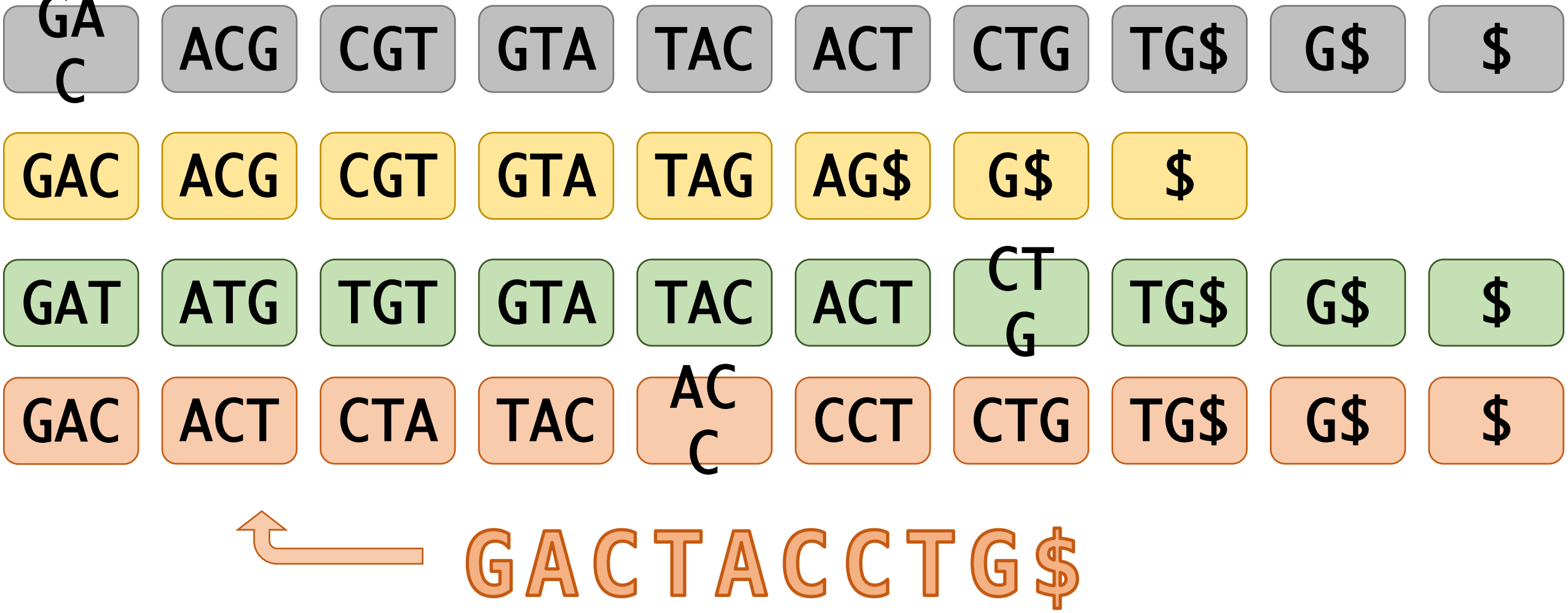

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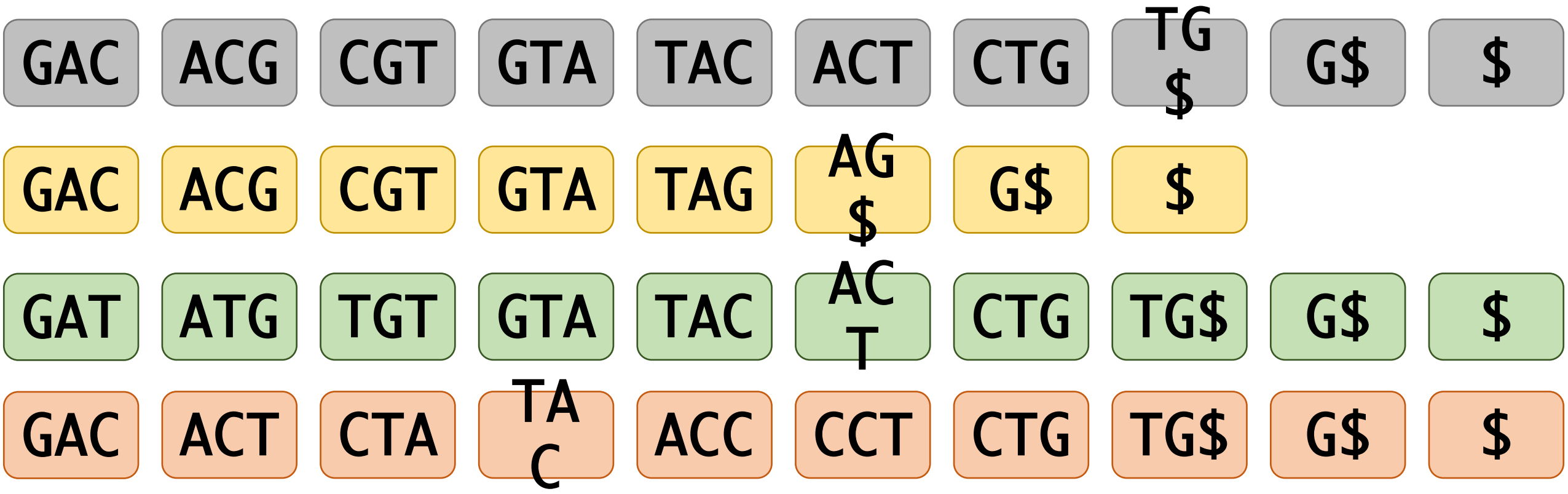

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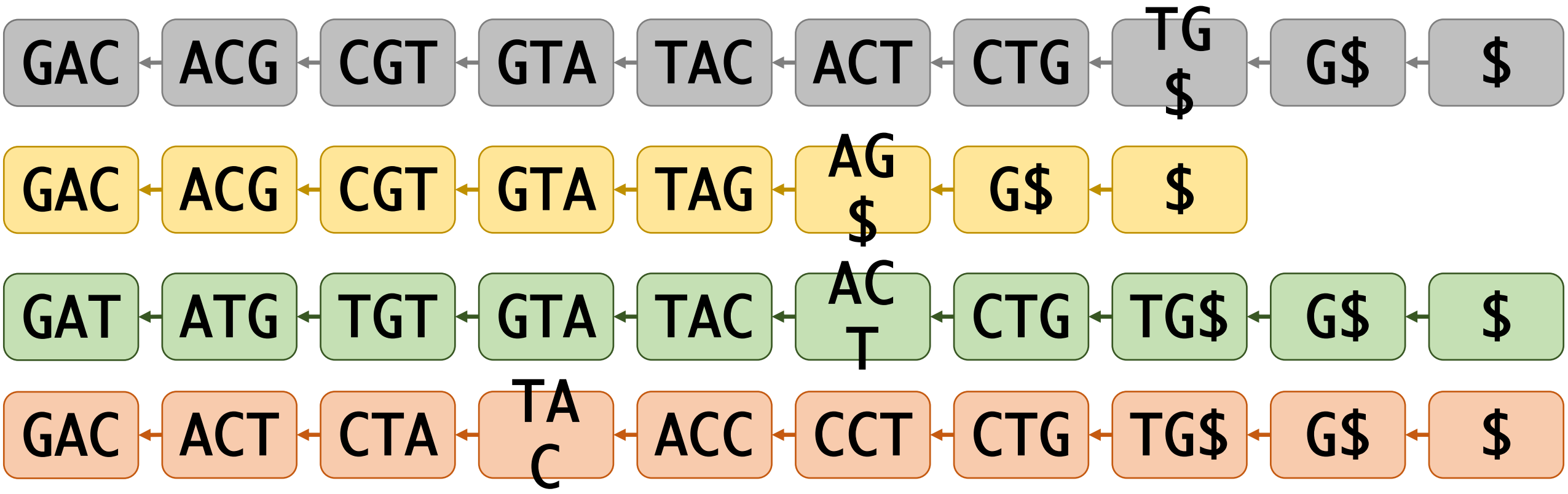

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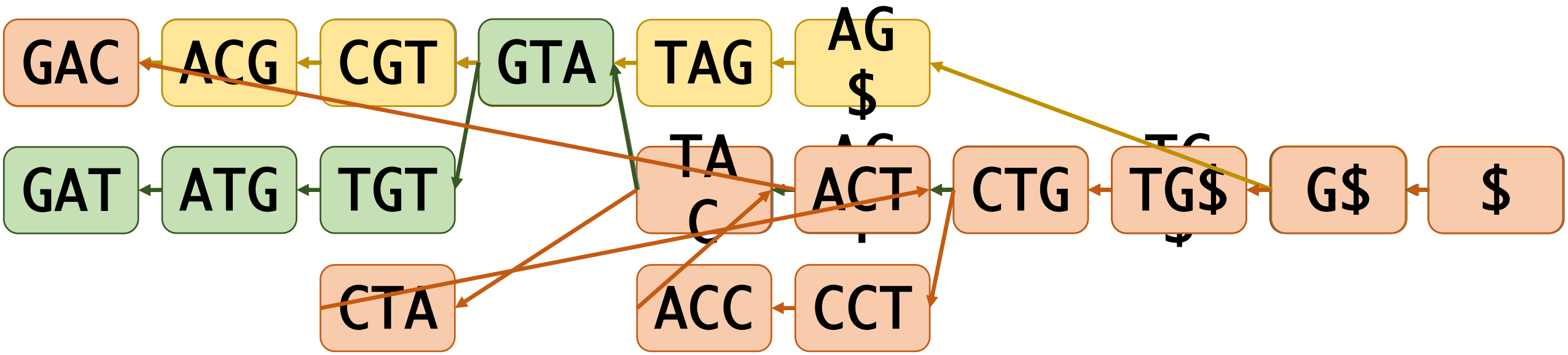

Genome coordinates are collapsed.

K = 4

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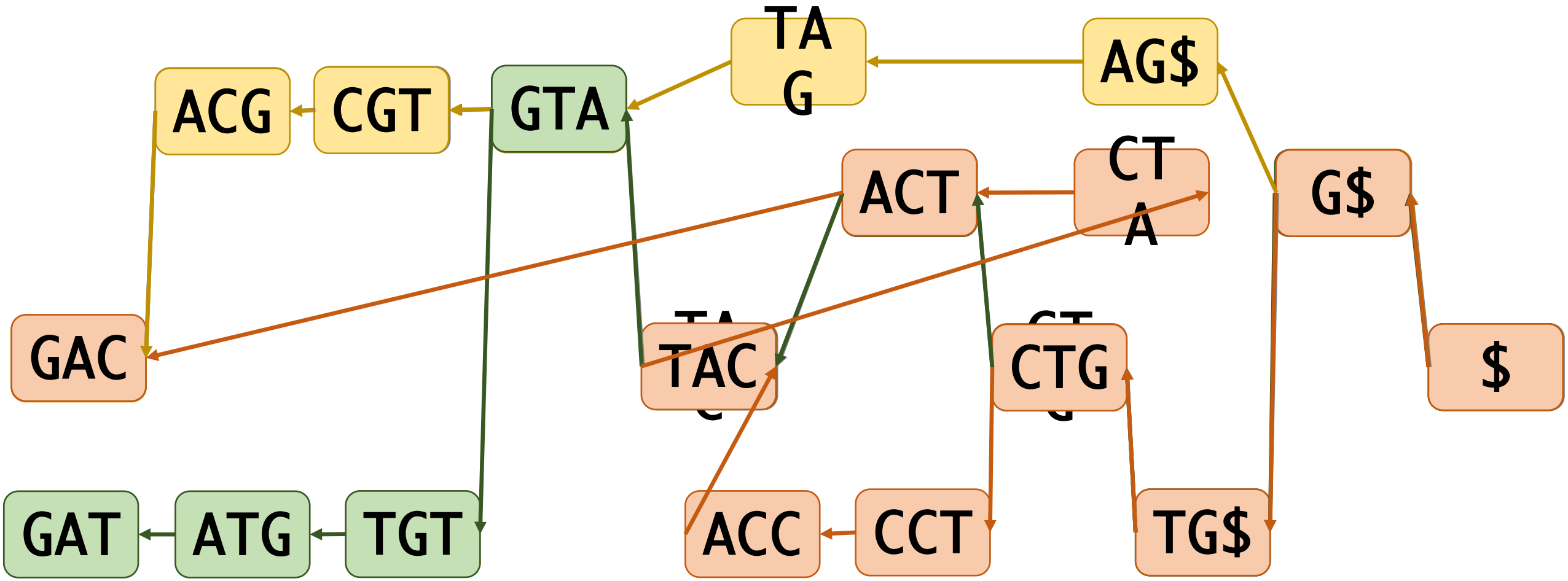

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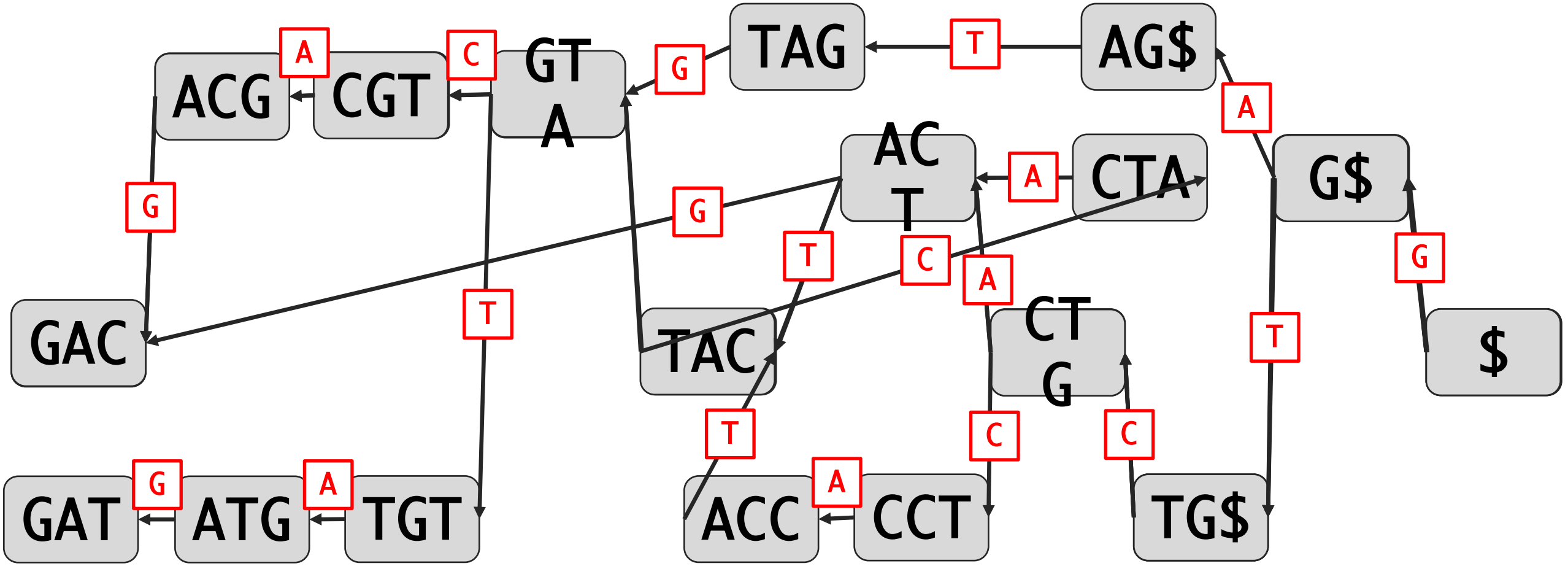

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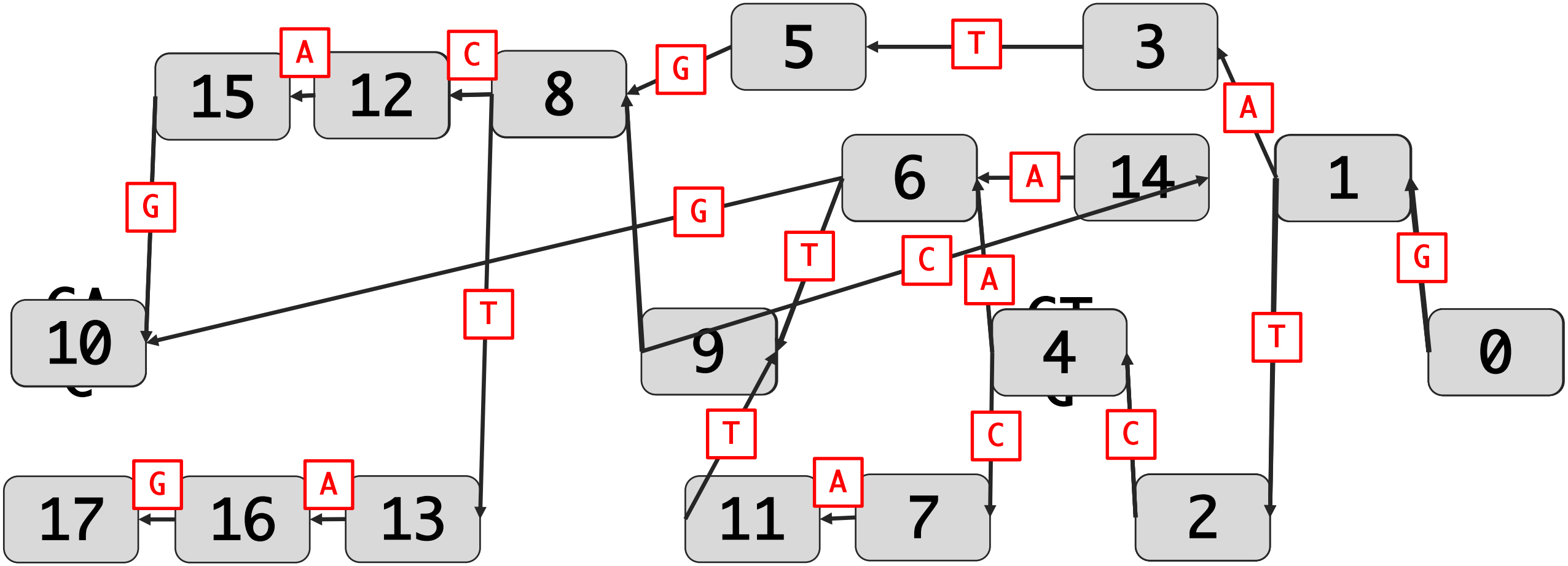


Genome coordinates are collapsed.

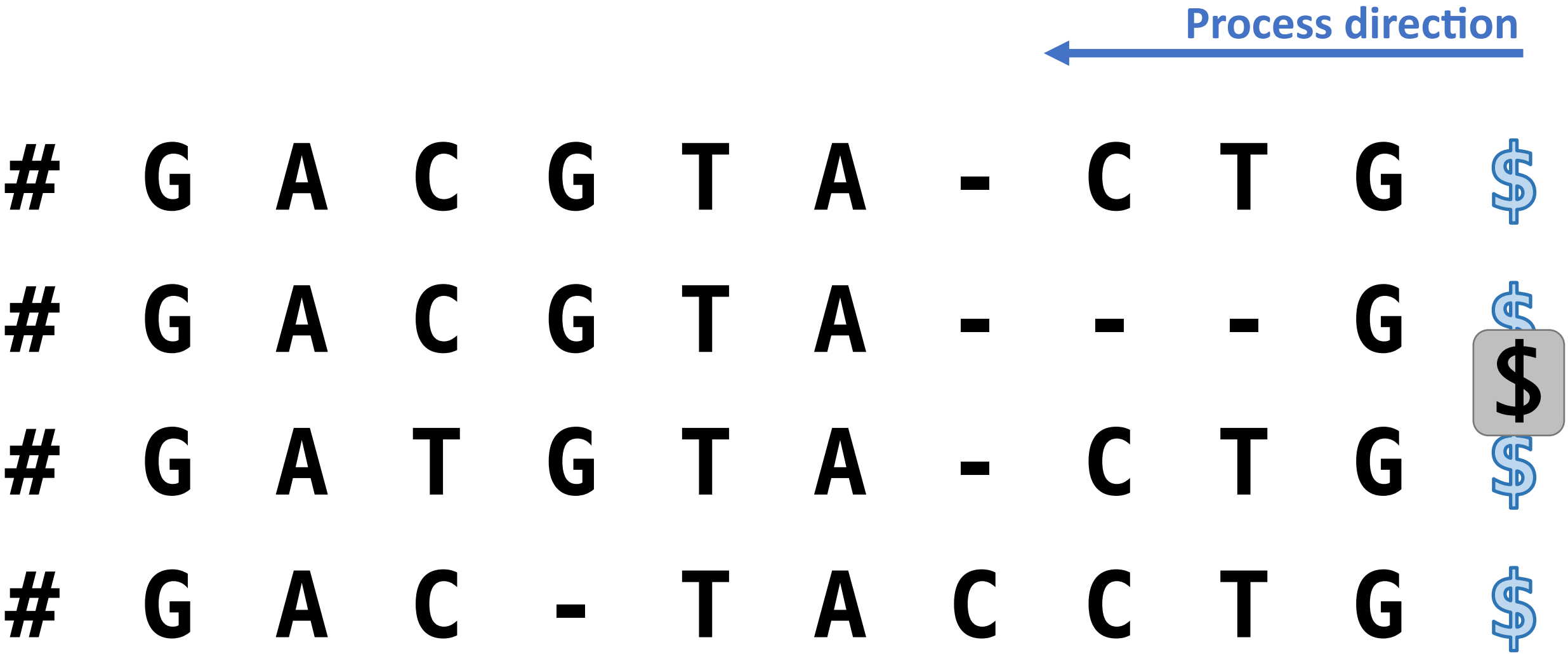
GCSA Reverse Deterministic Graph

```
G A C G T A - C T G
G A C G T A - - - G
G A T G T A - C T G
G A C - T A C C T G
```

GCSA Reverse Deterministic Graph


```
#  G  A  C  G  T  A  -  C  T  G  $
#  G  A  C  G  T  A  -  -  -  G  $
#  G  A  T  G  T  A  -  C  T  G  $
#  G  A  C  -  T  A  C  C  T  G  $
```

GCSA Reverse Deterministic Graph



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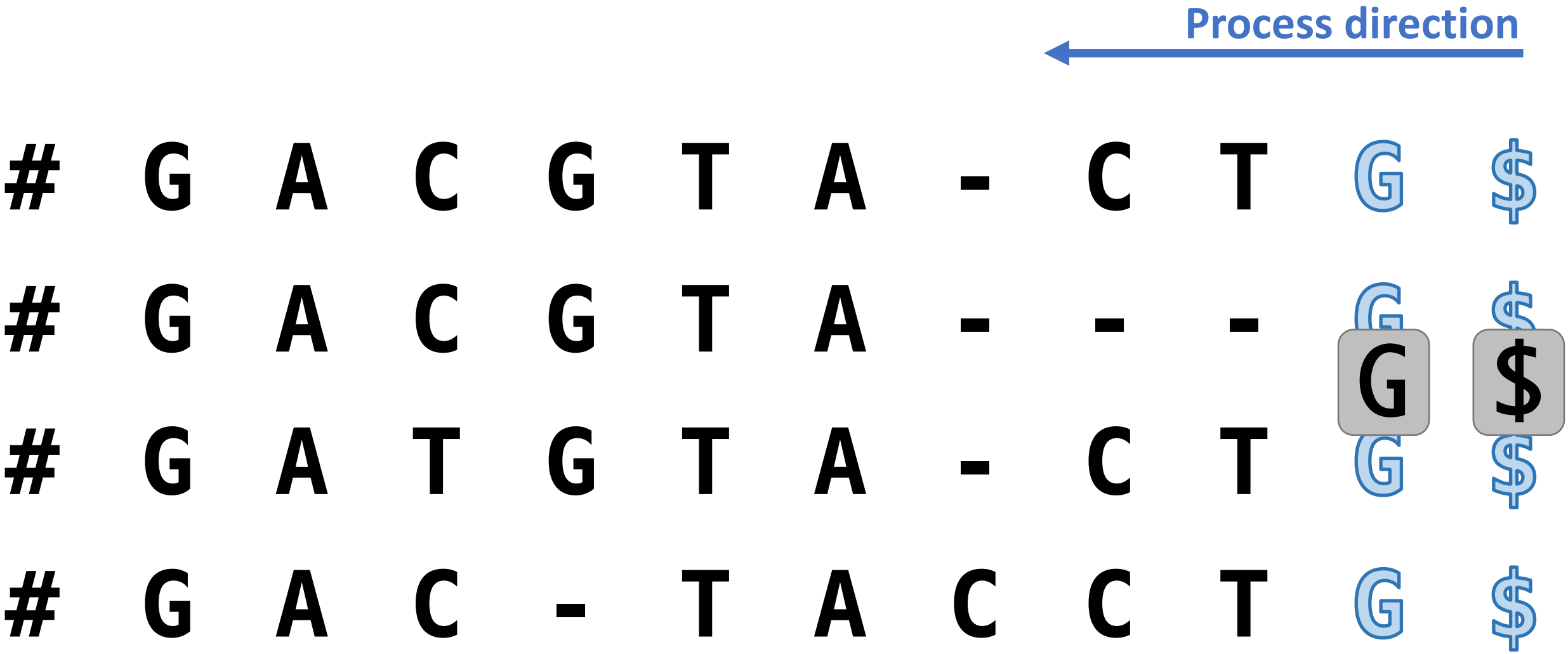

GCSA Reverse Deterministic Graph

Process direction

```
# G A C G T A - C T G $
# G A C G T A - - - G $
# G A T G T A - C T G $
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```

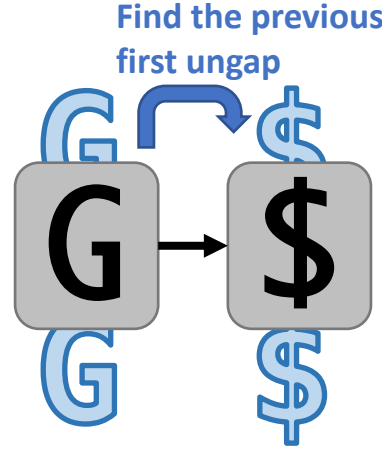

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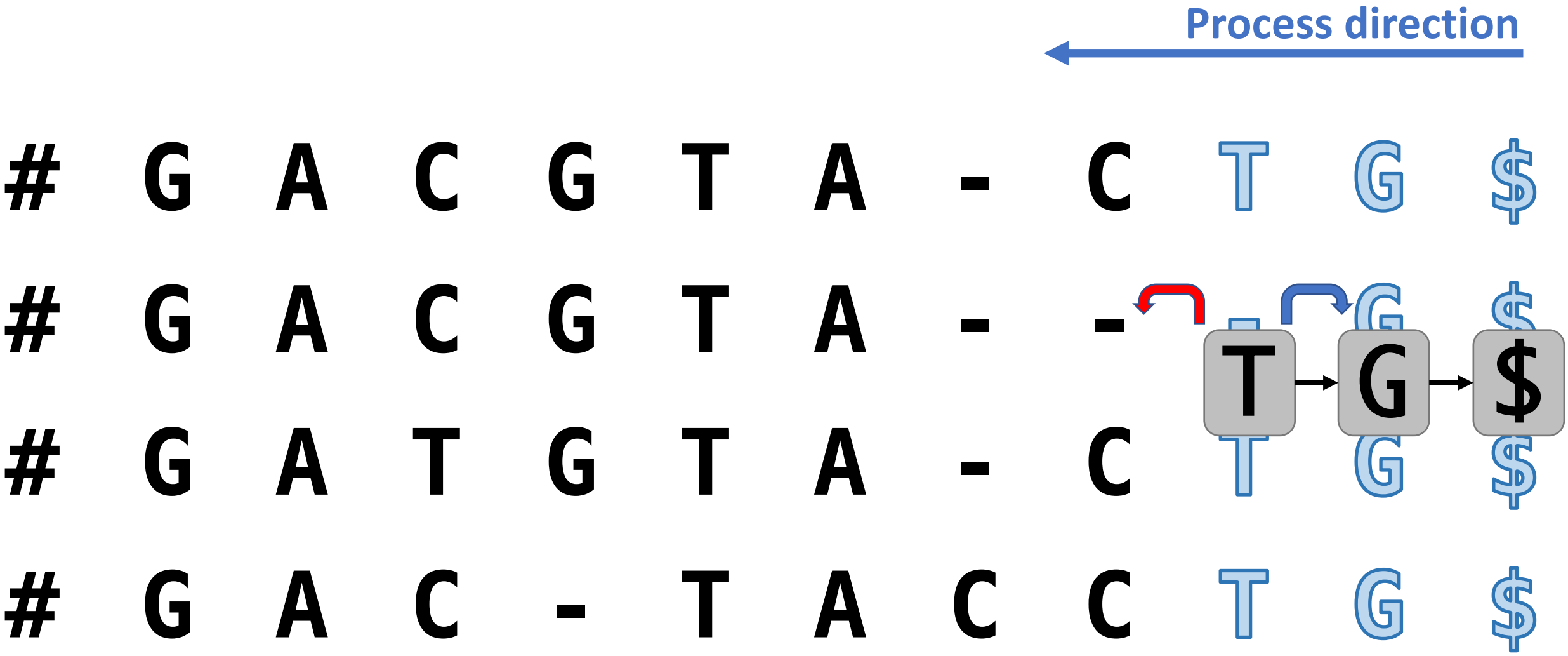

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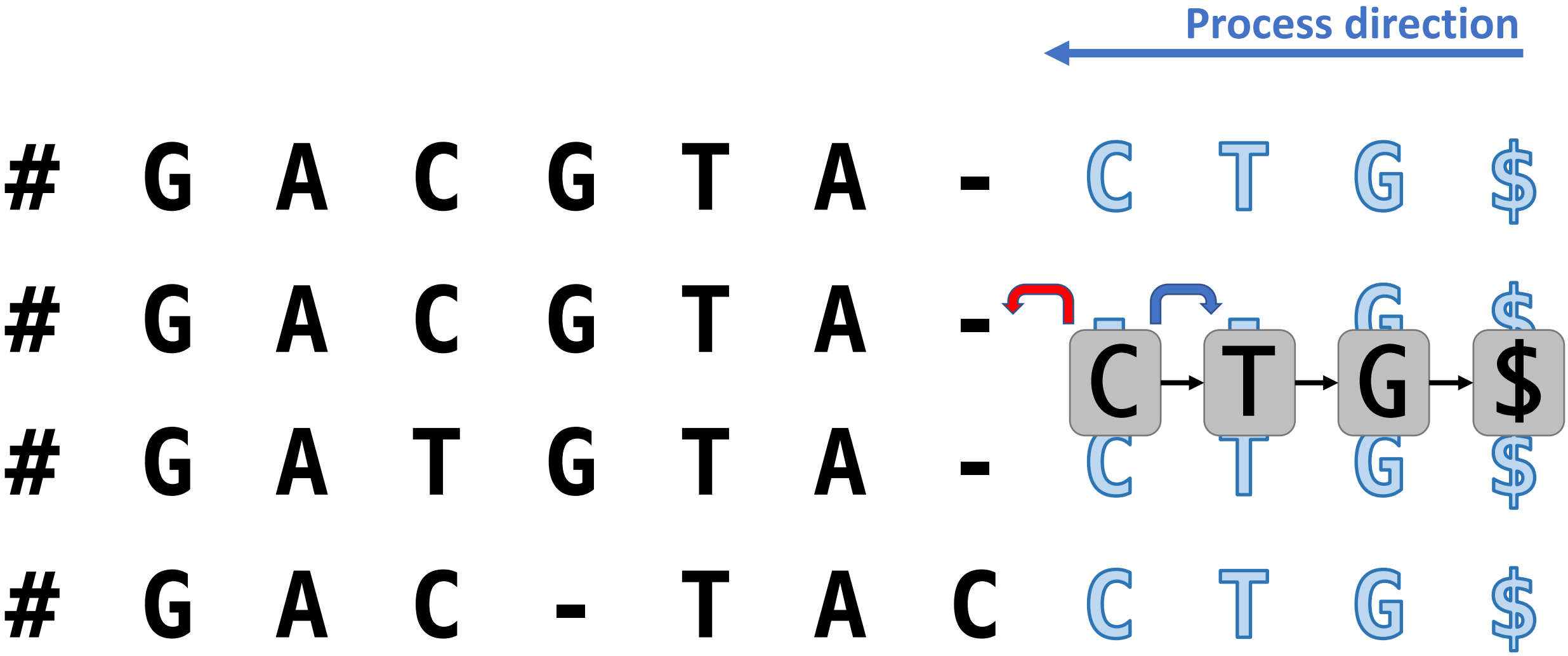

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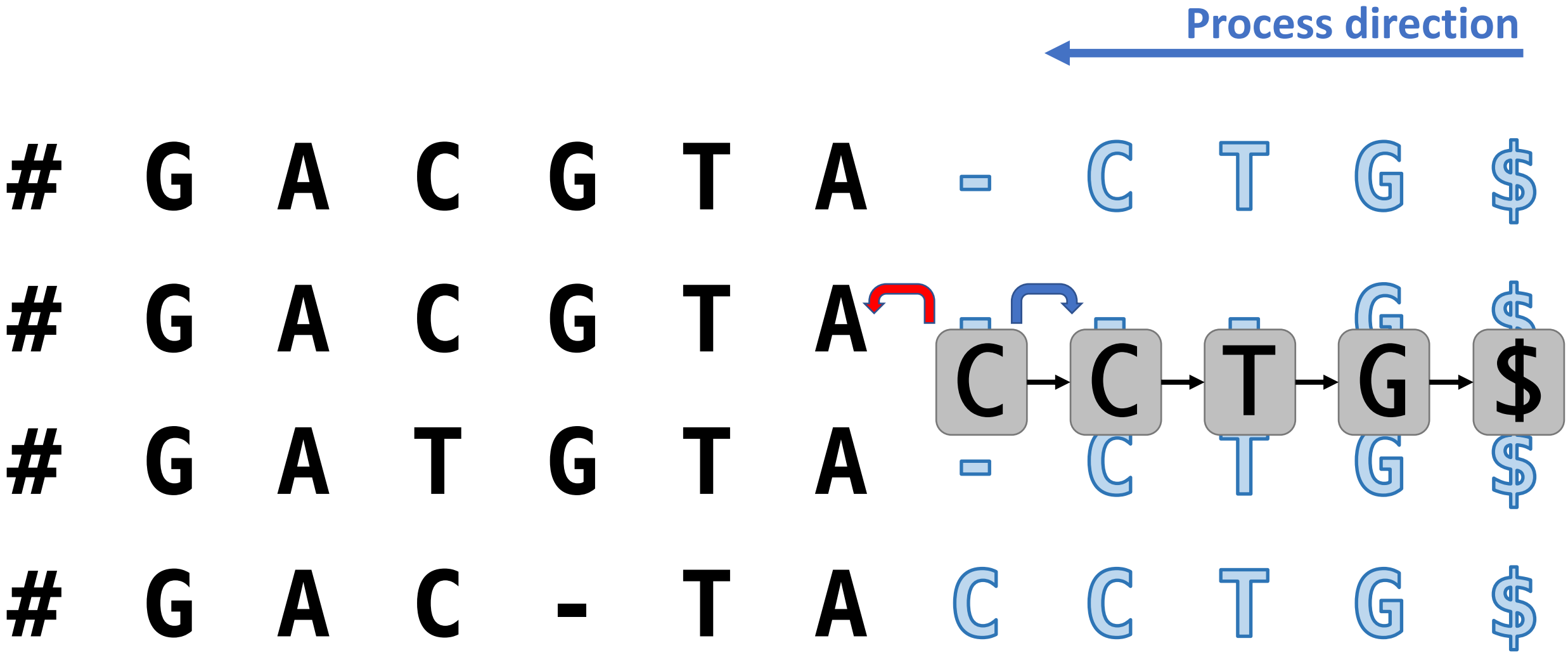

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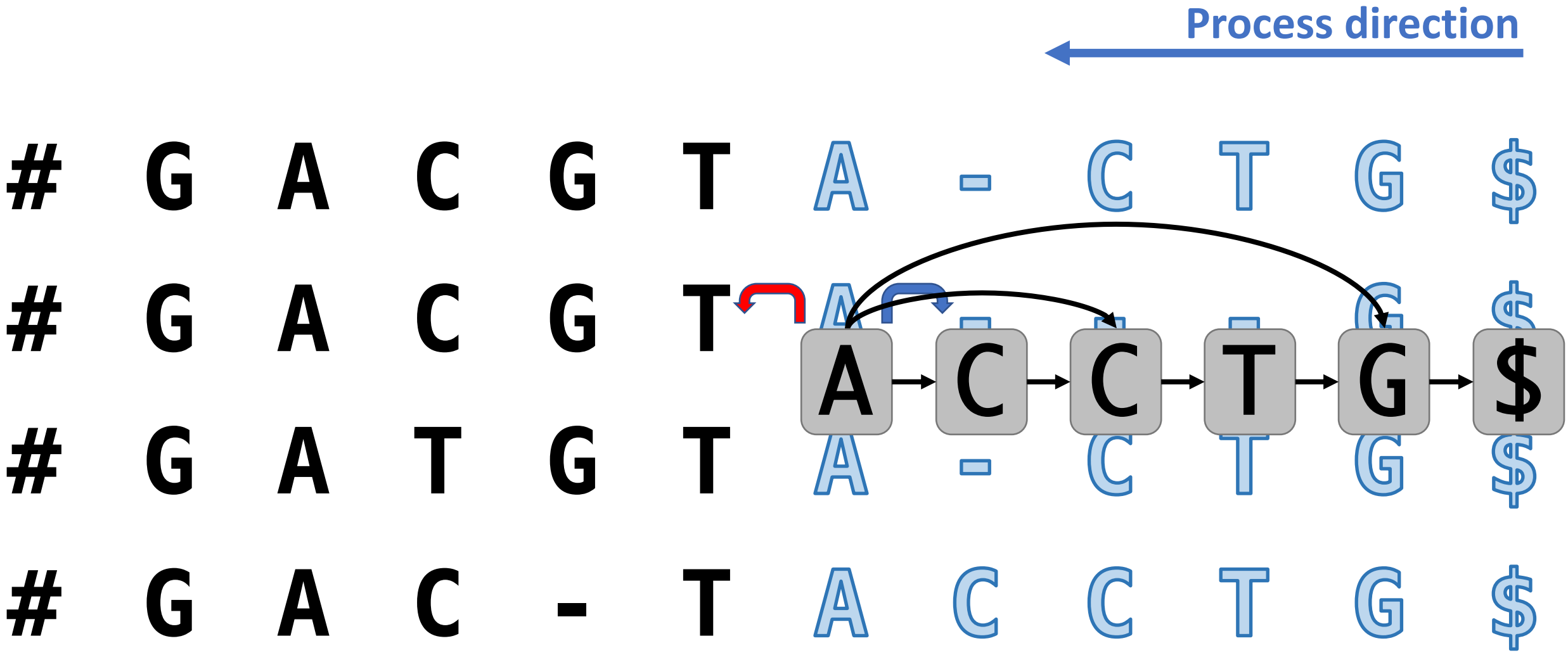

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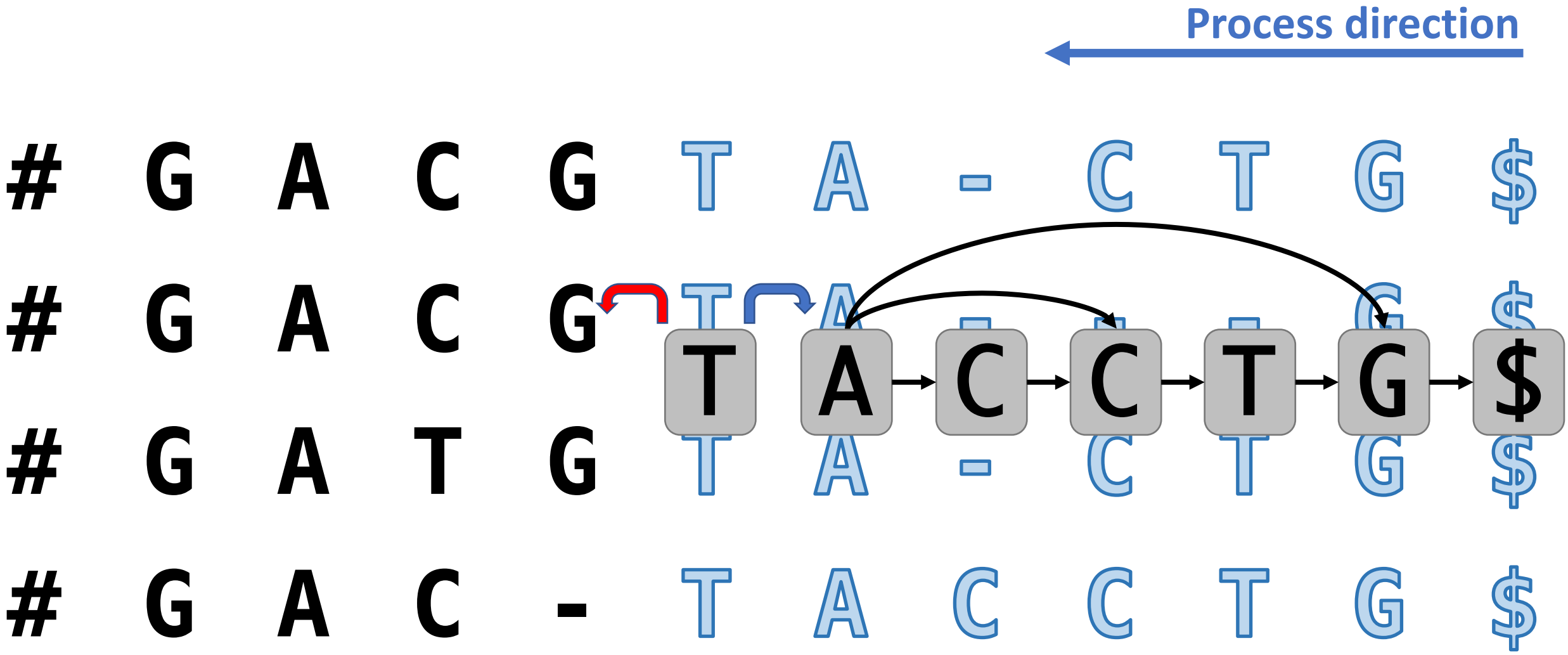

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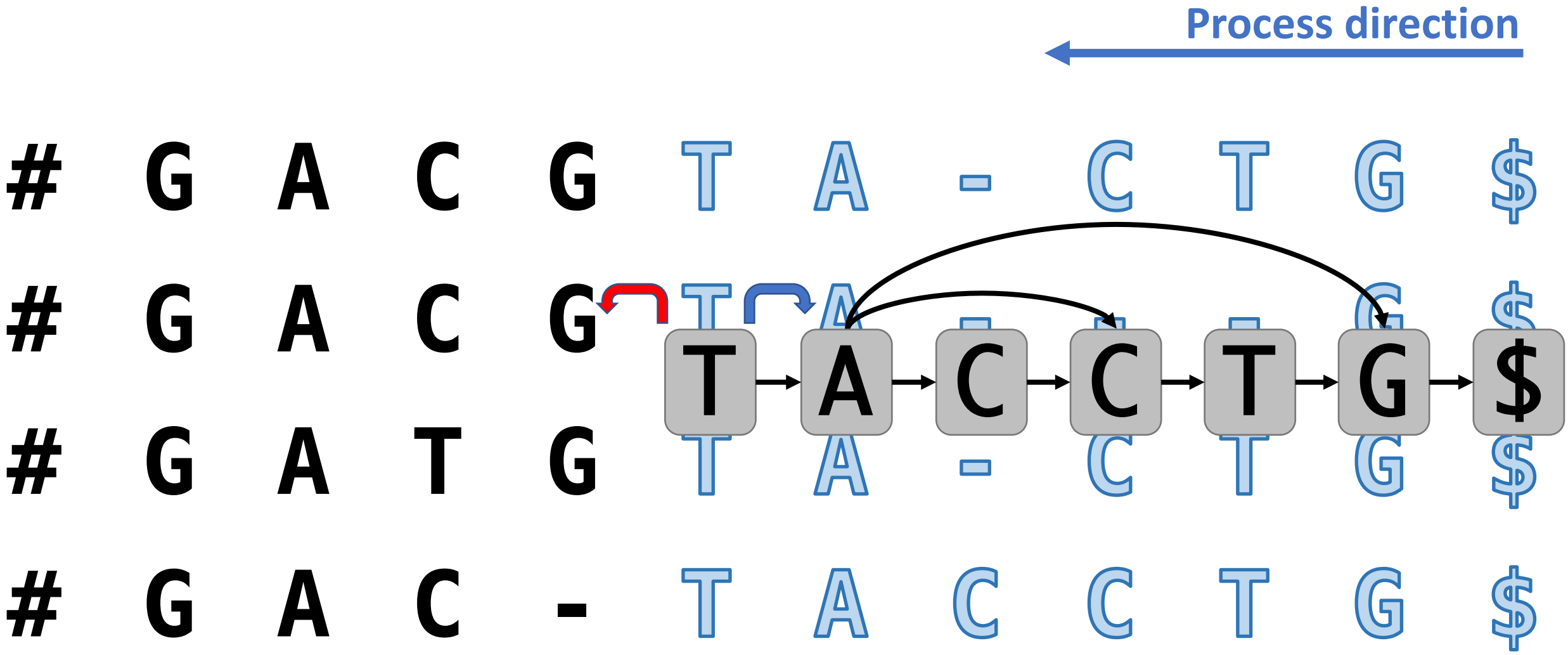

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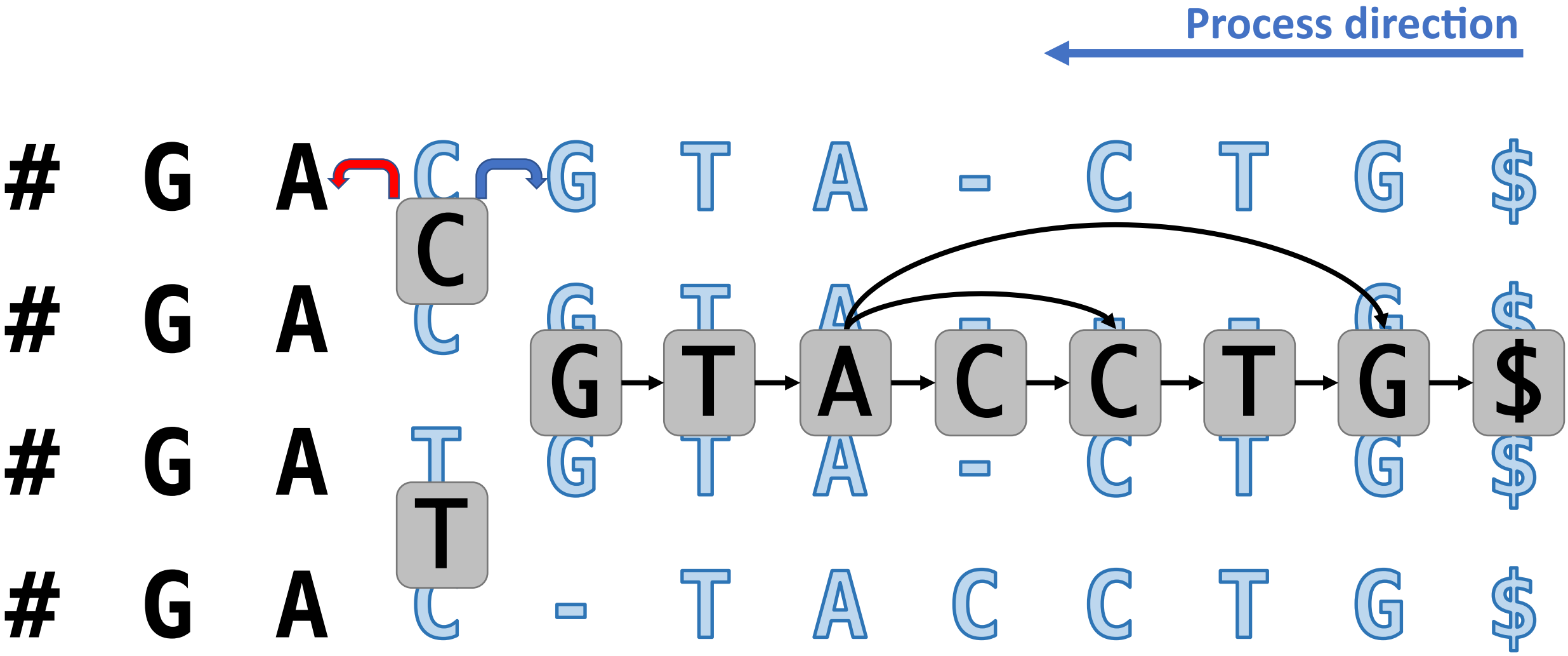

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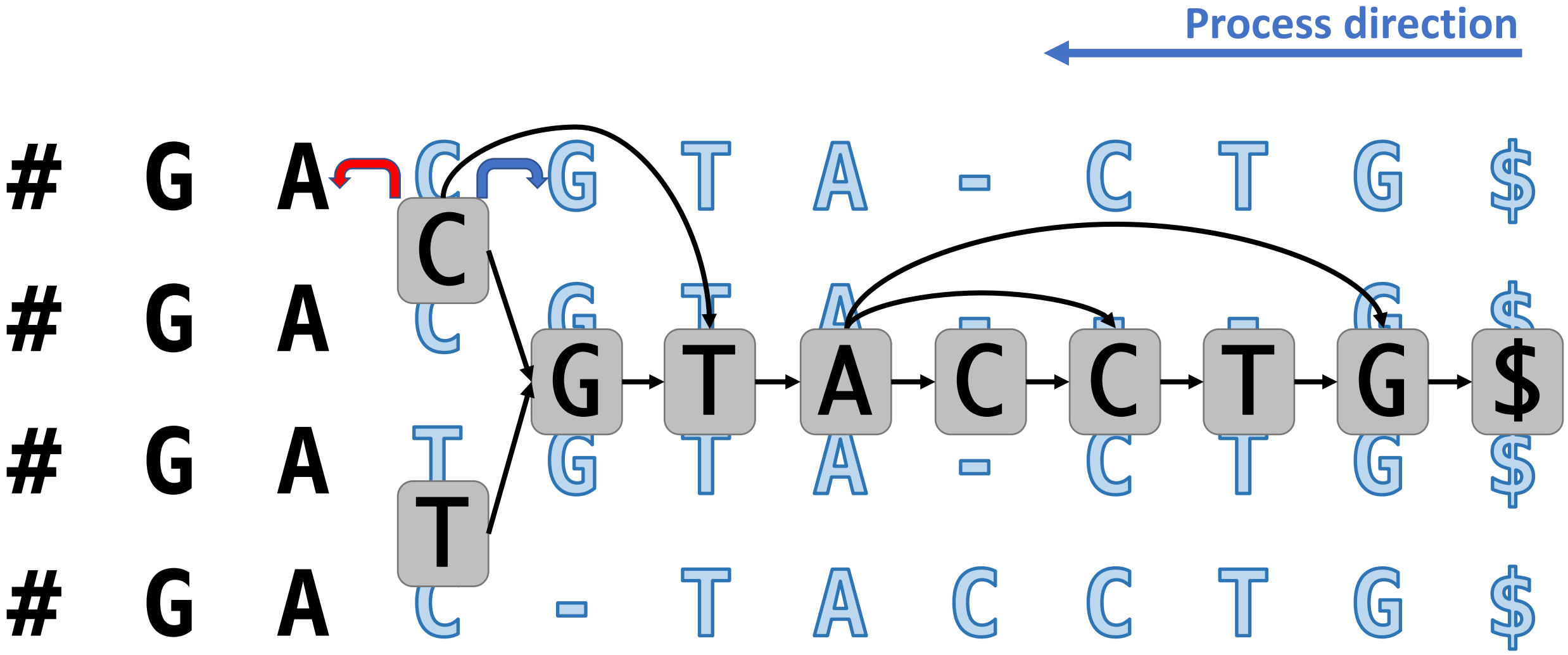

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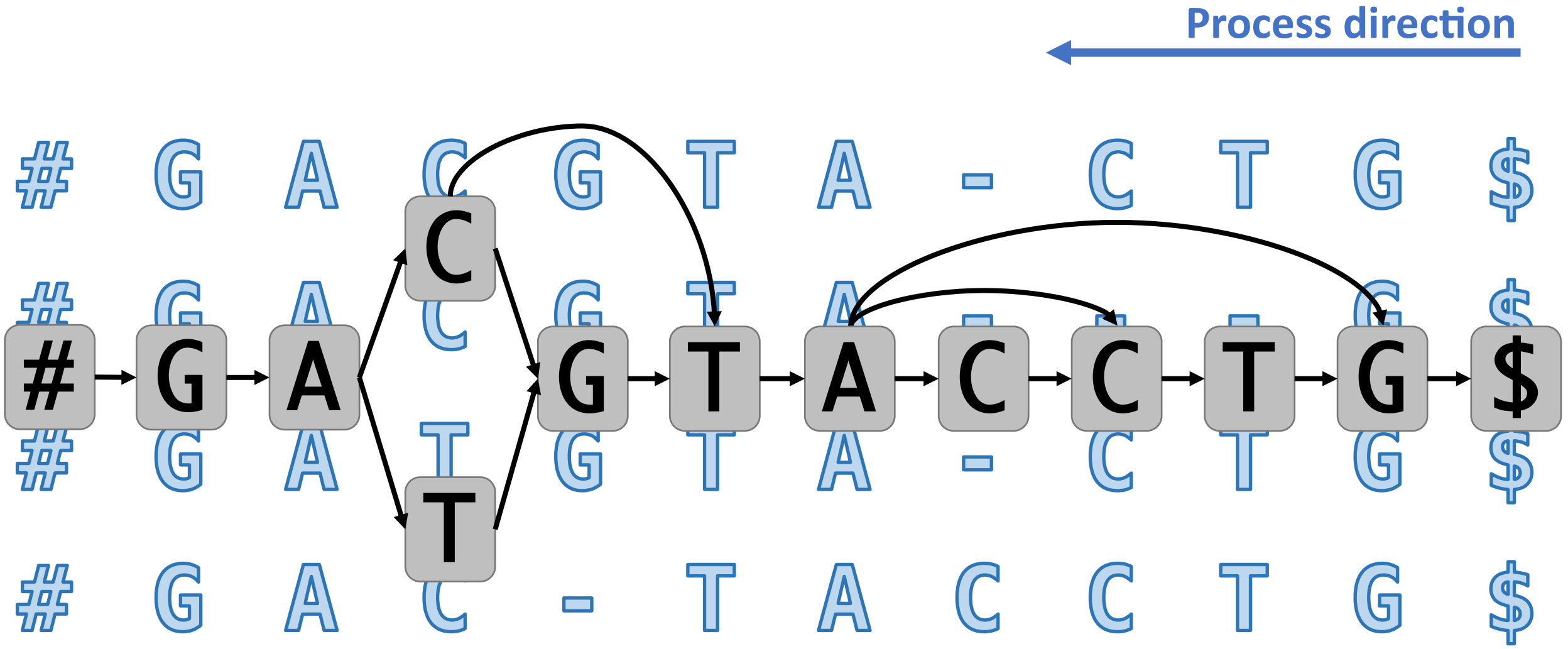

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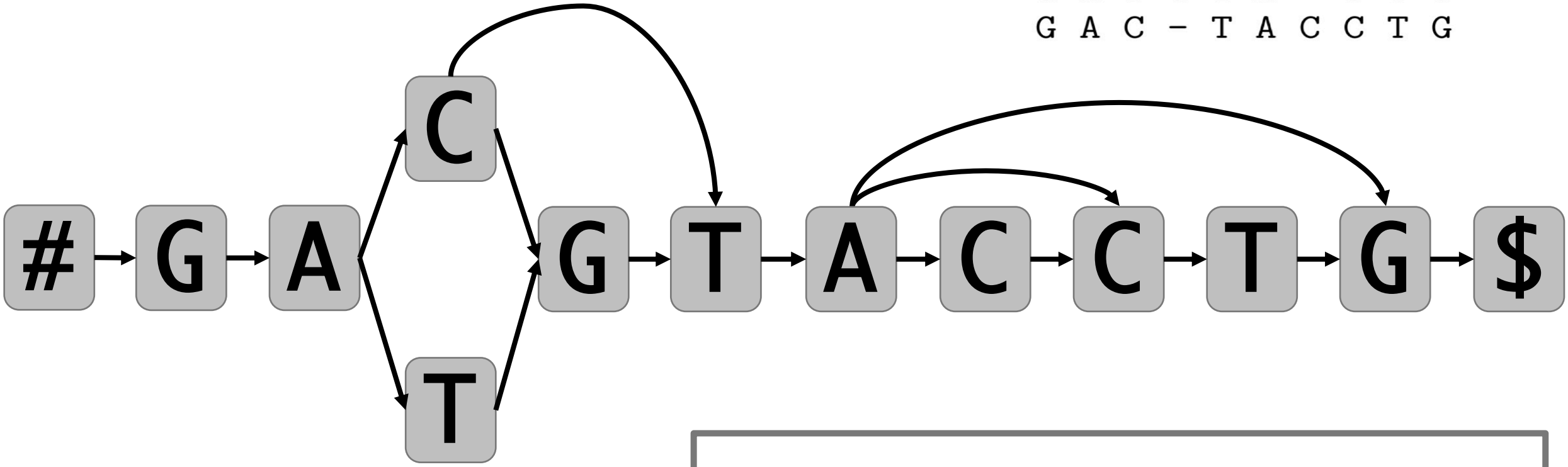
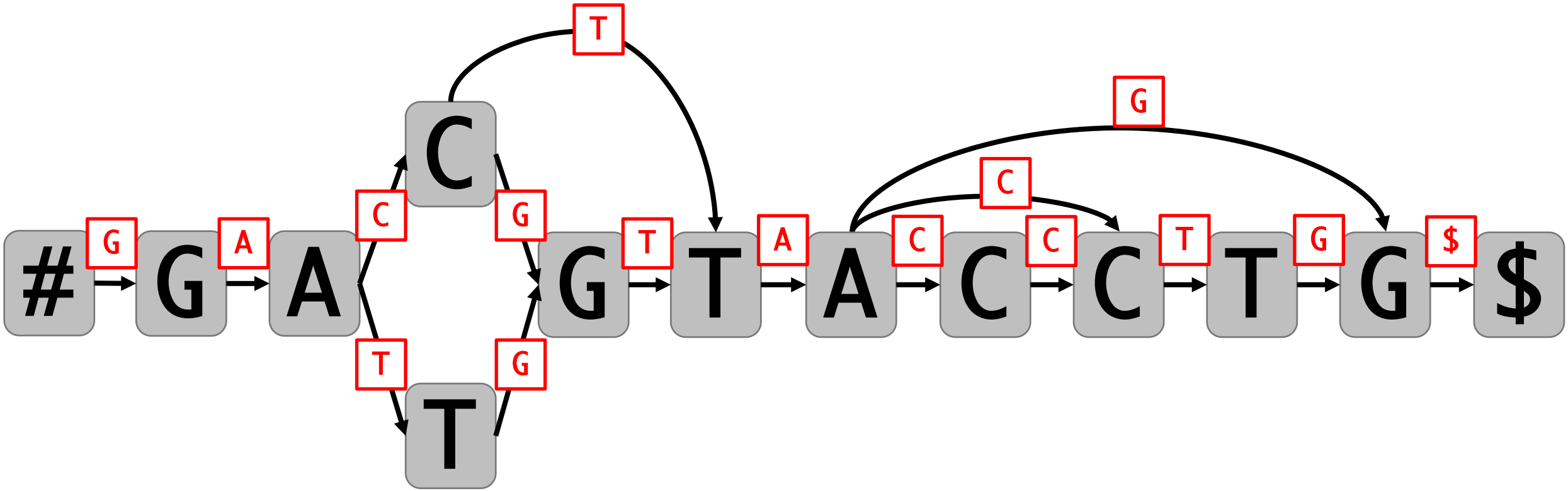


Automaton $\mathbf{A}$ is reverse deterministic if, for every node $v \in V$ and every character $c \in \Sigma \cup \{\#, \$\}$, there exists at most one node u such $label(u) = c$ and $(u, v) \in E$

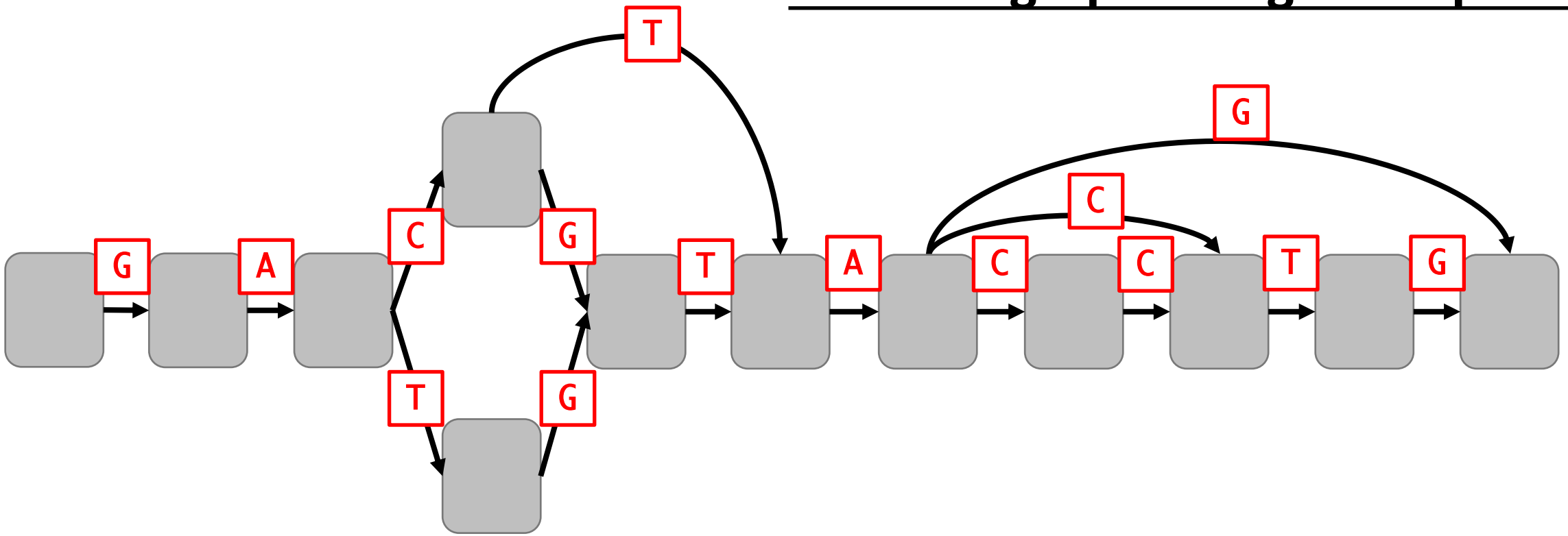
GCSA Reverse Deterministic Graph



Label the edges by the labels of their children.

GCSA Reverse Deterministic Graph

Wheeler graph recognition problem



Is it a Wheeler graph? => ✗ **Wheeler graph.**

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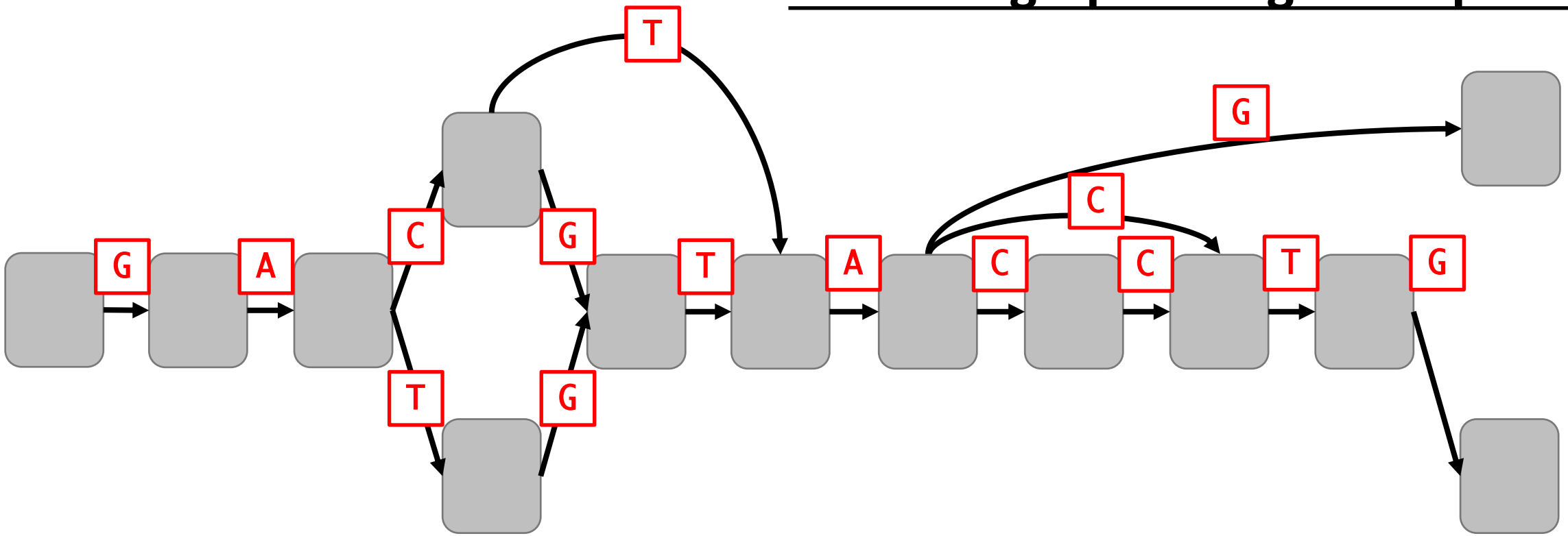

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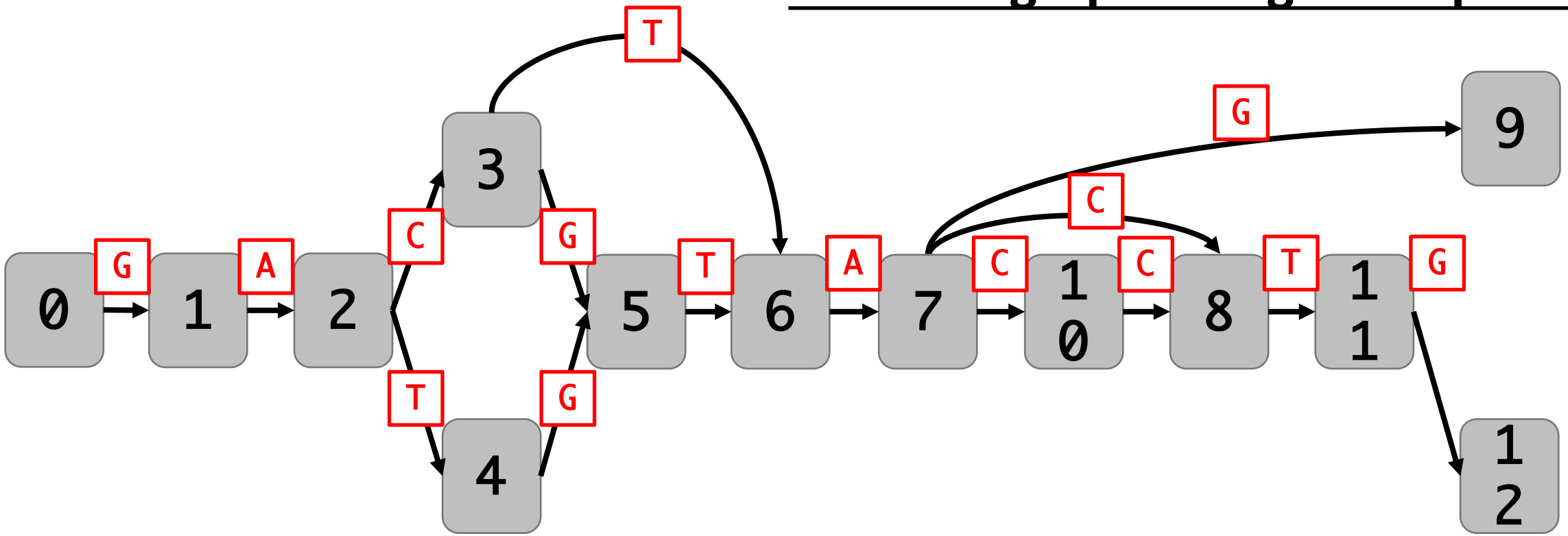

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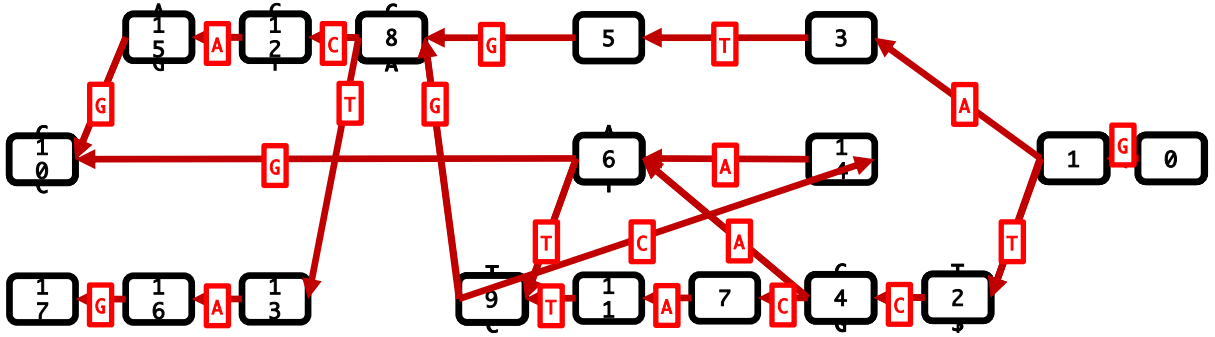
Potential application of Wheeler graph ?

```
G A C G T A - C T G
G A C G T A - - - G
G A T G T A - C T G
G A C - T A C C T G
```

nodes: 18
edges: 21

nodes: 13
edges: 14

De Bruijn Graph



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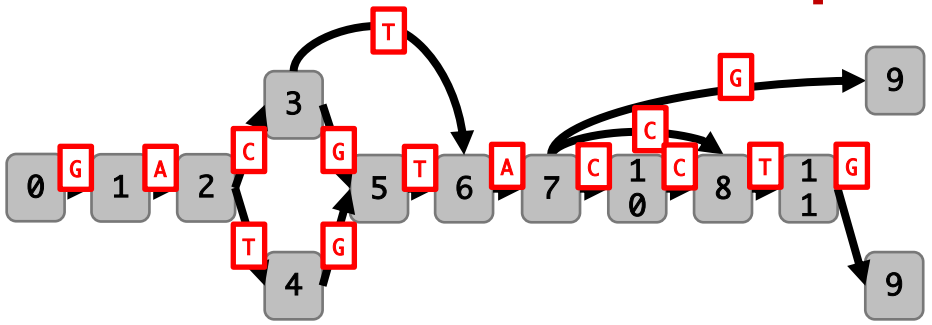
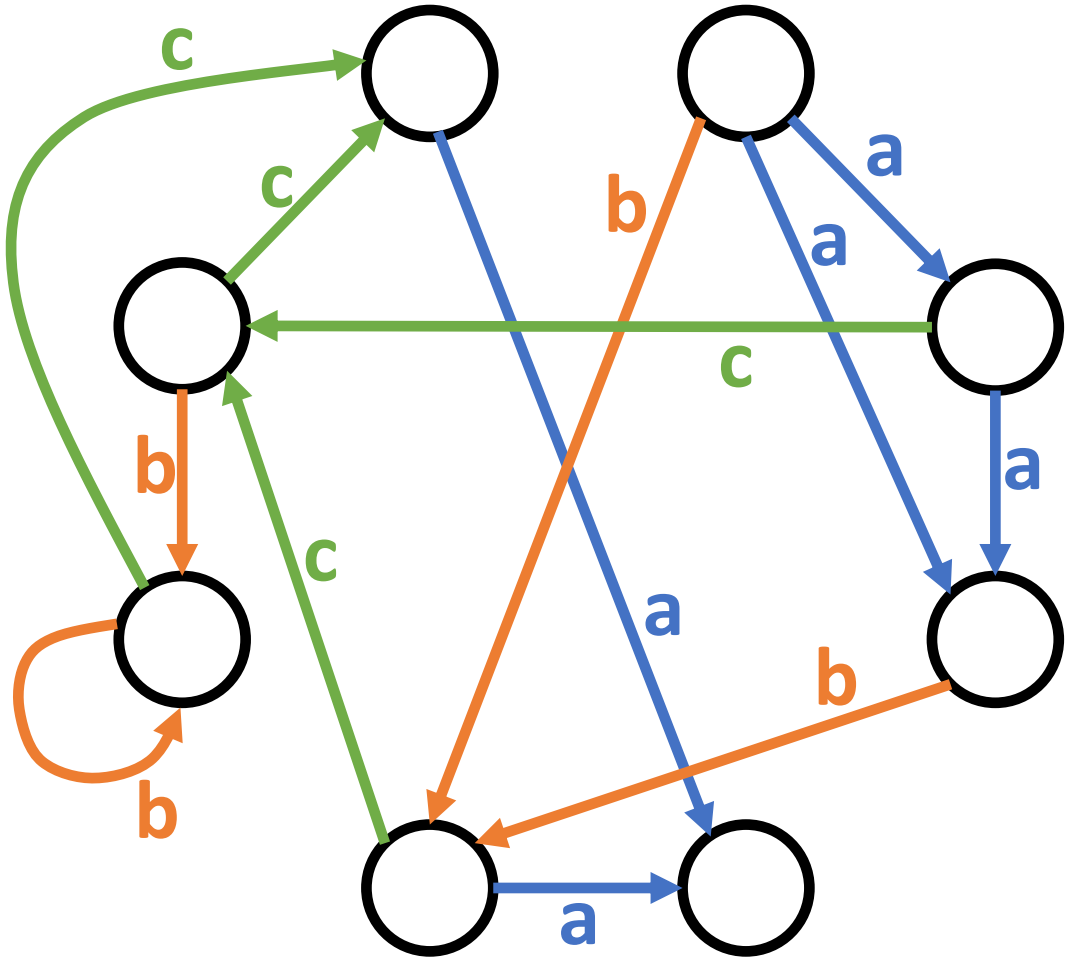


(2) Depending on K, DBG might be bigger than GSCA

Given an edge-labelled graph, is it a Wheeler graph?



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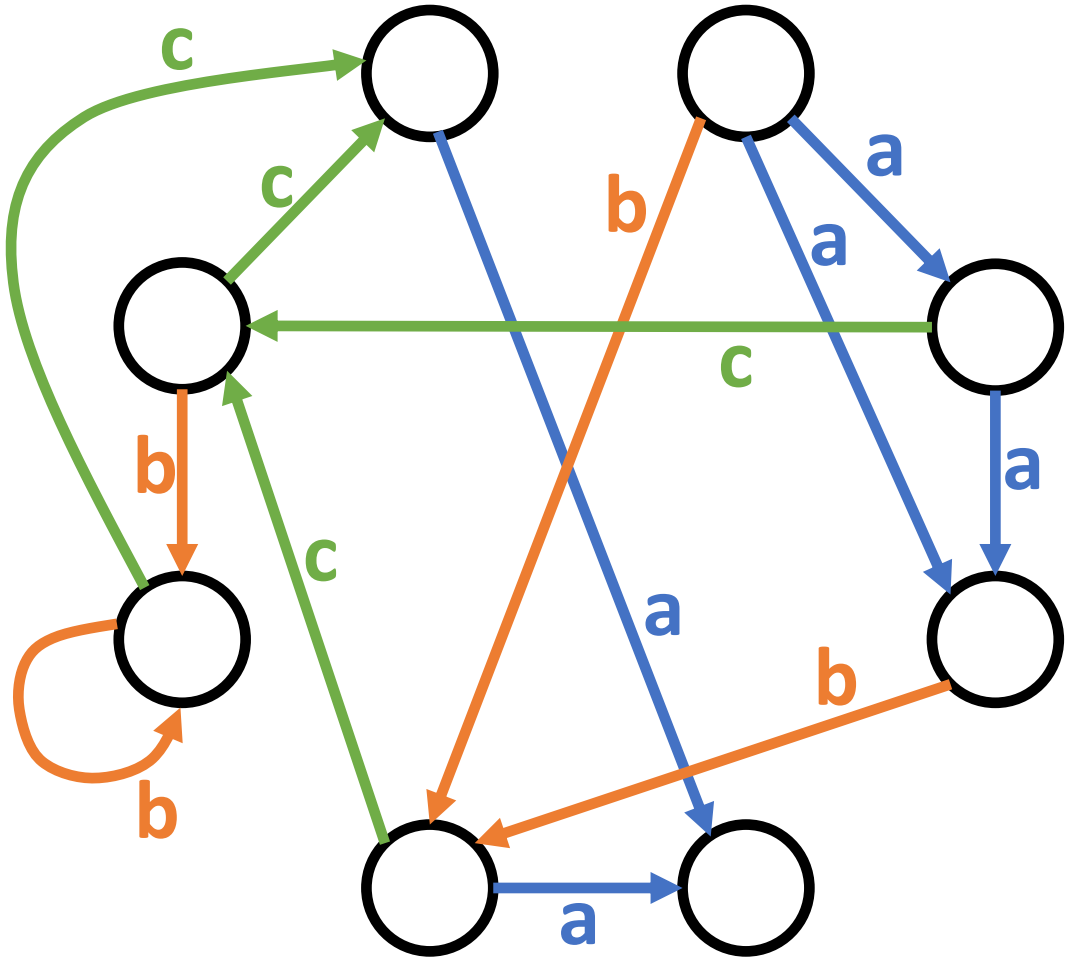

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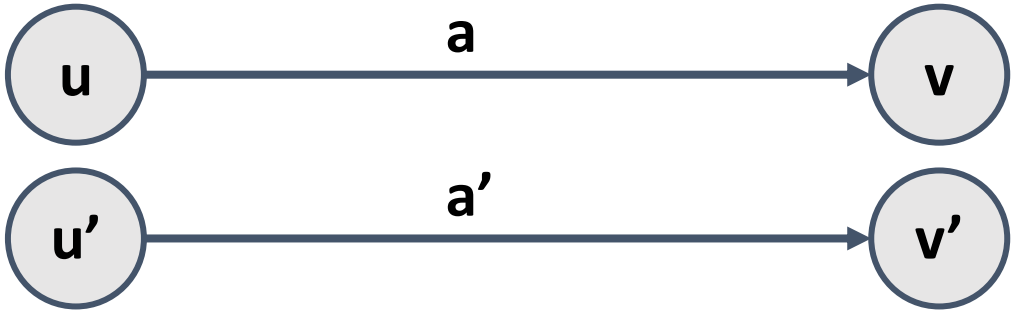

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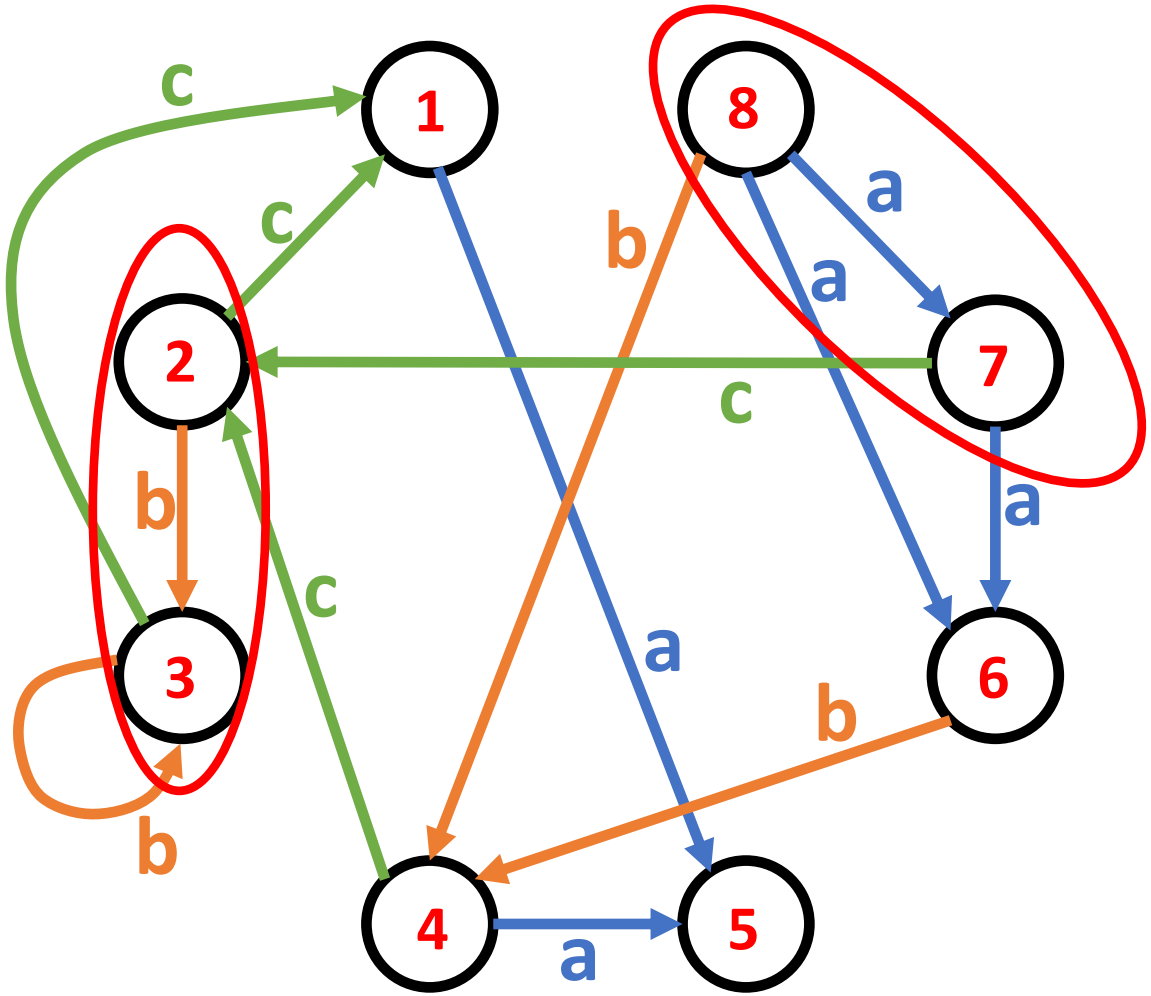

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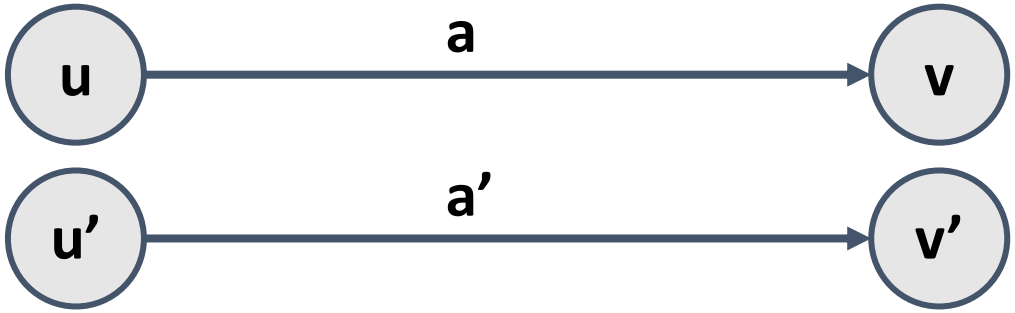

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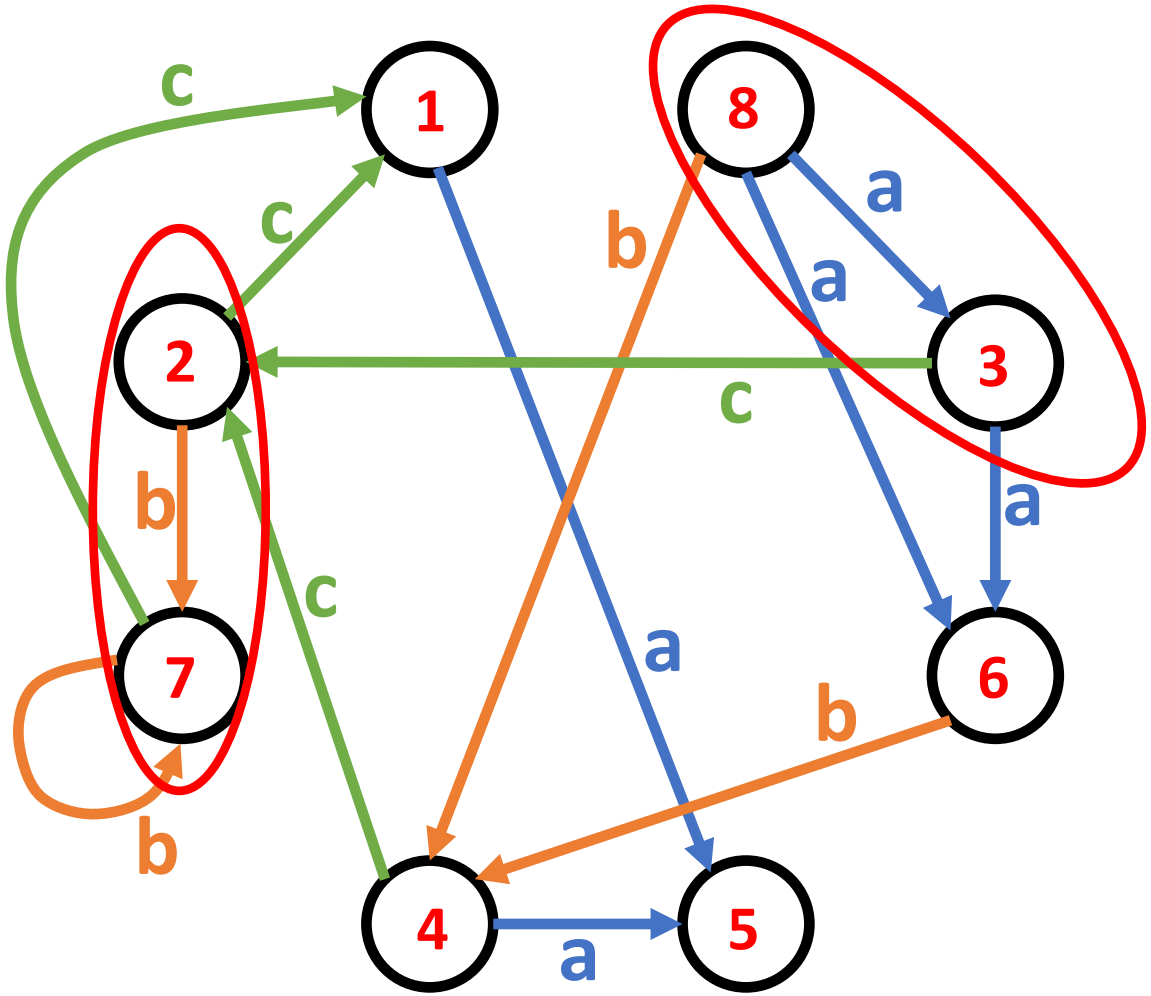

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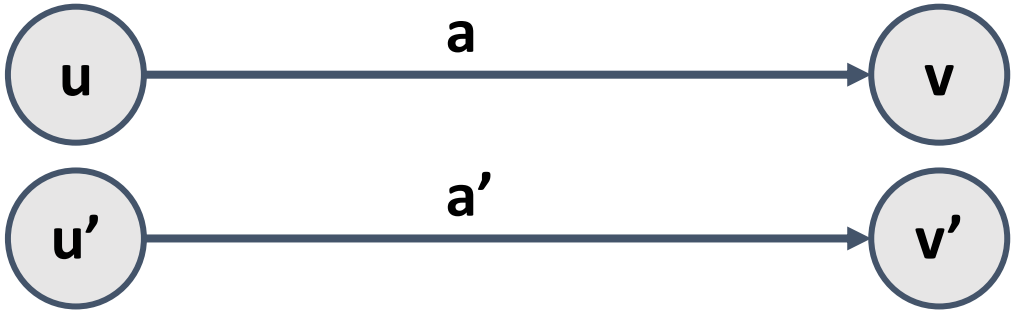
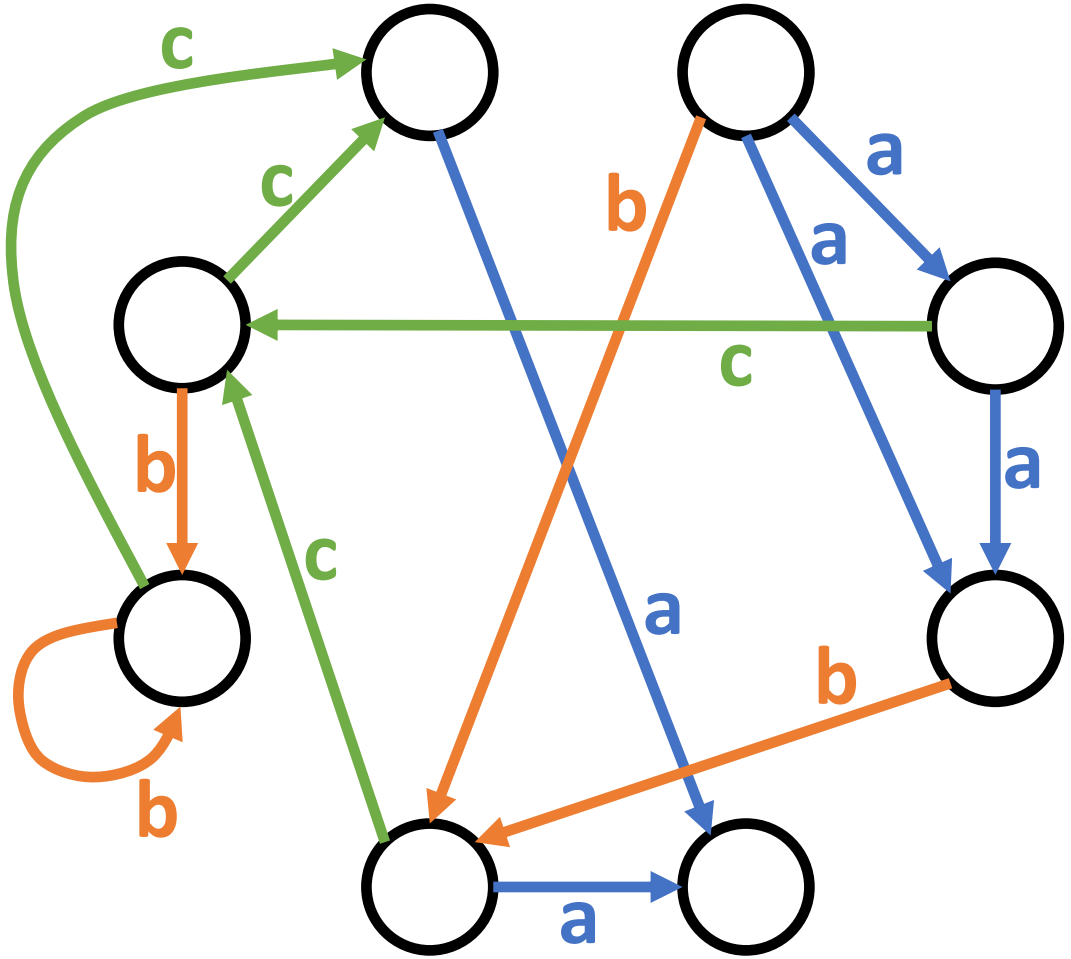


Given an edge-labelled graph, is it a Wheeler graph?



If we can come up a valid ordering =>

it is a Wheeler Graph

If not =>

it is not a Wheeler Graph

arXiv > cs > arXiv:1902.01960
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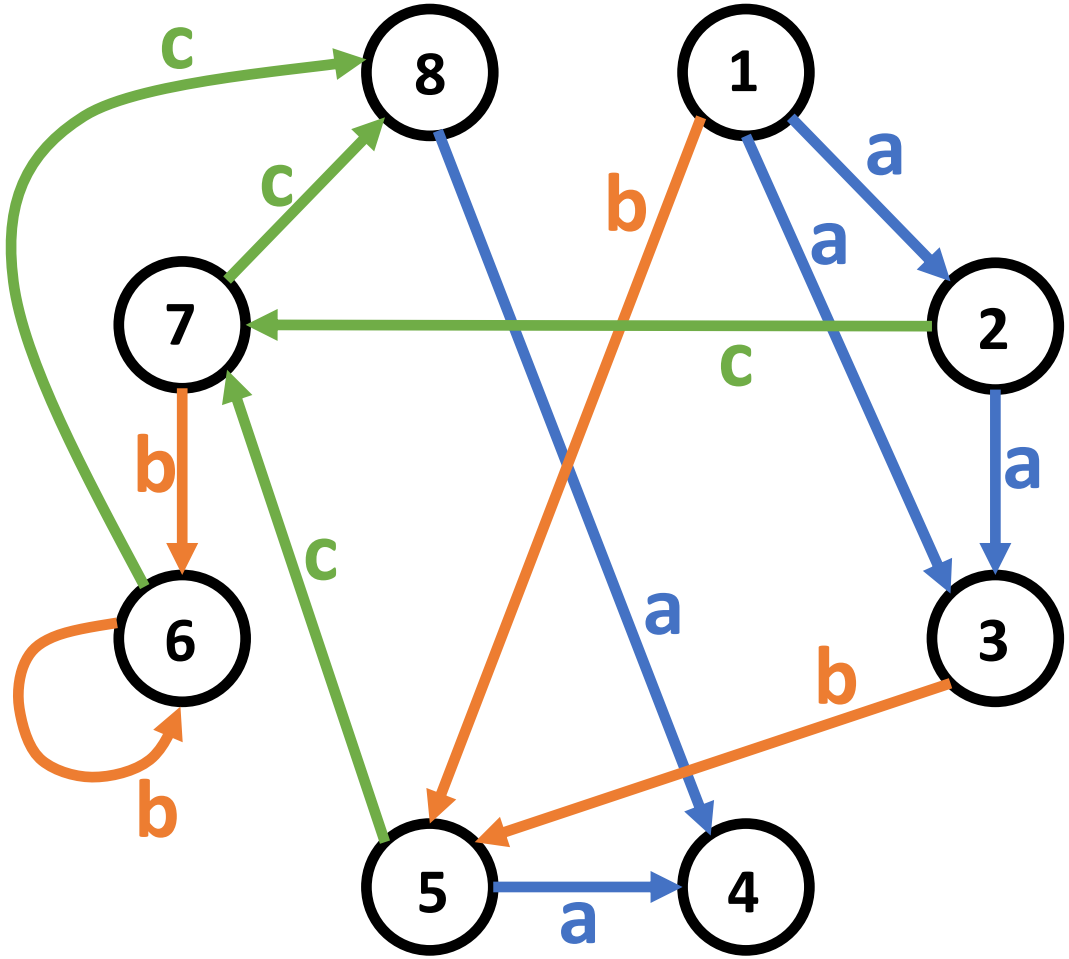
[Submitted on 5 Feb 2019 (v1), last revised 25 Feb 2019 (this version, v2)]

On the Hardness and Inapproximability of Recognizing Wheeler Graphs

Daniel Gibney, Sharma V. Thankachan

2019

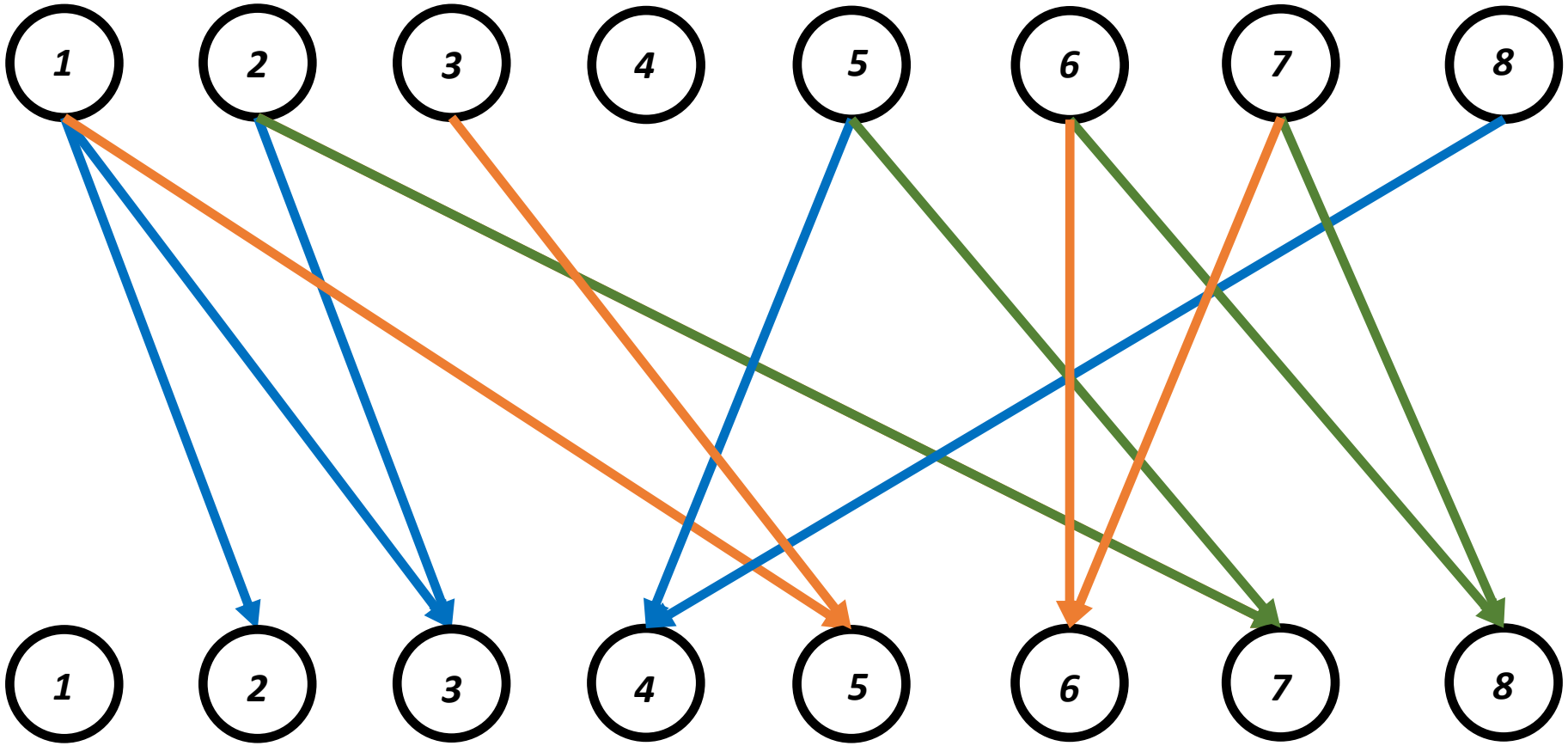
Given an edge-labelled graph, is it a Wheeler graph?



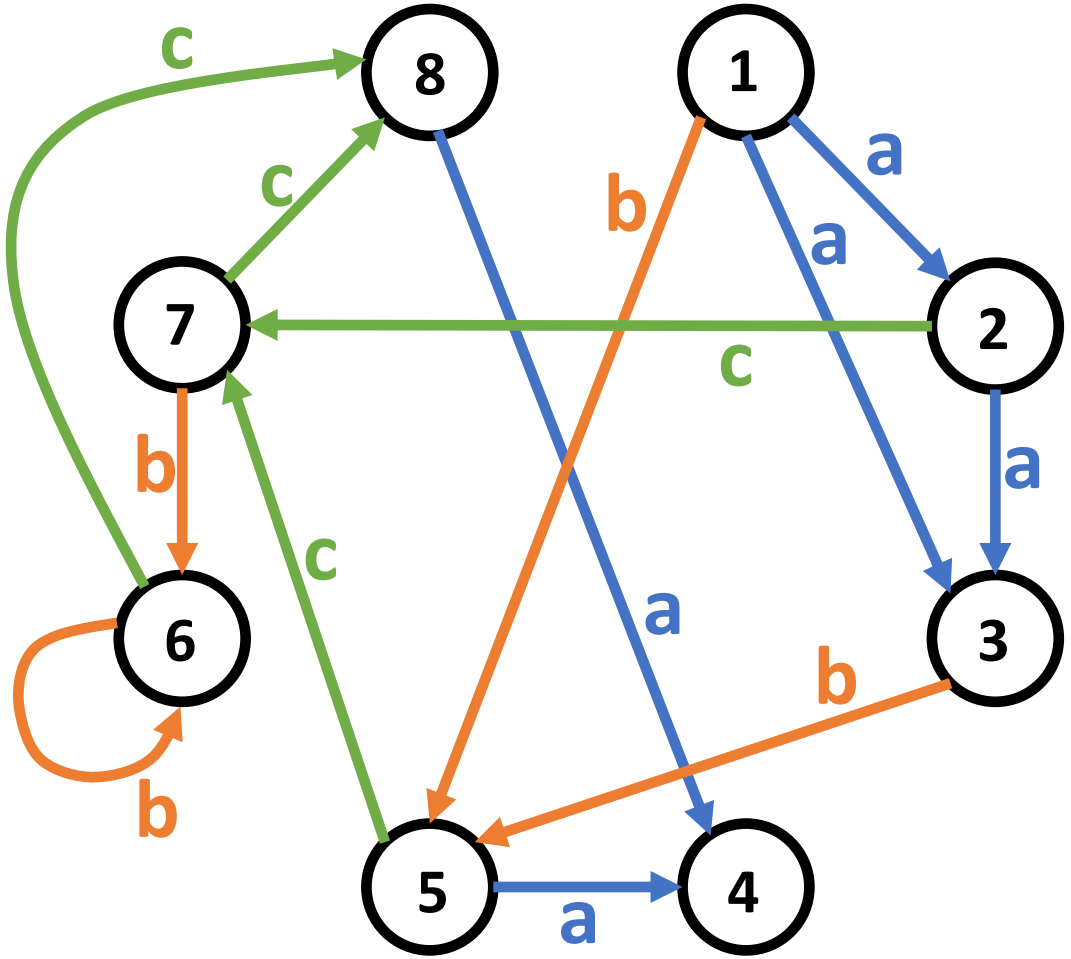
it is a Wheeler Graph

Wheeler graph recognition problem

Given an edge-labelled graph, is it a Wheeler graph?



State-of-the-art WG recognition algorithm



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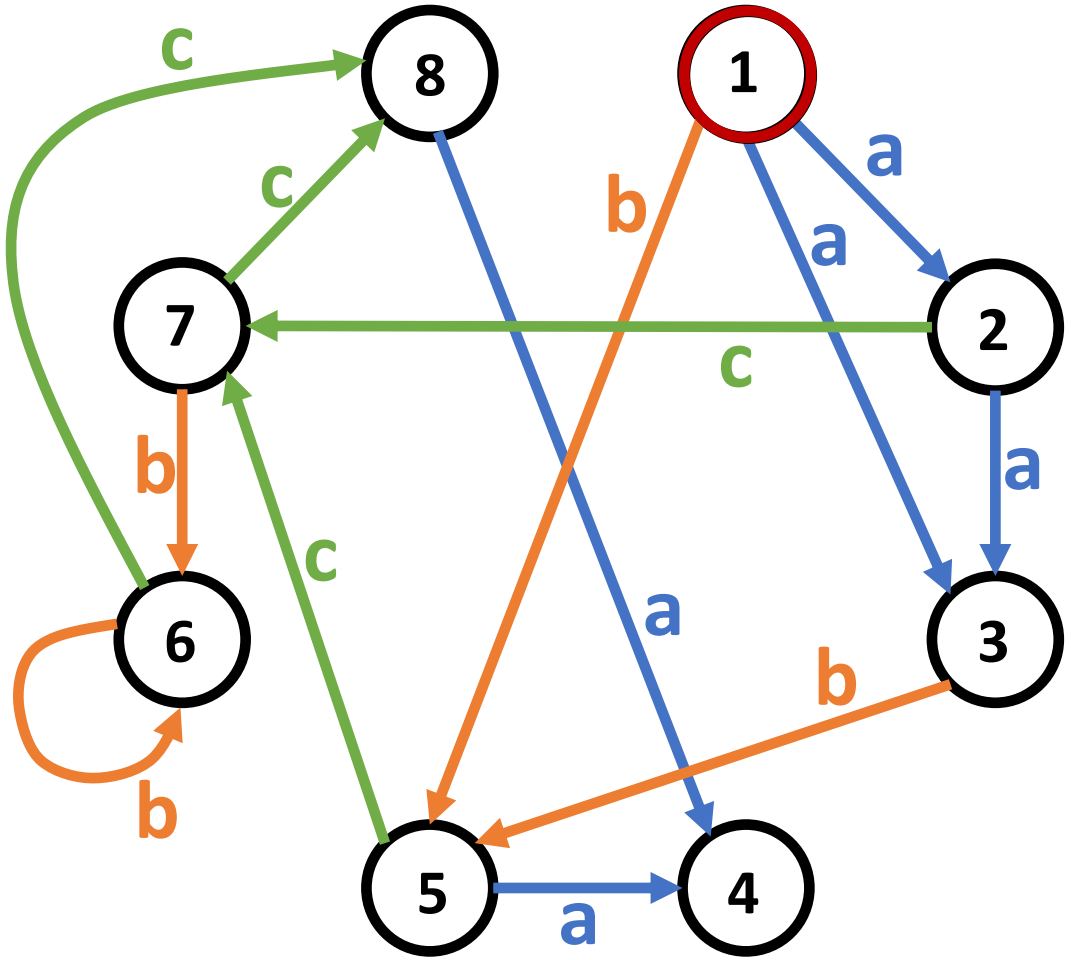
2019

How to encode a Wheeler Graph?



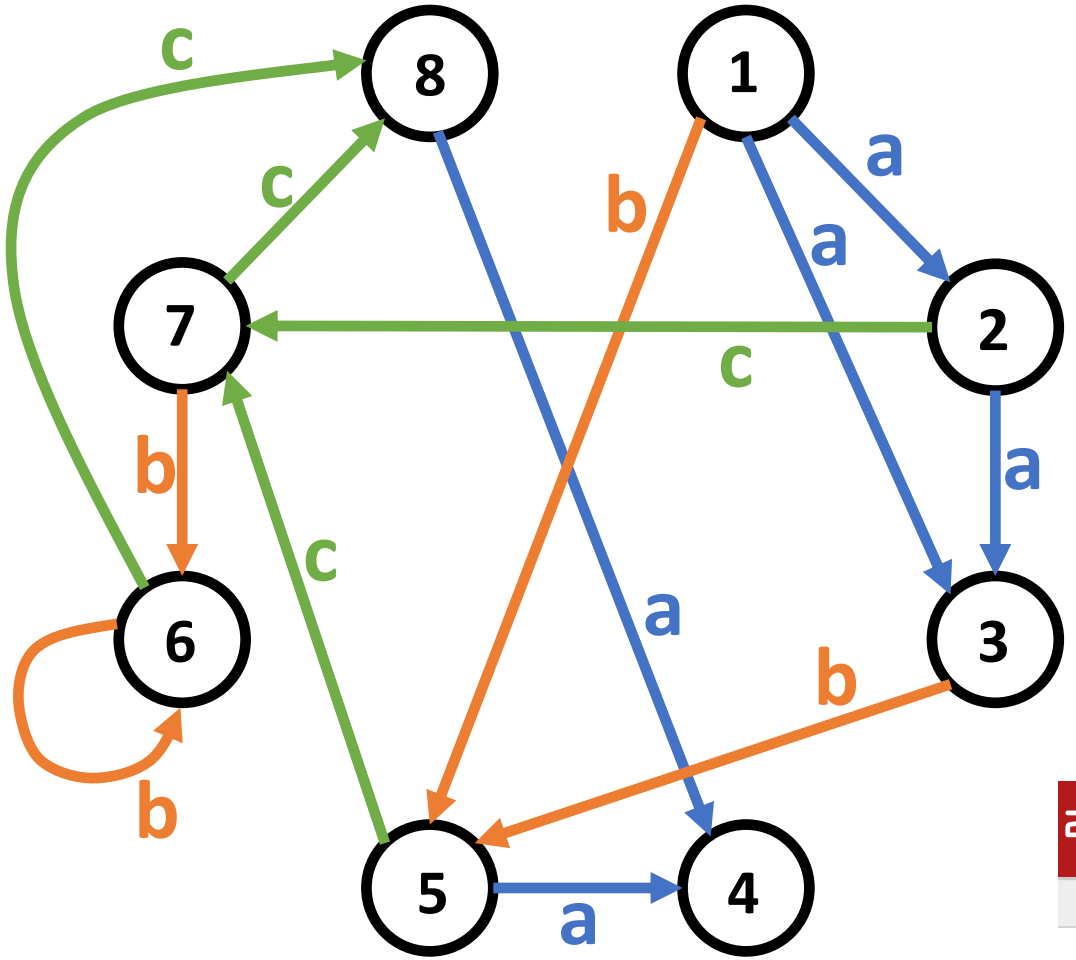
	1	2	3	4	5	6	7	8
O =	0001	001	01	1	001	001	001	01
L =	aab	ac	b		ac	bc	bc	a
I =	1	01	001	001	001	001	001	001

Wheeler graphs: A framework for BWT-based data structures ☆

Travis Gagie [a], Giovanni Manzini [b,c,*], Jouni Sirén [d]

2017

Gibney's & Thankachan's algorithm (G&T)



	1	2	3	4	5	6	7	8
O =	0001	001	01	1	001	001	001	01
L =	aab	ac	b		ac	bc	bc	a
I =	1	01	001	001	001	001	001	001

```
|O| = 13 + 8   (e + n)
|I| = 13 + 8   (e + n)
|L| = 13 * 2   (e * log(sigma))
```

arXiv > cs > arXiv:1902.01960

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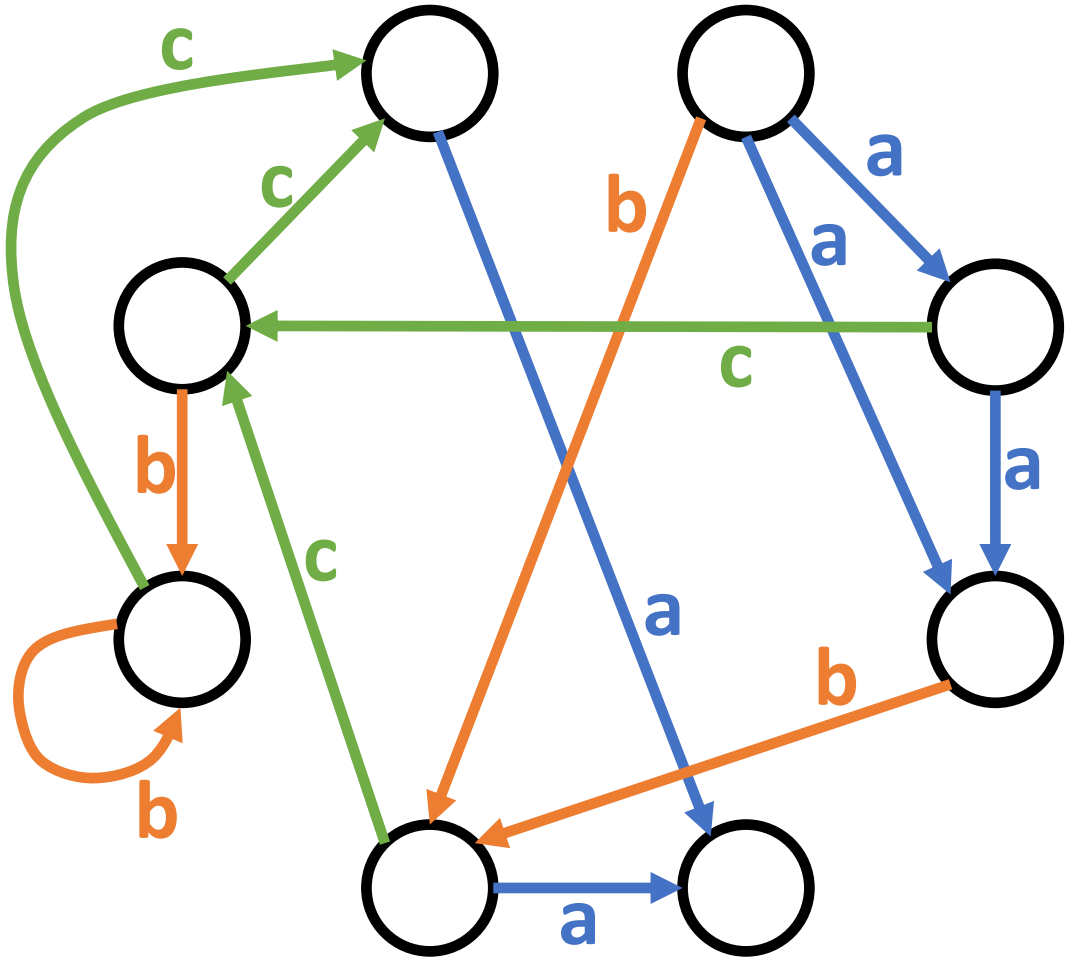


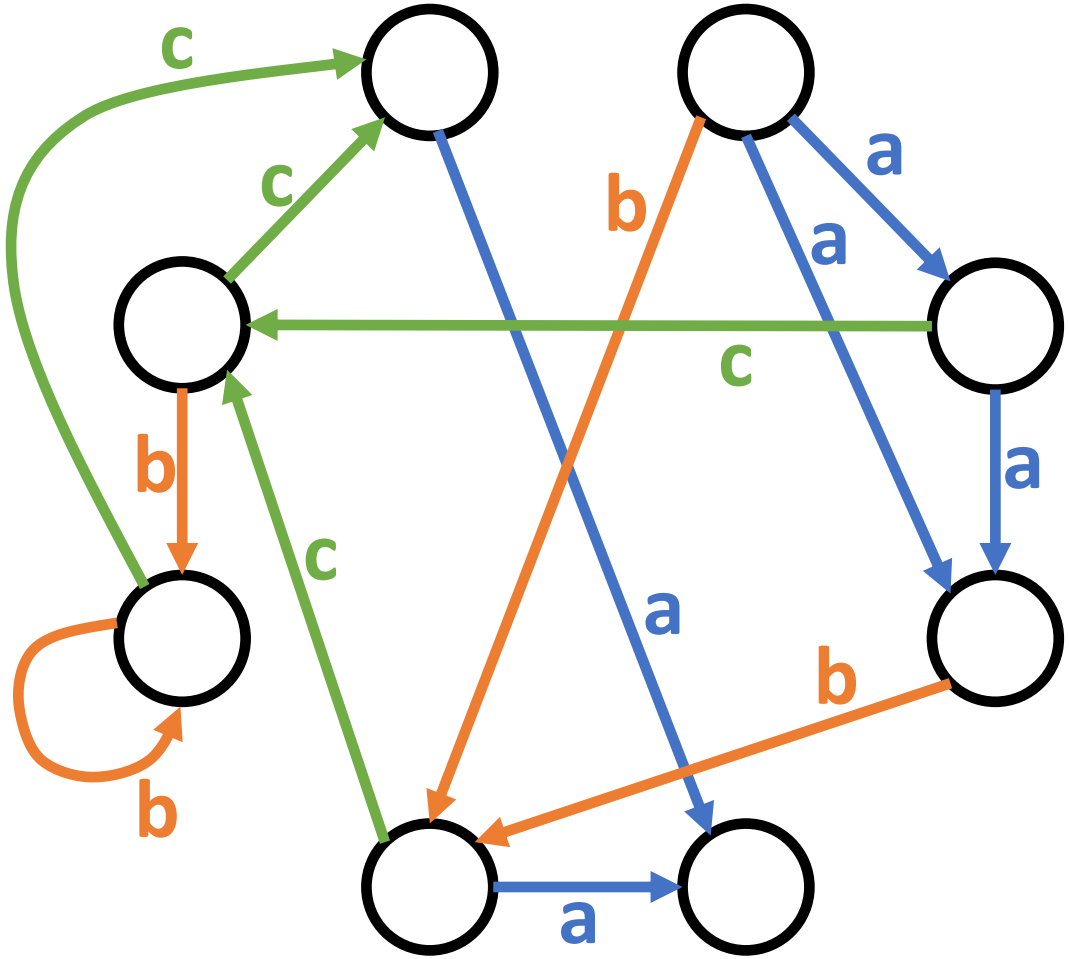

```
|O| = 13 + 8   (e + n)
|I| = 13 + 8   (e + n)
|L| = 13 * 2   (e * log(sigma))
```

Algorithm 1 IdentifyWheelerGraph(G)

for all $(O, I, L) \in S$ **do** $\quad |S| \leq 2^{2(e+n)+e \log \sigma}$
  if (O, I, L) defines a valid wheeler graph G' **then**
    convert G to undirected graph $\alpha(G)$
    convert G' to undirected graph $\alpha(G')$
    if $\alpha(G)$ and $\alpha(G')$ are isomorphic **then**
      return 'Wheeler Graph'
    end if
  end if
end for
return "Not a Wheeler Graph"

$$O(2^{O(e+n)+e \log \sigma})$$

Wheelie: WG recognition algorithm



Renaming heuristic

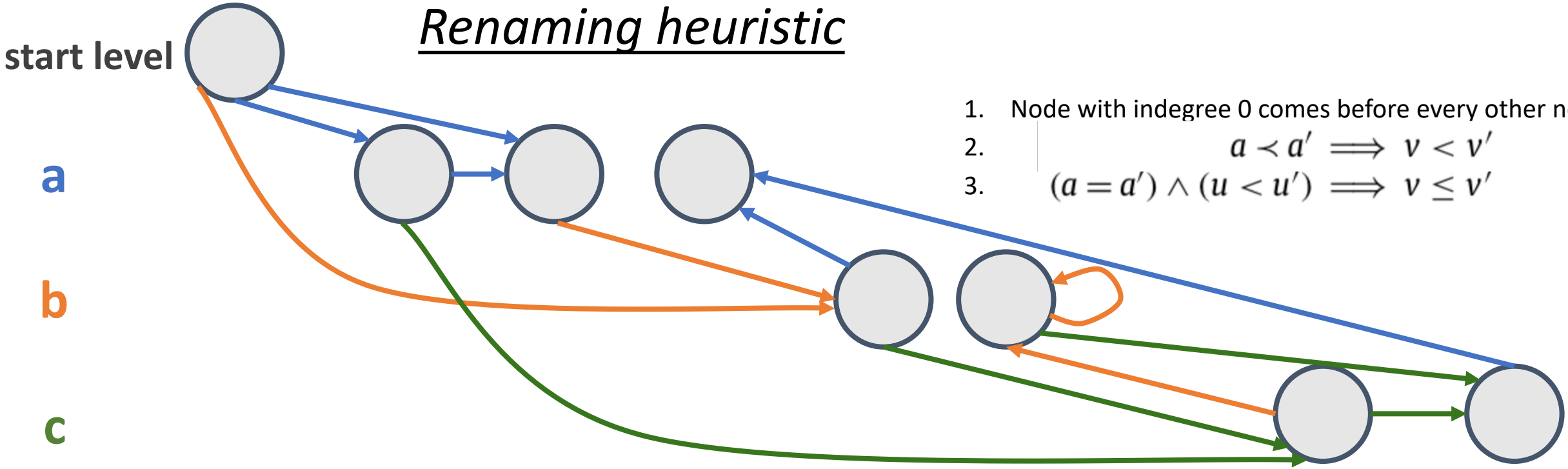
+

Solvers:

Permutation solver
- **Wheelie-PR**

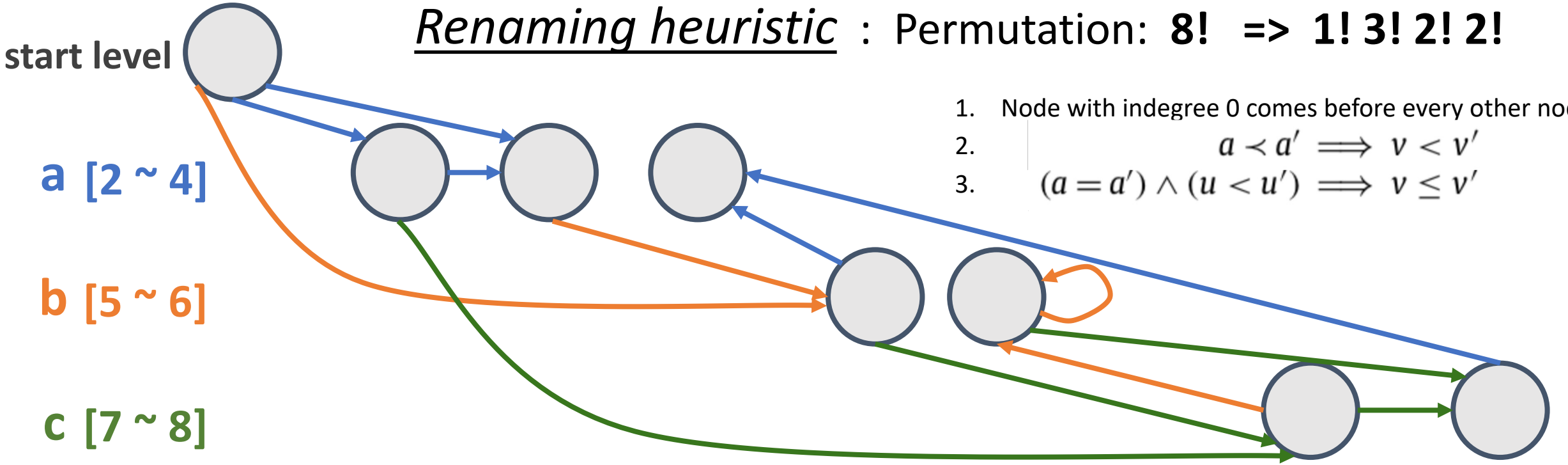
SMT solver:
- **Wheelie-SMT**

Renaming heuristic



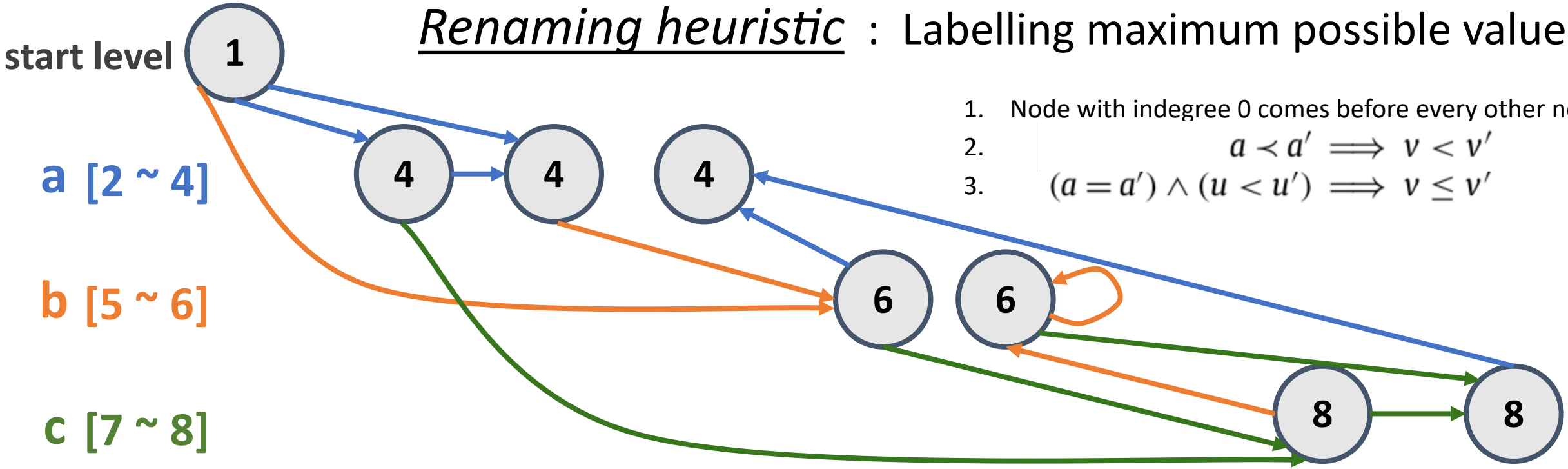
1. Node with indegree 0 comes before every other nodes.
2. $a \prec a' \implies v < v'$
3. $(a = a') \wedge (u < u') \implies v \leq v'$

Renaming heuristic : Permutation: **8! => 1! 3! 2! 2!**



1. Node with indegree 0 comes before every other nodes.
2. $$a \prec a' \implies v < v'$$
3. $$(a = a') \wedge (u < u') \implies v \leq v'$$

Renaming heuristic : Labelling maximum possible value



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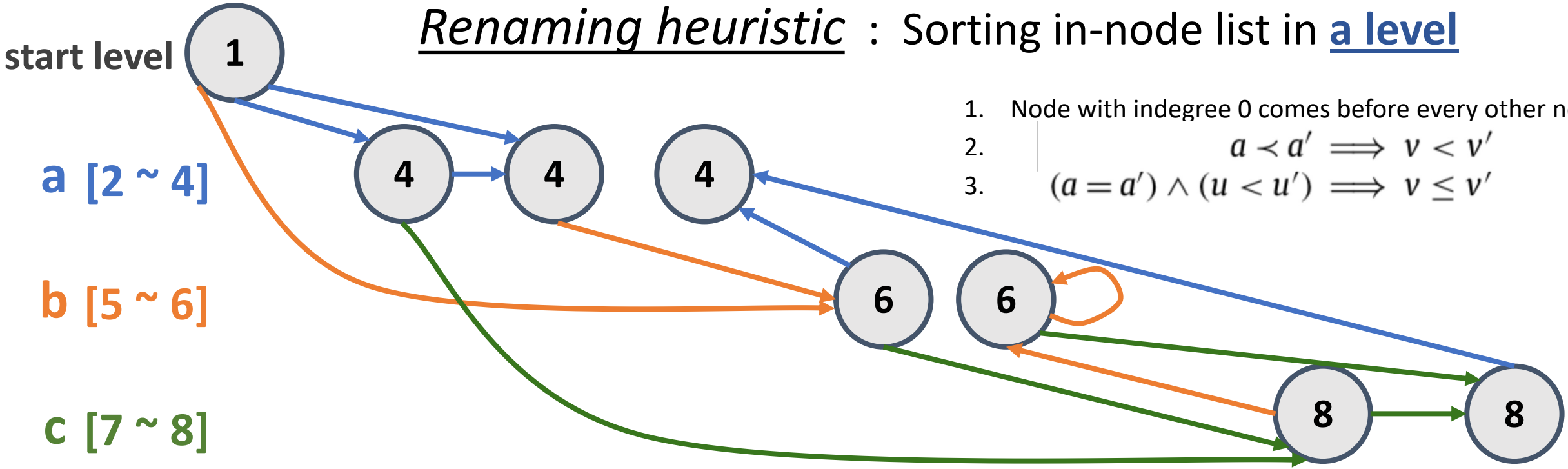
3. $$(a = a') \wedge (u < u') \implies v \leq v'$$

Renaming heuristic : Sorting in-node list in a level



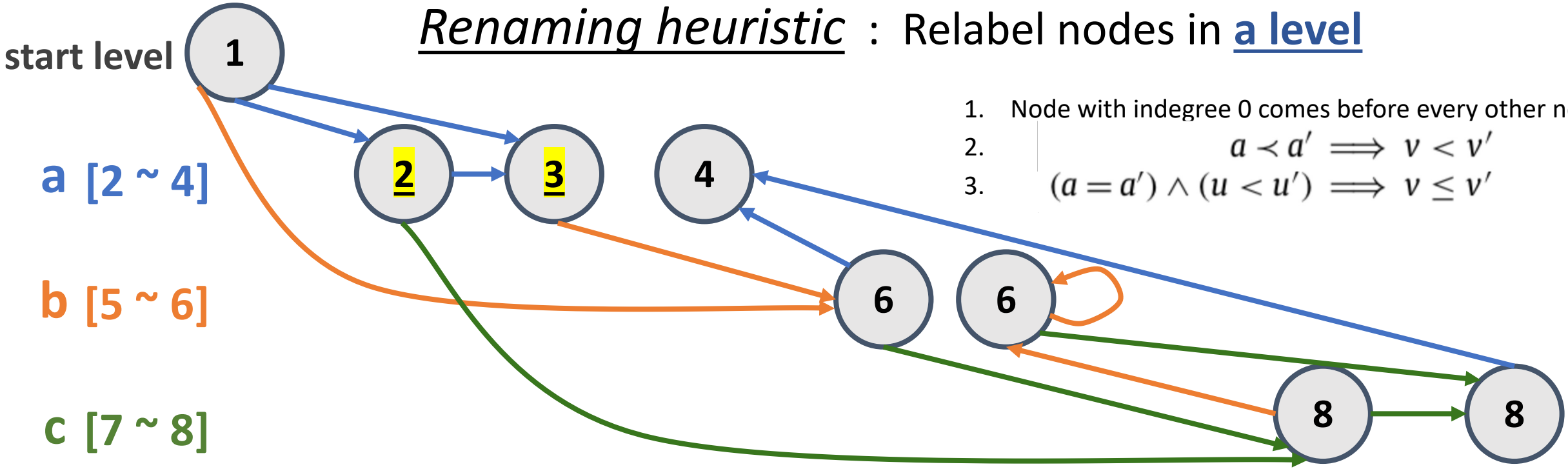
1. Node with indegree 0 comes before every other nodes.
2. $a \prec a' \implies v < v'$
3. $(a = a') \wedge (u < u') \implies v \leq v'$

In-node list:

start level
1: Ø

a level	b level	c level
4: 1	6: 1, 4	8: 4, 6
4: 1, 4	6: 6, 8	8: 6, 8
4: 6, 8		

Renaming heuristic : Relabel nodes in a level



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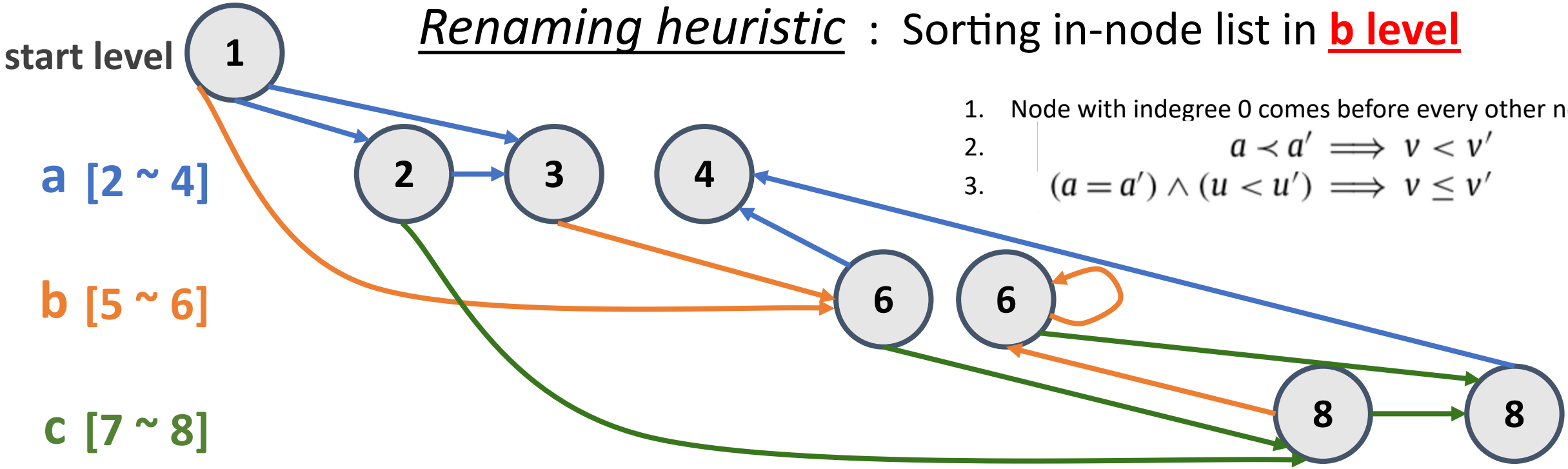
In-node list:

start level
1: Ø

a level	b level	c level
2: 1	6: 1, 3	8: 2, 6
3: 1, 4	6: 6, 8	8: 6, 8
4: 6, 8		

Renaming heuristic : Sorting in-node list in **b level**

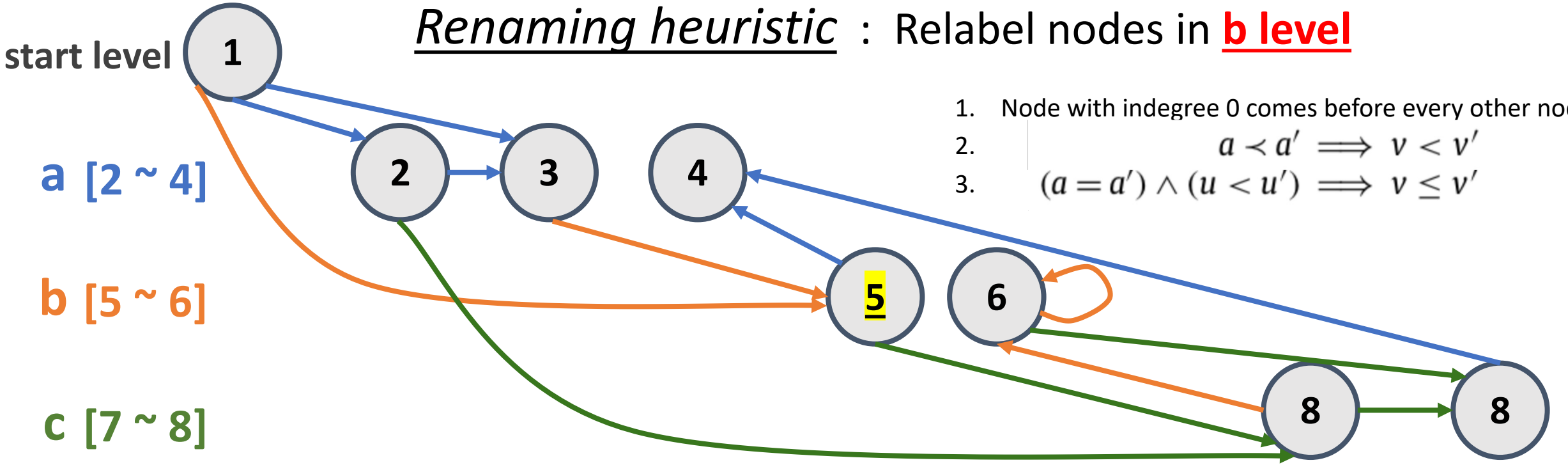


1. Node with indegree 0 comes before every other nodes.
2. $a \prec a' \implies v < v'$
3. $(a = a') \wedge (u < u') \implies v \leq v'$

In-node list:

start level	a level	b level	c level
1: Ø	2: 1	6: 1, 3	8: 2, 6
	3: 1, 4	6: 6, 8	8: 6, 8
	4: 6, 8		

Renaming heuristic : Relabel nodes in **b level**



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3. $(a = a') \wedge (u < u') \implies v \leq v'$

In-node list:

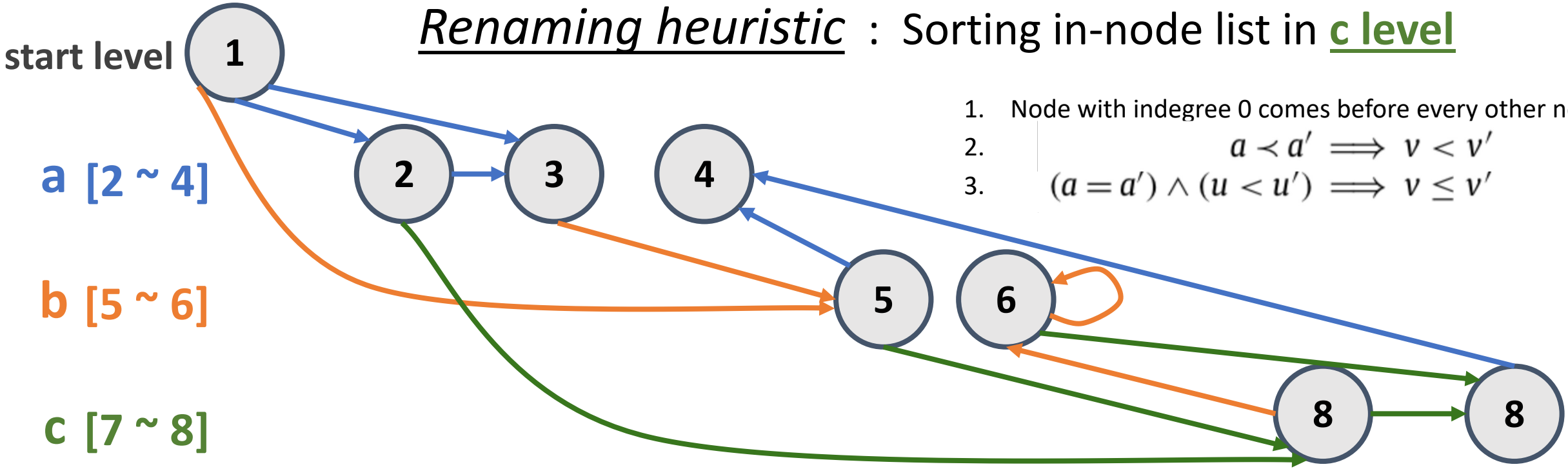
start level
1: Ø

a level
2: 1
3: 1, 4
4: 6, 8

b level
5: 1, 3
6: 6, 8

c level
8: 2, 5
8: 6, 8

Renaming heuristic : Sorting in-node list in c level

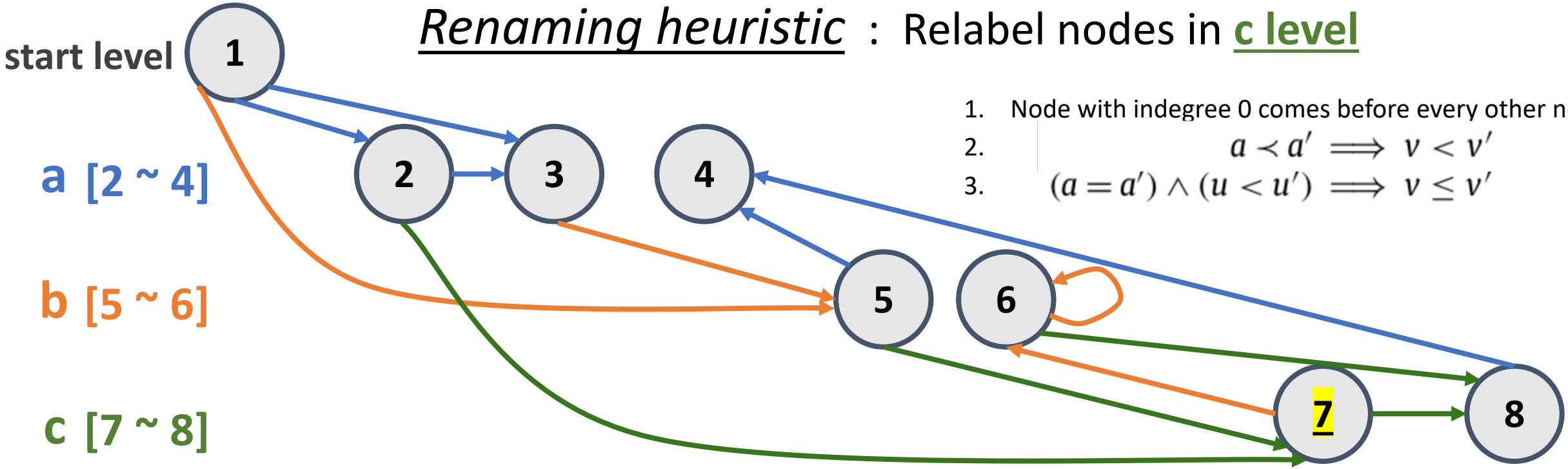


1. Node with indegree 0 comes before every other nodes.
2. $a \prec a' \implies v < v'$
3. $(a = a') \wedge (u < u') \implies v \leq v'$

In-node list:

start level	a level	b level	c level
1: Ø	2: 1	5: 1, 3	8: 2, 6
	3: 1, 4	6: 6, 8	8: 6, 8
	4: 6, 8		

Renaming heuristic : Relabel nodes in c level



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In-node list:

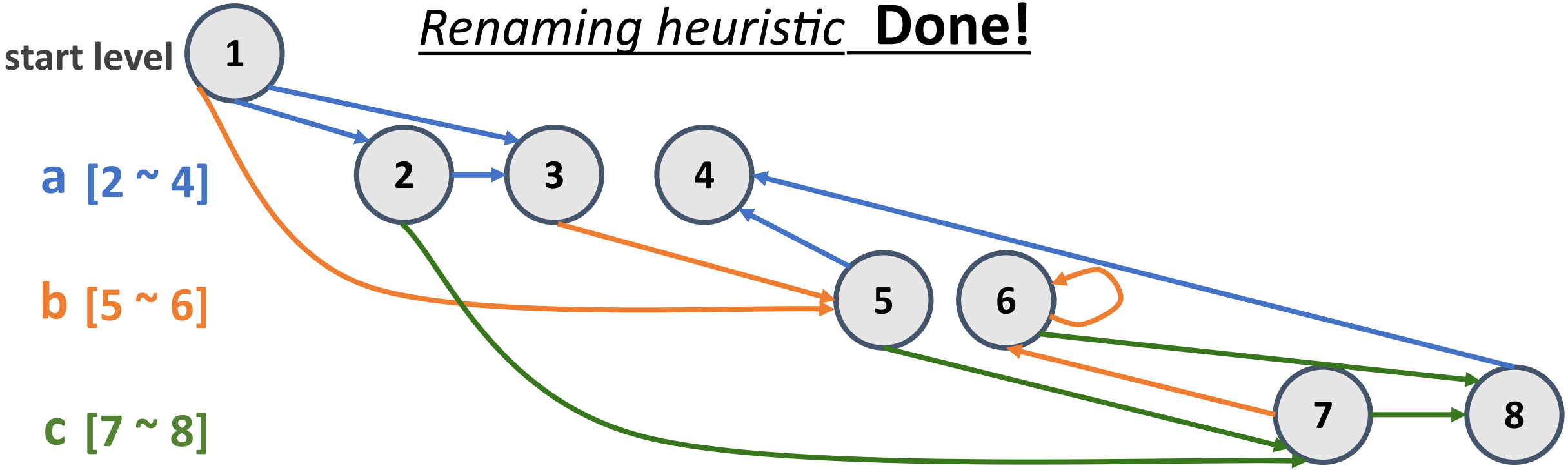
start level
1: Ø

a level
2: 1
3: 1, 4
4: 6, 8

b level
5: 1, 3
6: 7, 8

c level
7: 2, 6
8: 6, 8

Renaming heuristic **Done!**



In-node list:

start level
1: Ø

a level
2: 1
3: 1, 4
4: 6, 8

b level
5: 1, 3
6: 7, 8

c level
7: 2, 6
8: 6, 8

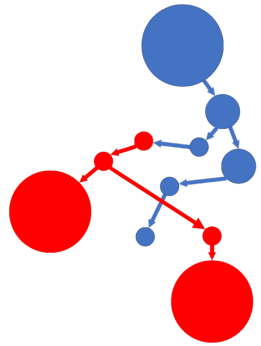
False

All nodes stabled

True

Solvers { Wheelie-PR, Wheelie-SMT

Our Contribution



WGT
Wheeler Graph Toolkit

- A Wheeler graph visualizer: bipartite representation

- ***Implemented the first Wheeler graph recognizer***

- Wheeler graph *generators*: Random WG / Trie / DBG / RDG

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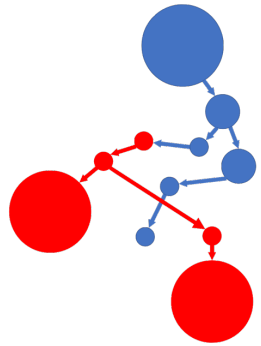

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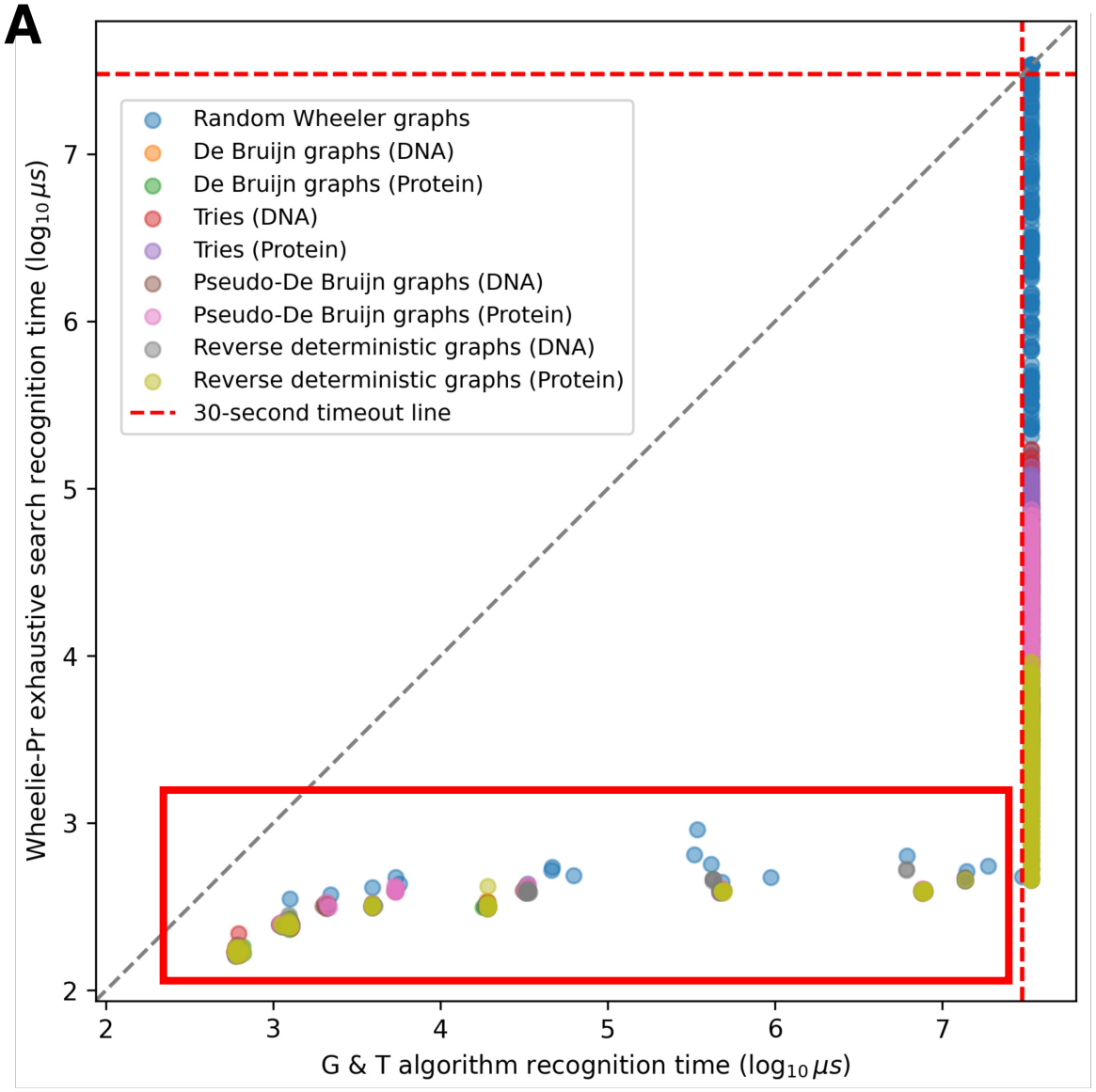
Comparing Wheelie-PR to G&T's algorithm

Timeout: 30 sec

25 multiple orthologue alignments (GENCODE REST API),

DNA & amino acid (AA) sequences.



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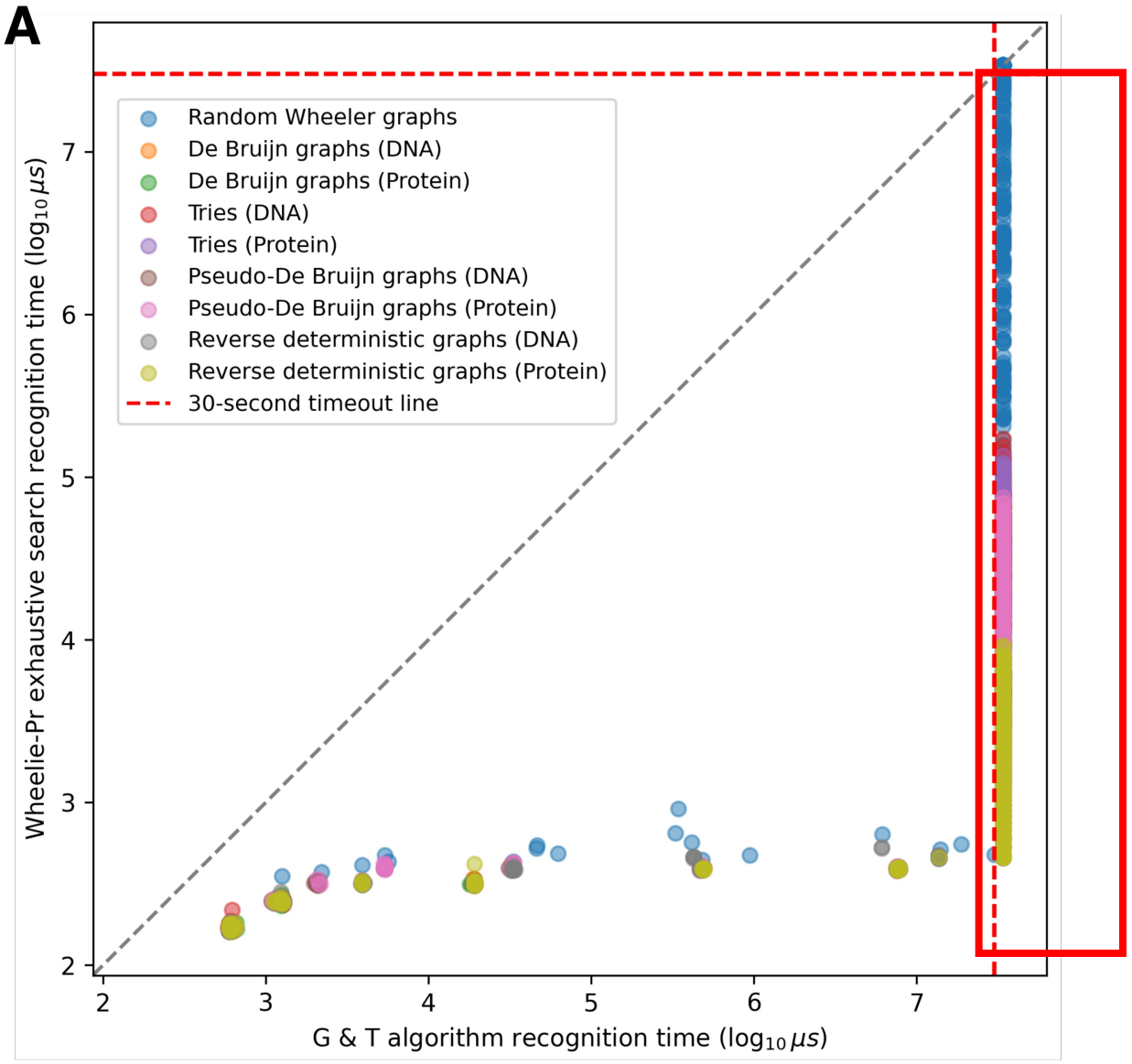

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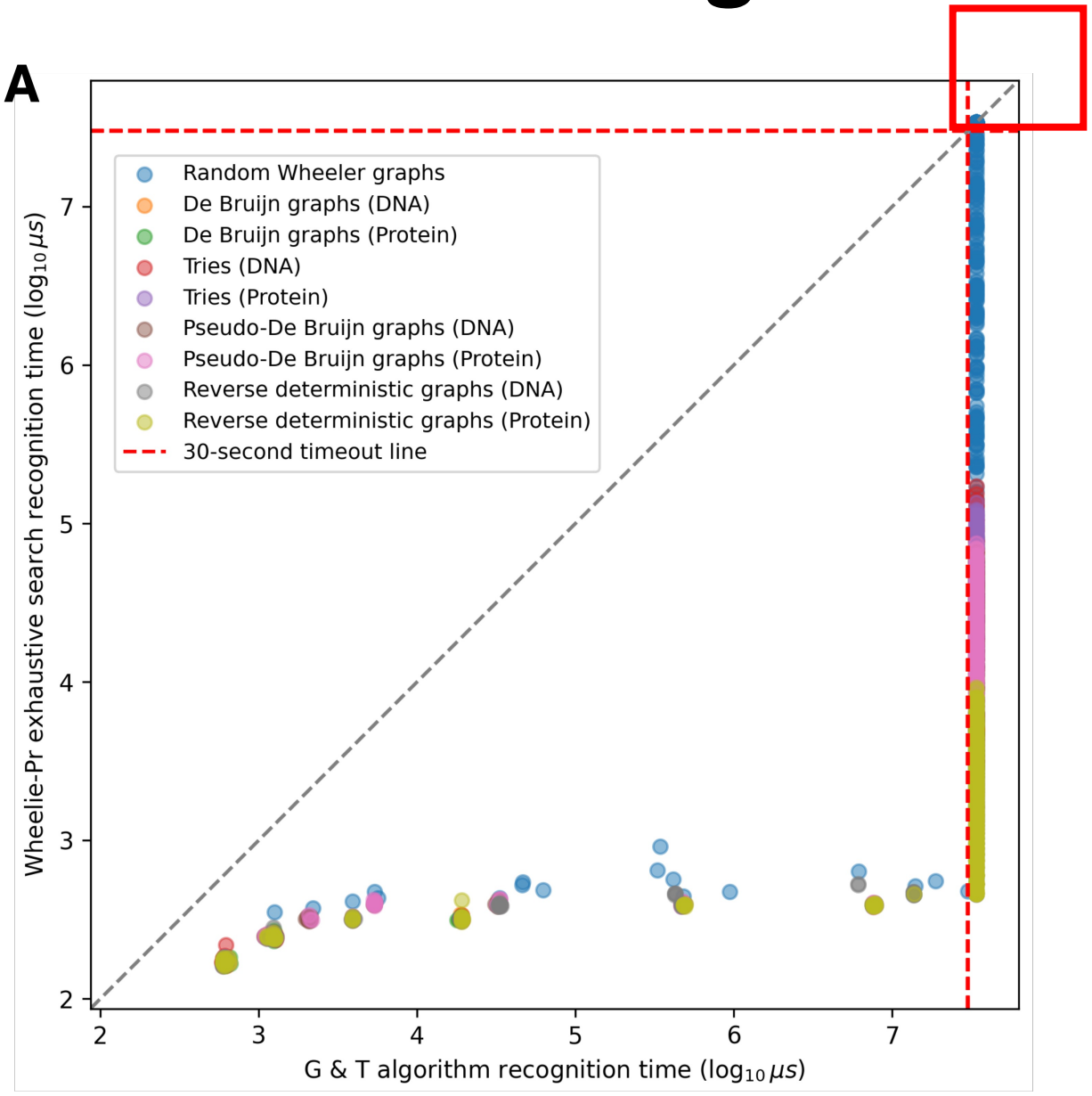

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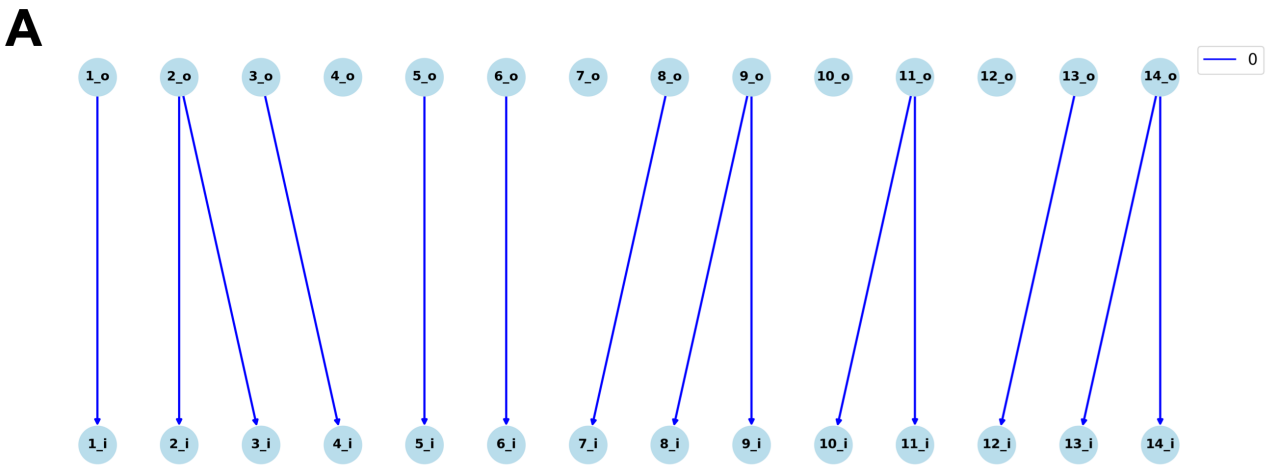
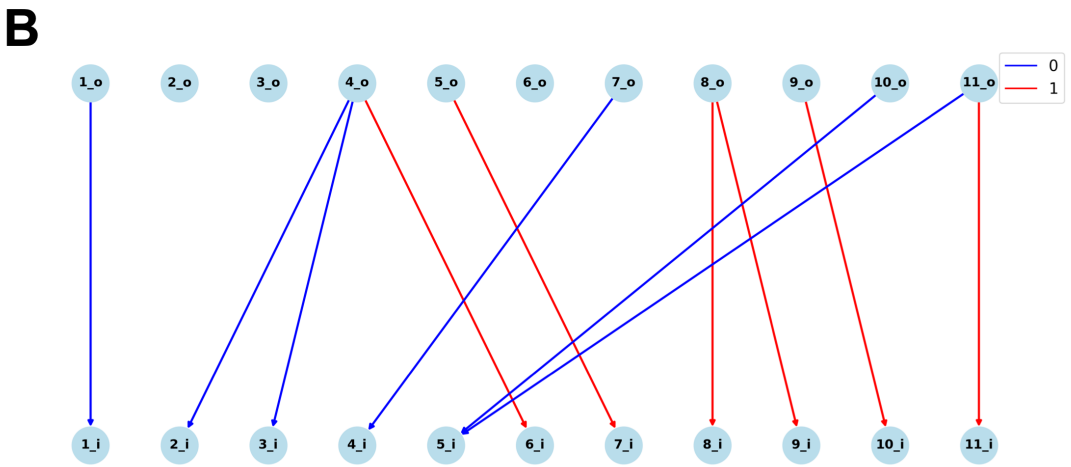
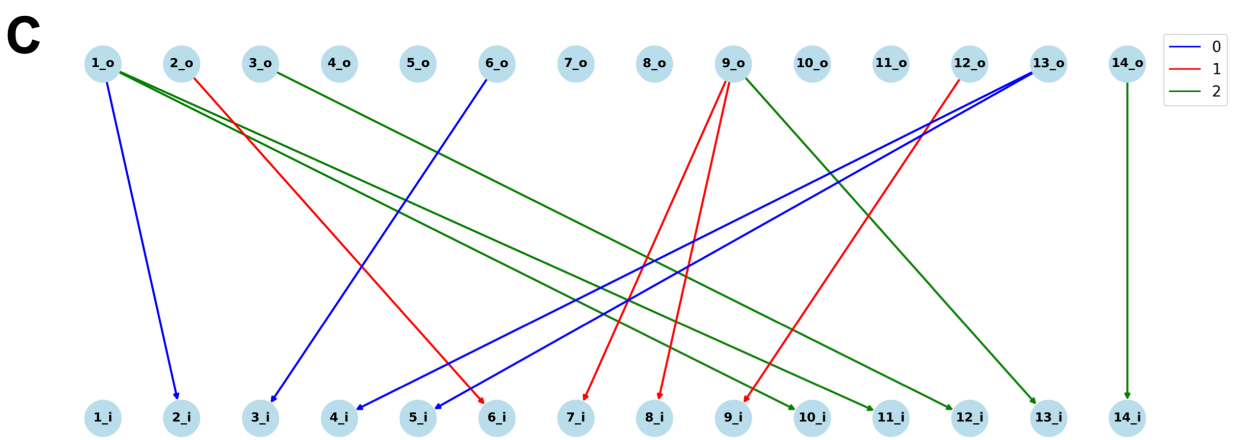
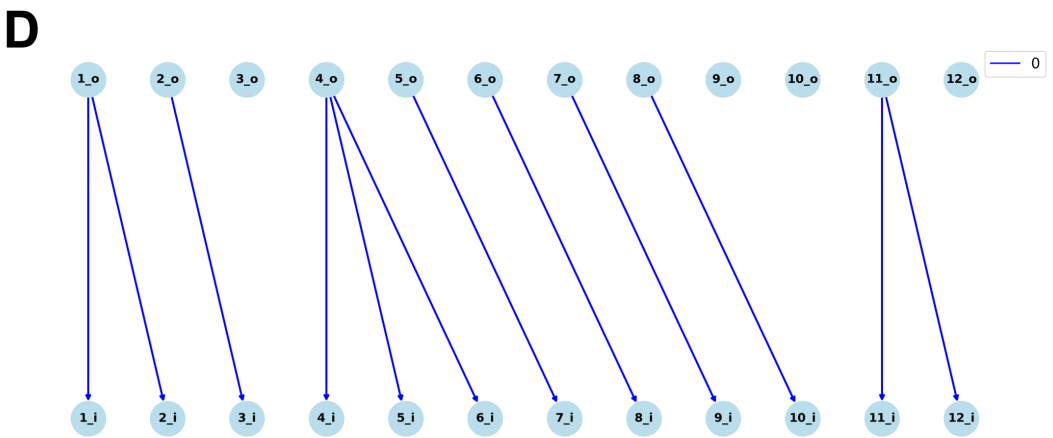








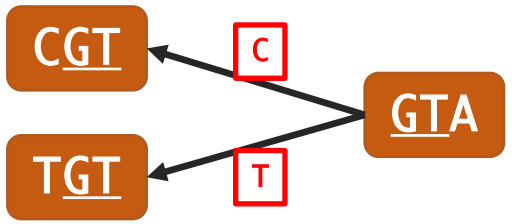
Hardness of Wheeler Graphs: d-NFA

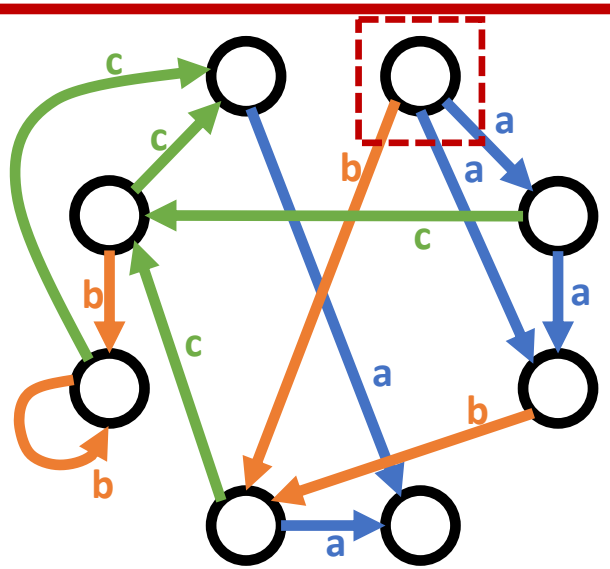
- A linear sequence can always be encoded as a Wheeler graph
  - Sorted Suffix order of reversed T (T^R)
  - It is **1-NFA** (simplest Wheeler Graph)

Definition

d-NFA : describing a Wheeler Graph where all nodes have ≤ d outgoing same-label edges, and at least one node has exactly d outgoing same-label edges.

- Harder graph: d-NFA, d > 1
  - 2 edges labelled as a coming out from the node
- Other 1-NFA Wheeler graphs
  - DeBruijn graph

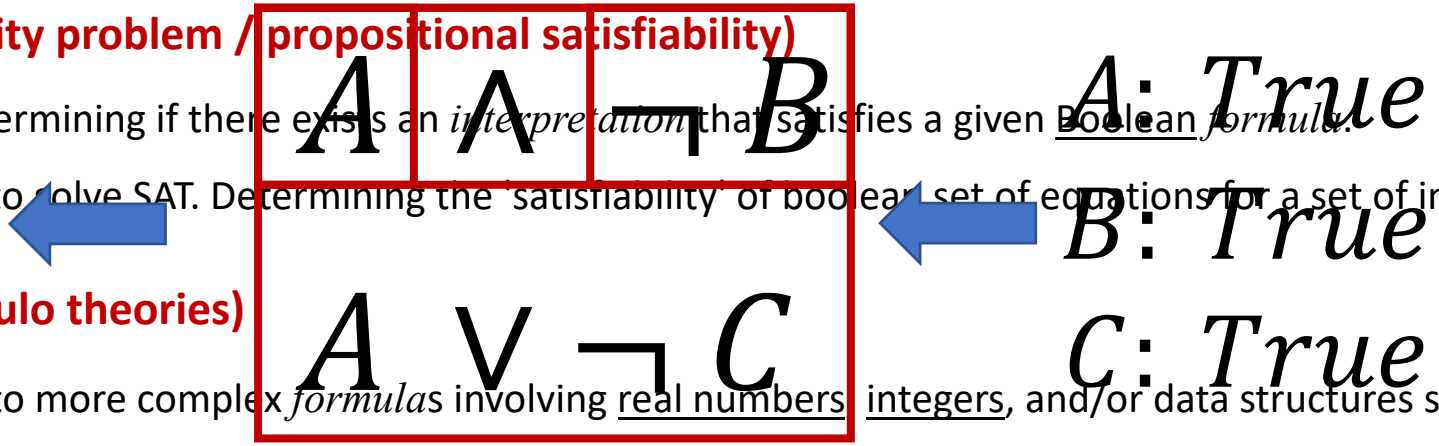




Satisfiability modulo theories (SMT)

- An ***atom*** is a basic unit of a logical expression (predicate) which can be `True` or `False`
- A ***literal*** is either an *atom* or its negation (¬).
- A ***formula*** is a set of *literals (atoms)* connected by Boolean connectives (∧, ∨, ¬),
- A ***theory*** is a set of *formulas* in the formal language
- An ***interpretation*** is an assignment of meanings to a *theory* and predicate symbols within the theory.

- **SAT (Boolean satisfiability problem / propositional satisfiability)**
  - is the problem of determining if there exists an *interpretation* that satisfies a given Boolean *formula*.
  - **SAT solver**: program to solve SAT. Determining the "satisfiability" of boolean set of equations for a set of inputs.
- **SMT (Satisfiability modulo theories)**
  - SMT generalizes SAT to more complex *formulas* involving real numbers, integers, and/or data structures such as lists, arrays, bit vectors, and strings.
  - decides the satisfiability of a first-order *formula* with respect to one or more background *theories*.



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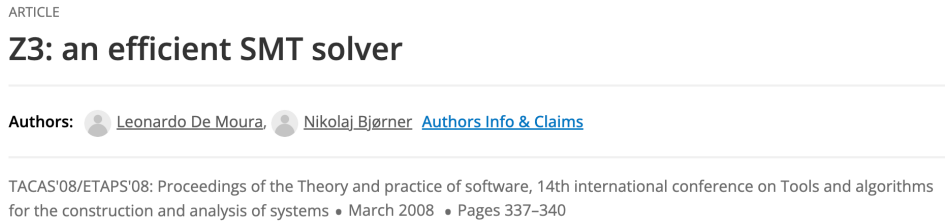
  - decides the satisfiability of a first-order *formula* with respect to one or more background *theories*.
- Only consider the **theory of *Integer Difference Logic (IDL)***,
  - requires *atoms* to be of the form $xi - xj \leq c$
- **A theory solver** decides the satisfiability of a conjunction of *literals*.
  - ***IDL theory solver*** => the Bellman-Ford algorithm (polynomial time).
- **SMT solver = SAT solver + IDL theory solver**
  - Input: a formula
  - Output: an assignment to the variables if the formula is satisfiable / unsatisfiable.

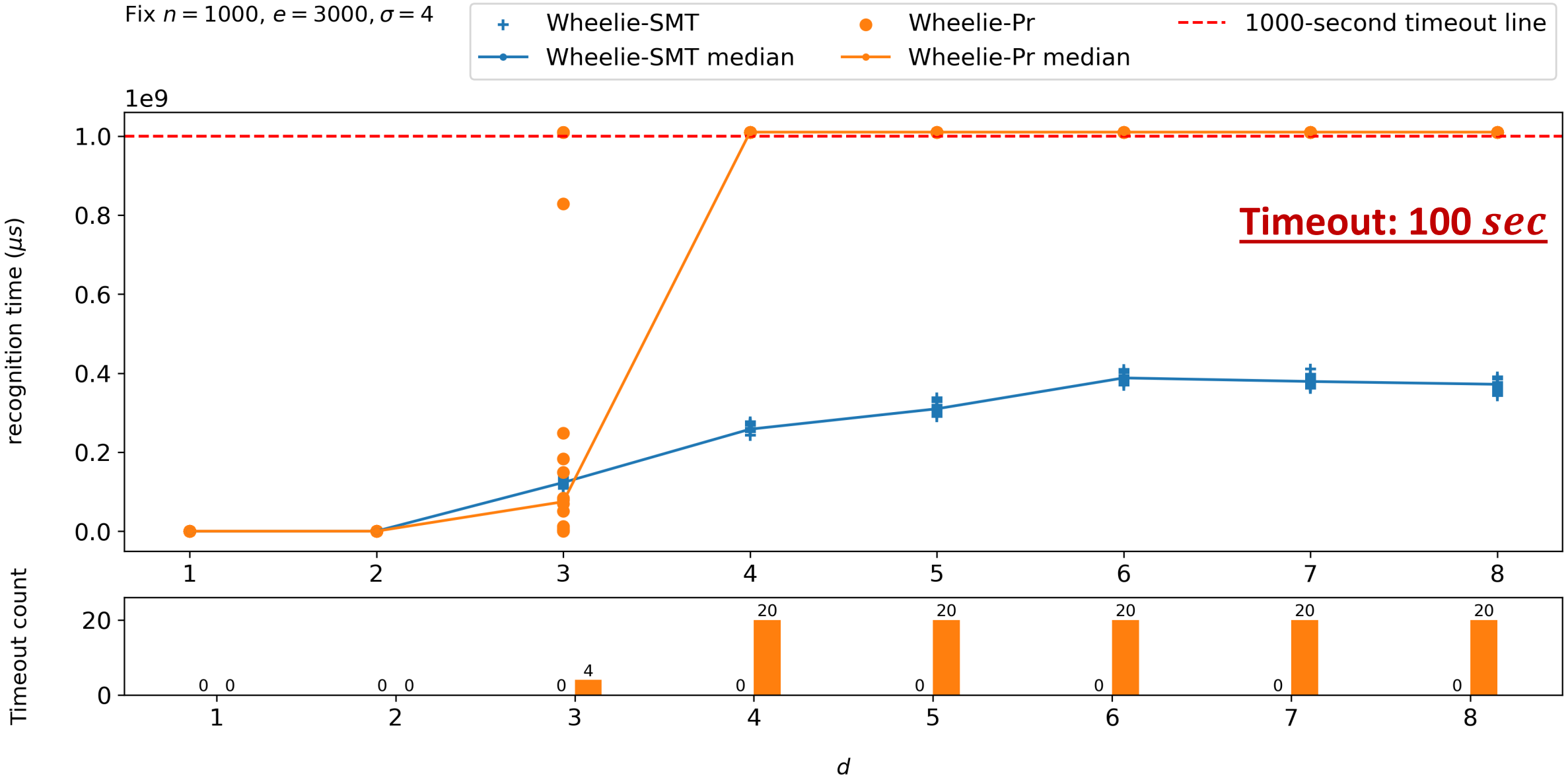

ARTICLE

Z3: an efficient SMT solver

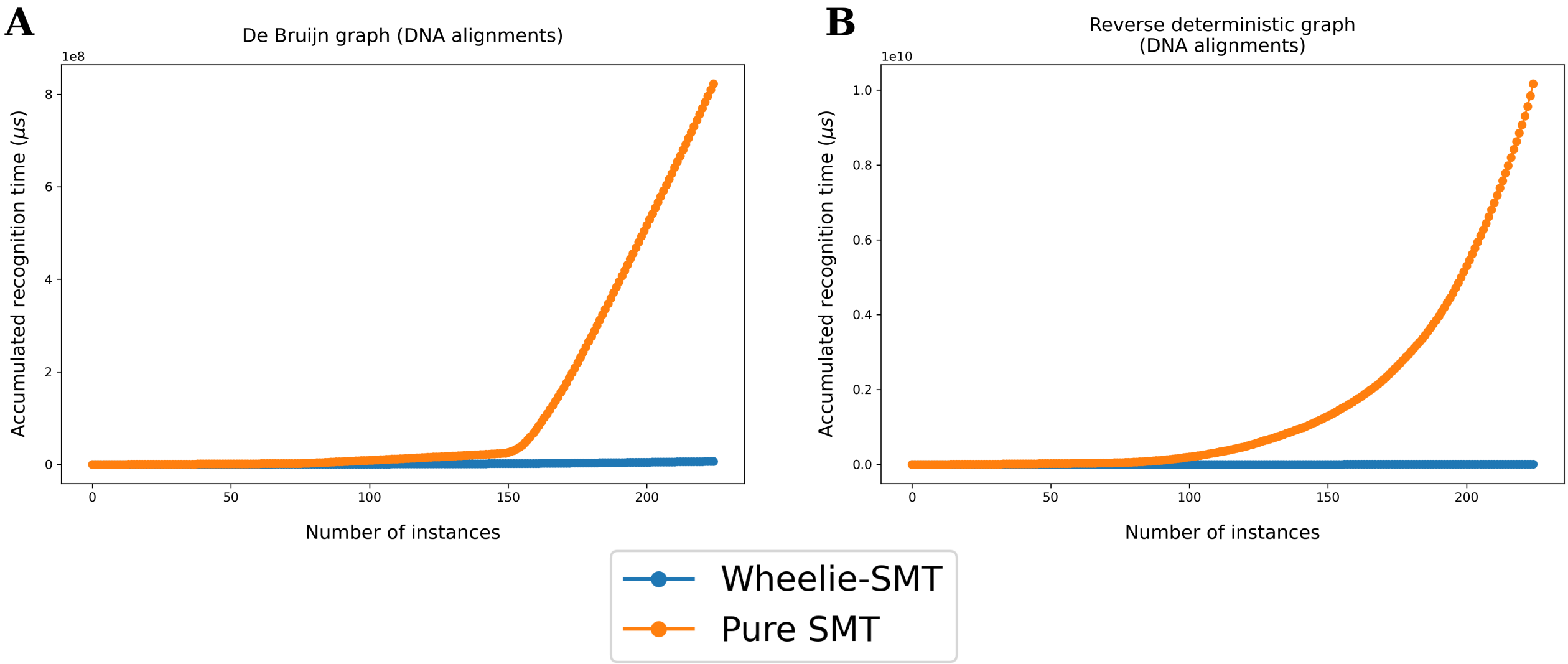
Authors: Leonardo De Moura, Nikolaj Bjørner Authors Info & Claims

TACAS'08/ETAPS'08: Proceedings of the Theory and practice of software, 14th international conference on Tools and algorithms for the construction and analysis of systems • March 2008 • Pages 337–340

Wheelie_SMT vs Wheelie_PR (d-NFA)



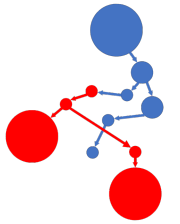
Wheelie_SMT vs Pure SMT



Conclusion

- A new Wheeler graph **recognizer**
  - Renaming heuristic + SMT
- A Wheeler graph **visualizer**: bipartite representation
- Wheeler graph **generators**: Random WG / Trie / DBG / RDG
- the recognizer is effective up to 3-NFA's, xx nodes.

Acknowledge



WGT
Wheeler Graph Toolkit

Project advisors:

Ben Langmead

Sanjit A Seshia

Co-first author:

Pei-Wei Chen

My PhD advisors:

Steven Salzberg

Mihaela Pertea

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R35GM139602 (MP.)
R01HG011392 (BL.)

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