Counting simple cycles

in the *de Bruijn* graph

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Minimizers in bioinformatics

word of length k

Definition *(minimizer)*. A minimizer scheme selects within each sliding window of w k-mers over a string S, the smallest of those k-mers (breaking ties on leftmost), with respect to some order $\mathcal{O}$.

Eg.

$$S = \texttt{ATTCCTAGA}$$

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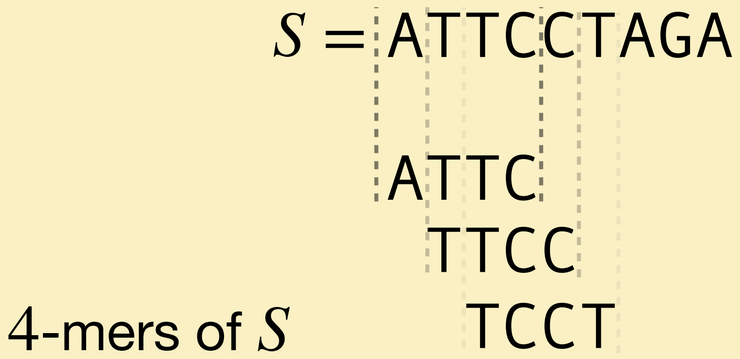

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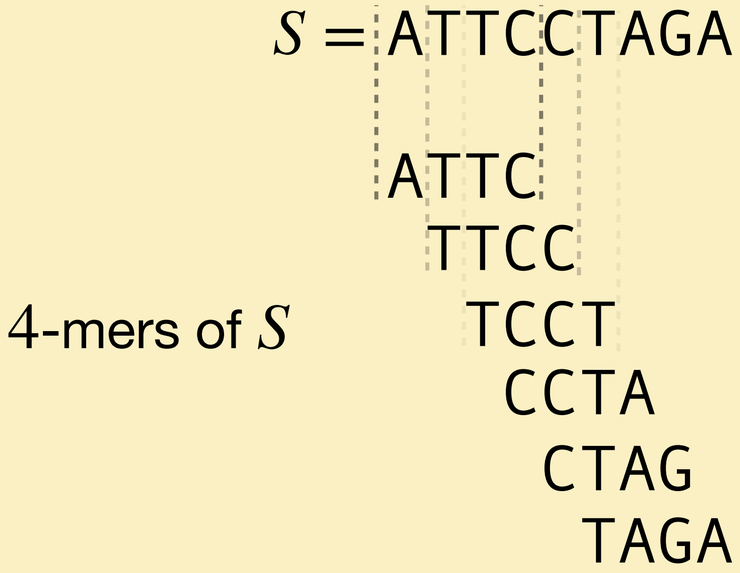

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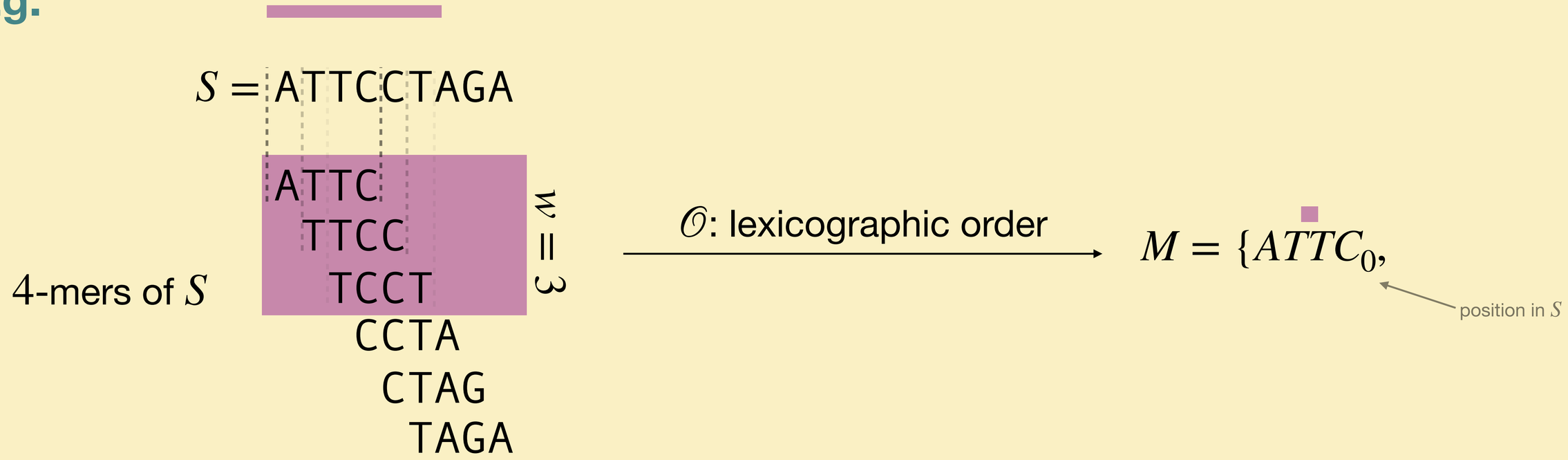

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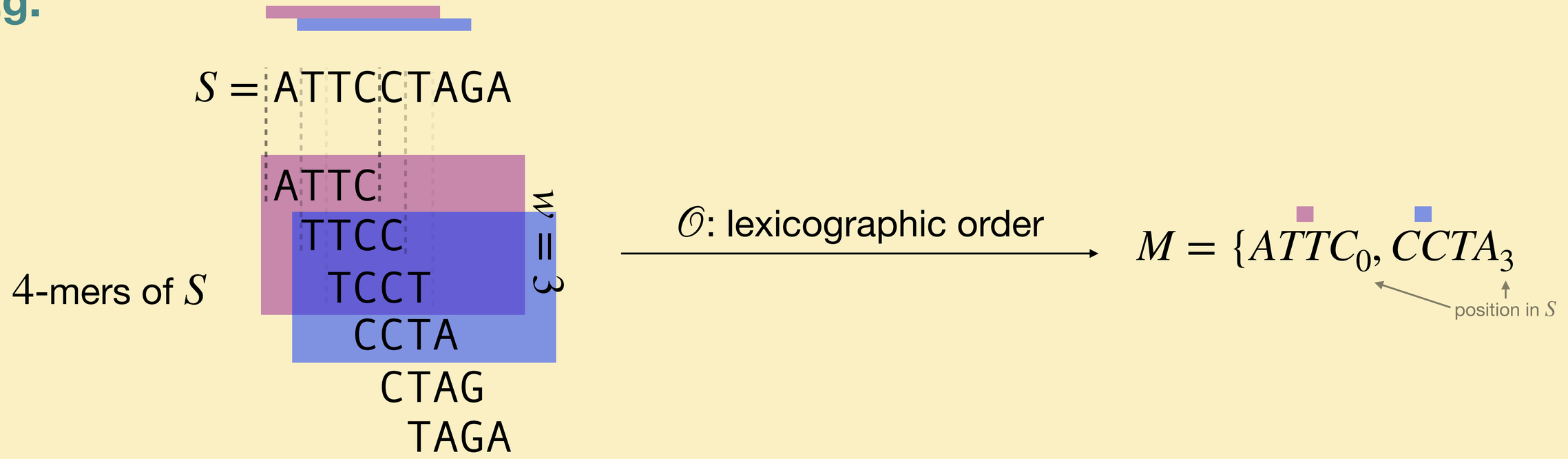

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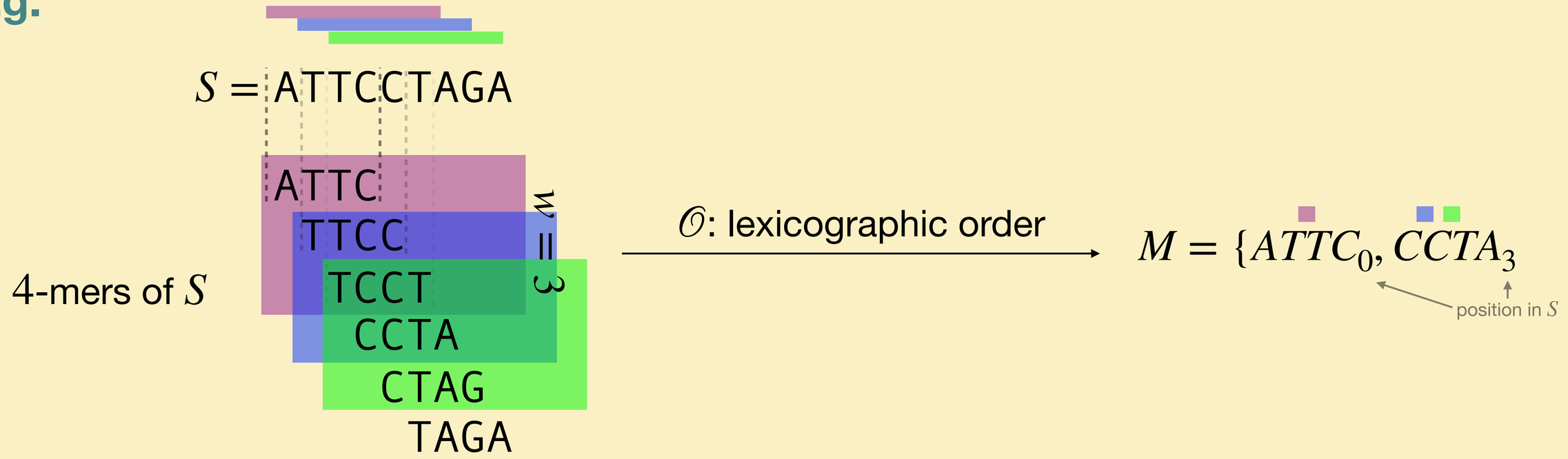

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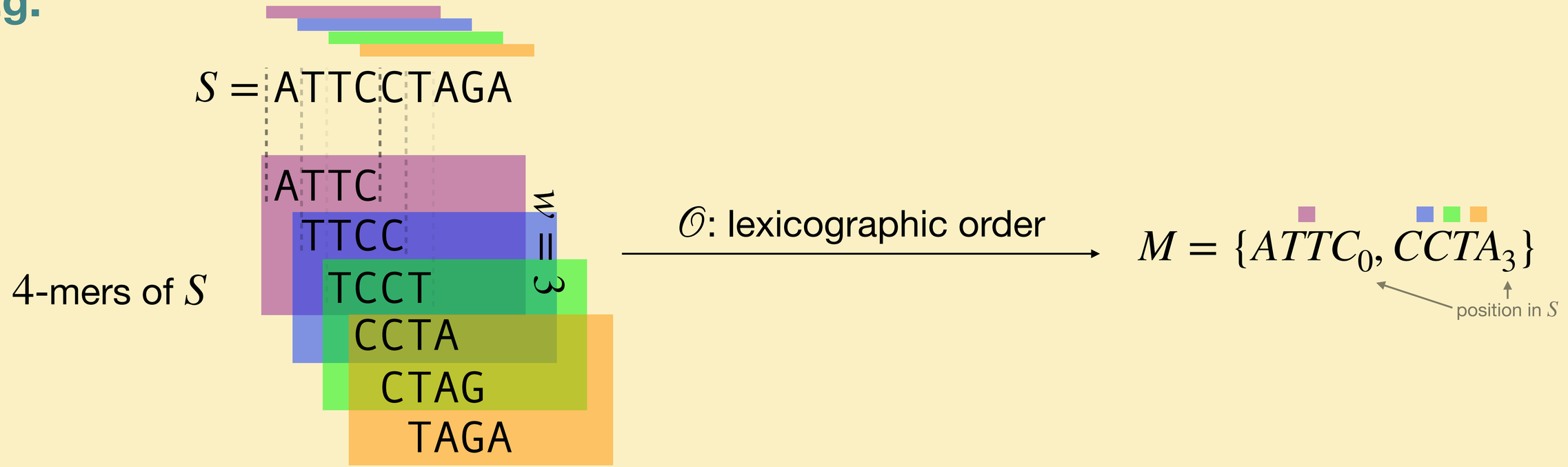

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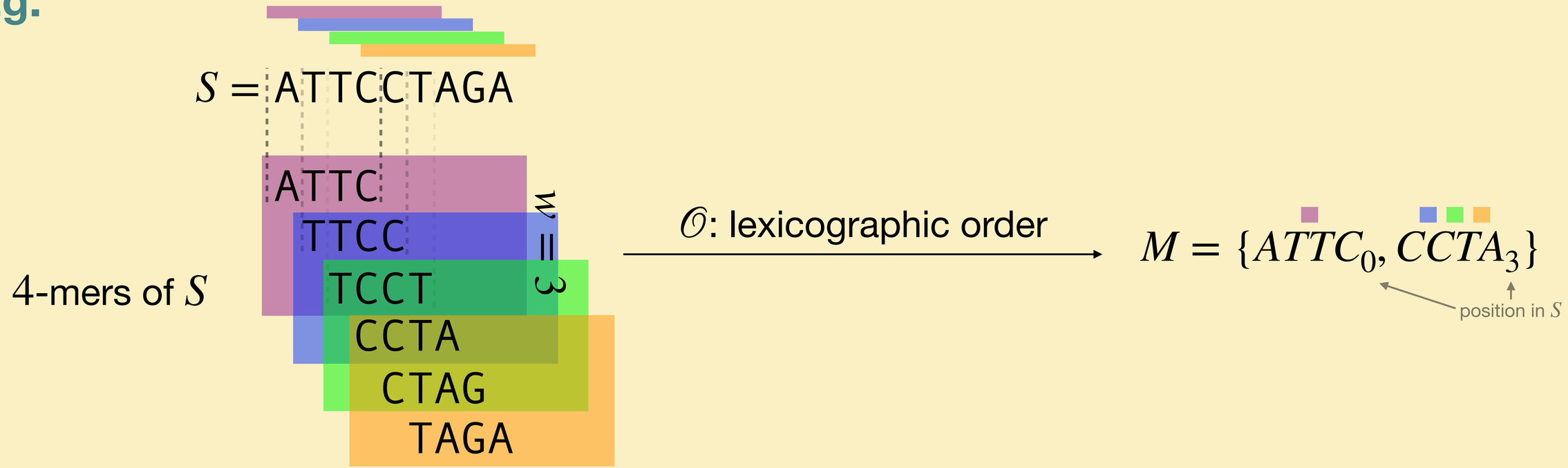


Typically, it holds that $|\mathscr{G}| \gg |\mathrm{sp}^k(\mathscr{G})| \gg |\mathrm{mnz}^{k,w,\mathcal{O}}(\mathscr{G})|$.

set of genomes — set of k-mers — set of minimizers

⇒ good for big data era

Applications of minimizers

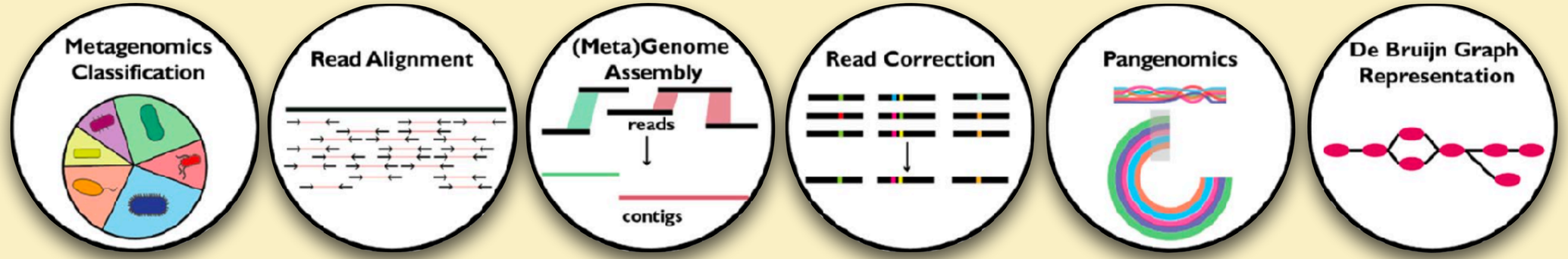
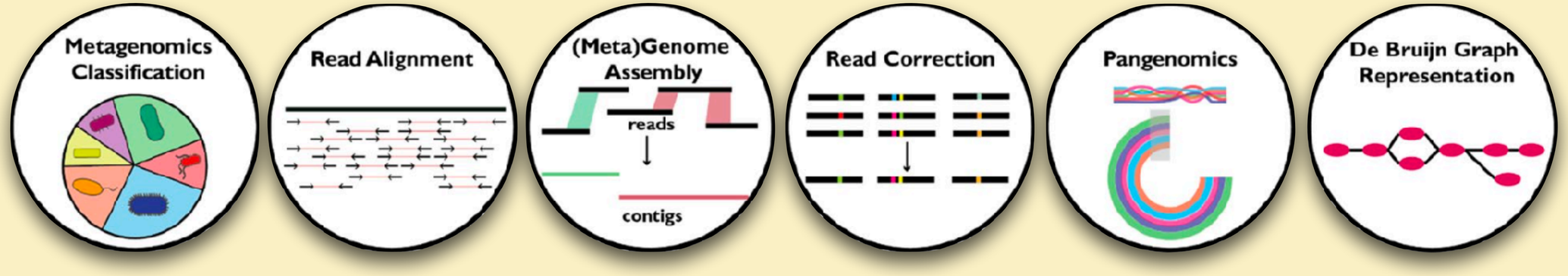


Figure from Ndiaye et al. "When less is more: sketching with minimizers in genomics" (2024)

Applications of minimizers



The sparser the better. The (specific) density of a minimizer scheme on a string S is

$$D = \frac{|\,\mathrm{mnz}^{k,w,\mathcal{O}}(S)\,|}{|S| - w - k + 2}\,.$$

It ranges somewhere within $1/w$ and 1.

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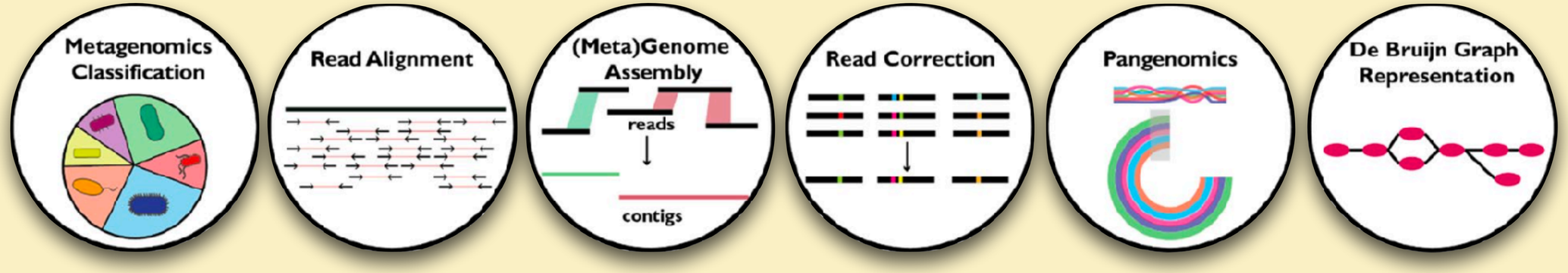

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- 1: every k-mer is selected
- $1/w$: a k-mer is selected as soon as it enters the windows and as long as it lies within it

Extremal examples *(on lexicographic order, $k = 4$, $w = 3$).*

- $S =$ CCACCACCACC (D = $1/w$)
- $S =$ AAAAAAAAAAAA (D = 1)

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Worst-case density of greedy minimizers

Definition *(greedy minimizer)*. The tie breaking rule favors the last selected minimizer, and takes the rightmost otherwise. This greatly reduces the density.

Eg.

Minimizer

Greedy minimizer

Sliding windows

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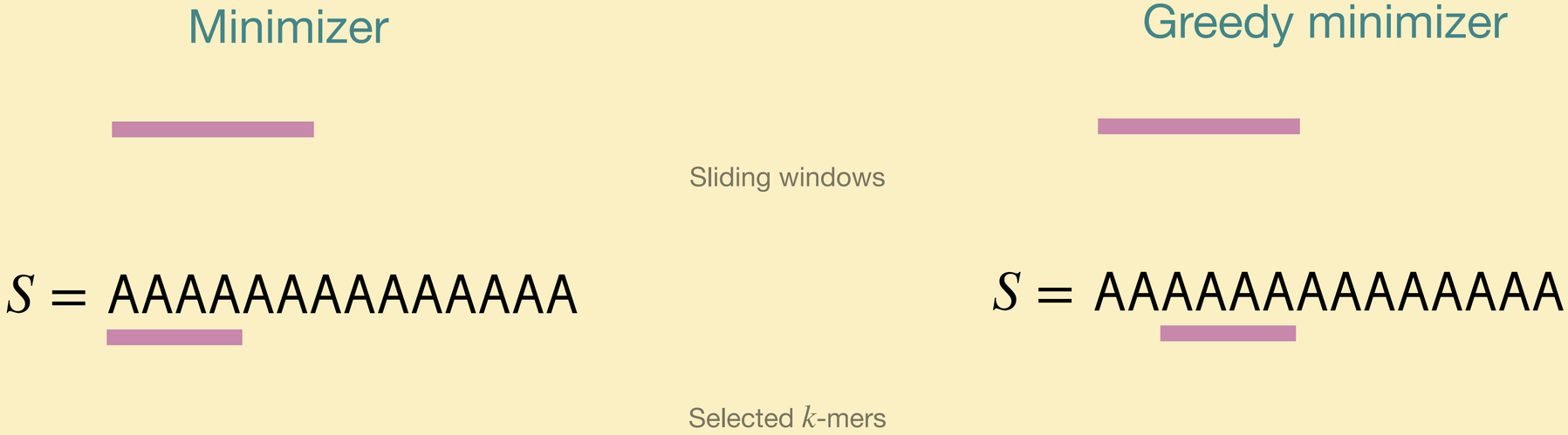

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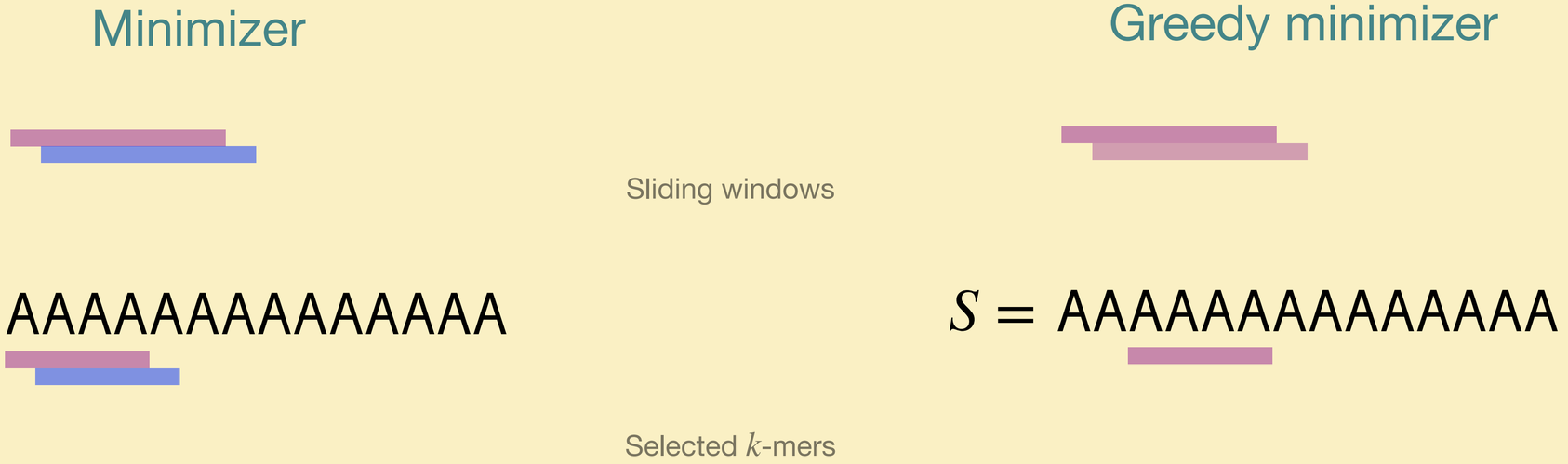

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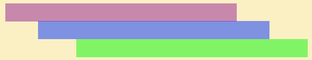

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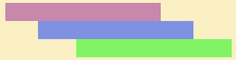

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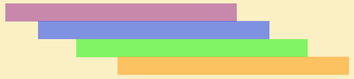

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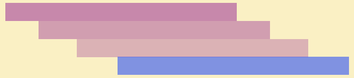

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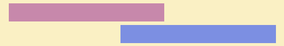

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Sliding windows

Selected k-mers

Greedy minimizer

D = $1/w$

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Eg.

Minimizer

D = 1

Sliding windows

Selected k-mers

Greedy minimizer

D = $1/w$

Research question. Given w and k, come with a couple $(\mathcal{O}, S)$ such that the specific density of the greedy minimizer $(w, k, \mathcal{O})$ on S is maximal.

What makes density increase?

Observation. There are two mechanisms that cause a greedy minimizer to change selected k-mer between consecutive windows:

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Research question *(rough reformulation)*. Come with an ordering on the vertices of the *de Bruijn* graph of order k such that there exist an increasing-then-decreasing path as long as possible in this dBG.

de Bruijn graphs

de Bruijn graph

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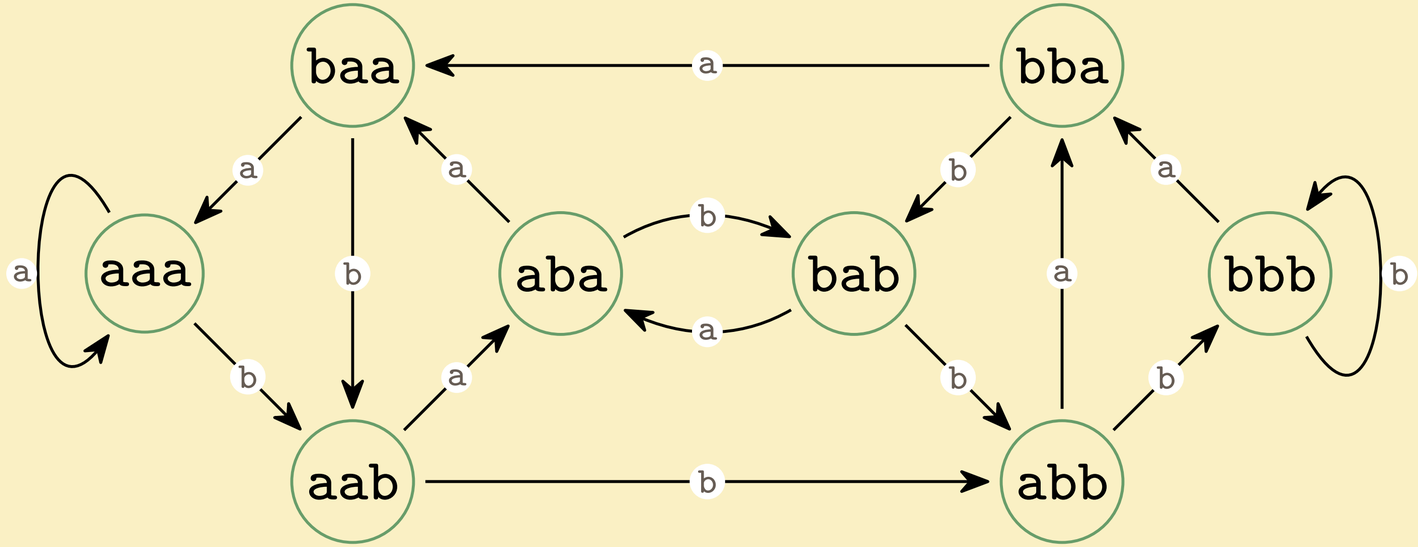

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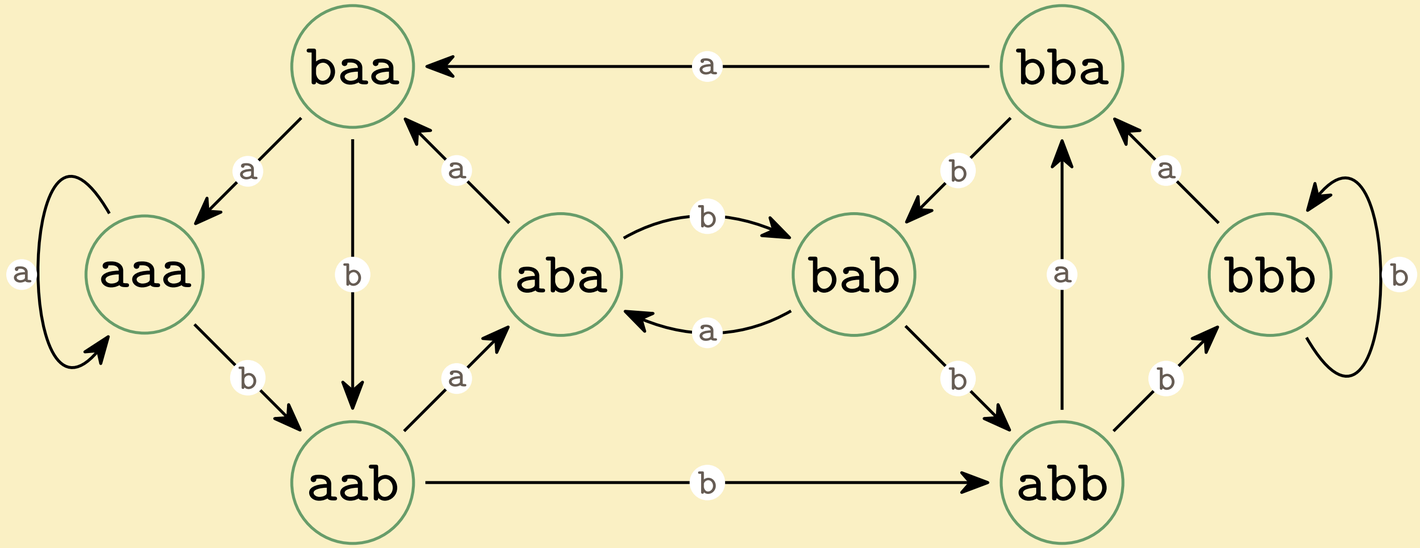

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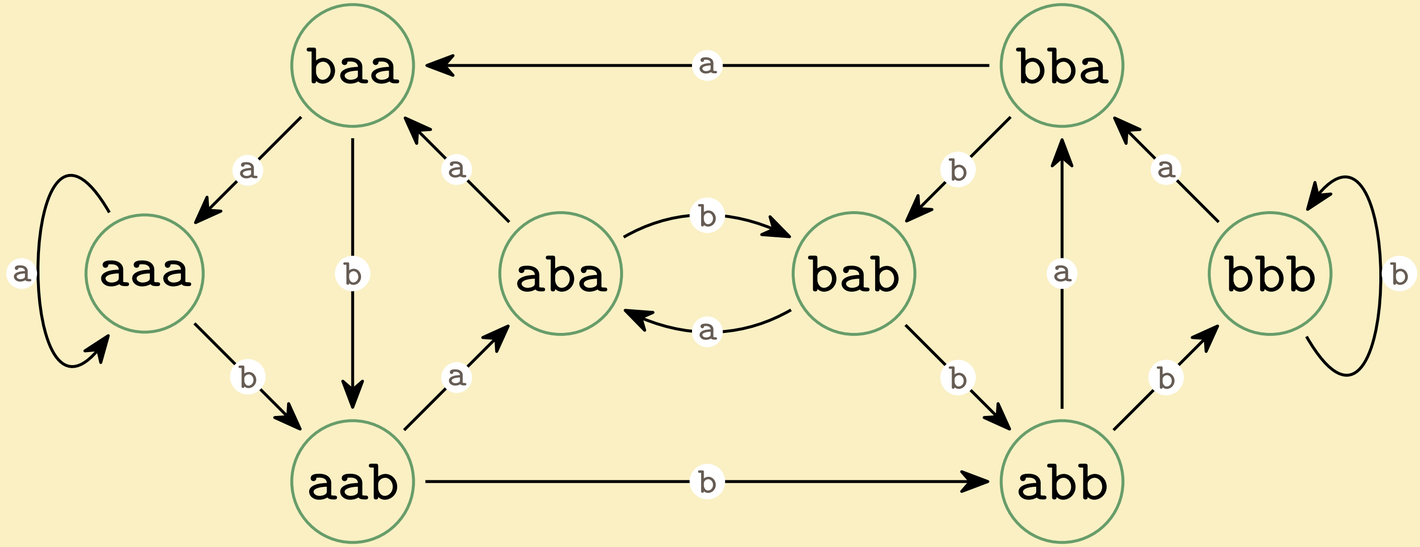

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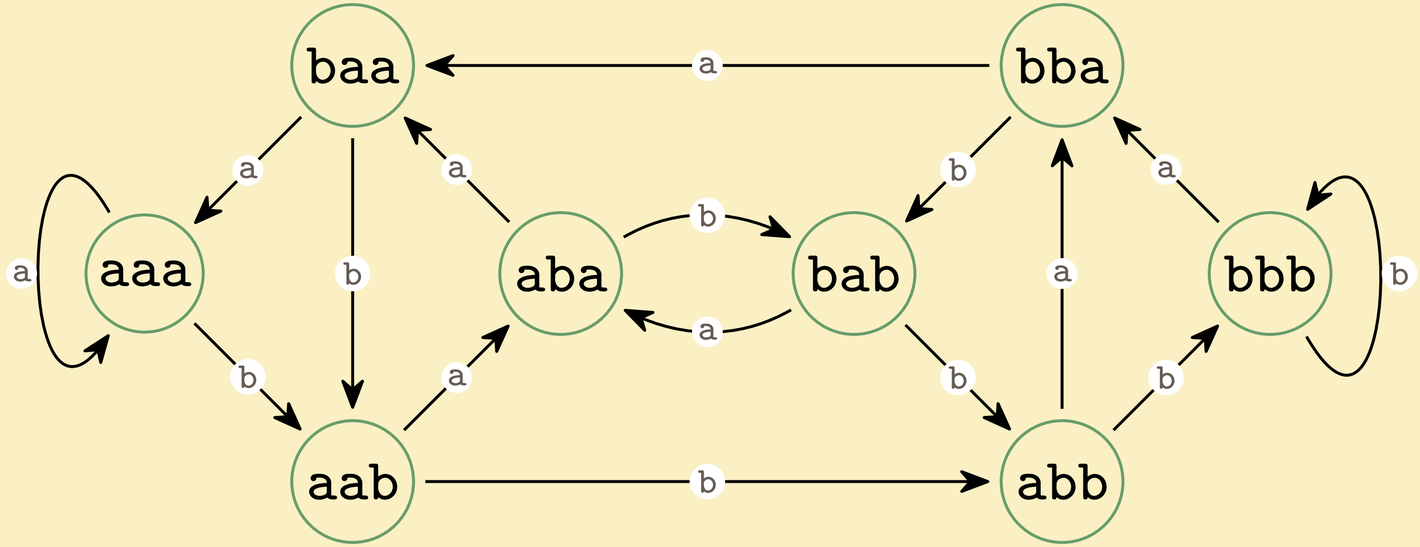

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Interest. Sliding windows (minimizers, compression schemes)

Counting simple cycles in the *de Bruijn* graph

Question. How many simple cycles of length ℓ live within the *de Bruijn* graph of order n over an alphabet made of σ letters?

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Outline.

- A bijection from simple cycles to a restriction of Lyndon words
- Reformulation of the state of knowledge
- Extending knowledge on simple cases (+ conjecture)
- A small CLI interface to count/enumerate simple cycles for the curious

Correspondence with restricted class of Lyndon words

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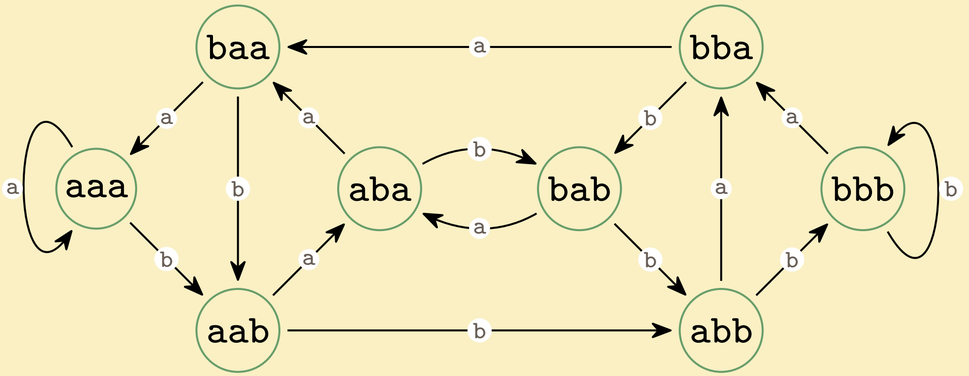
Lyndon word

Powering

Sliding window



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Lyndon word ab

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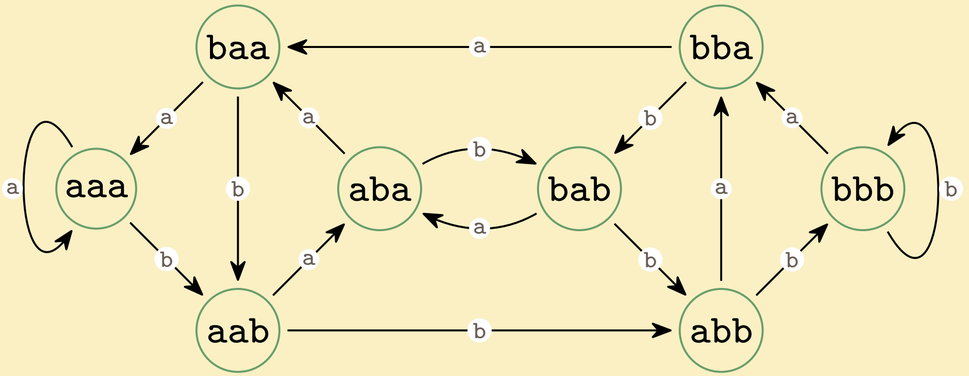

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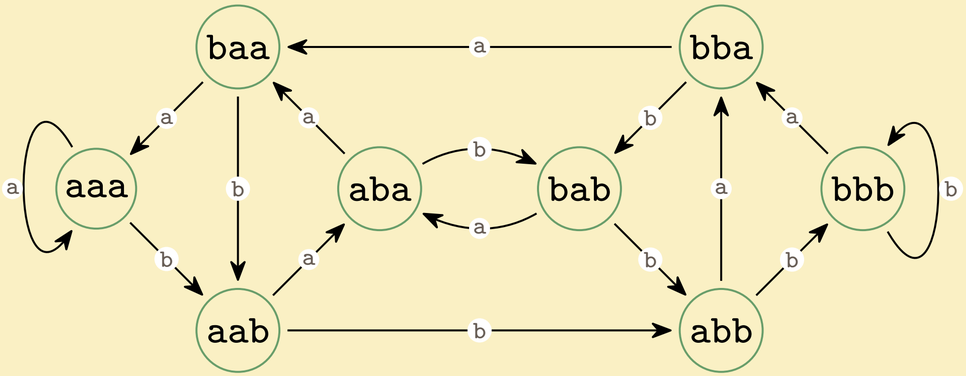
Sliding window	



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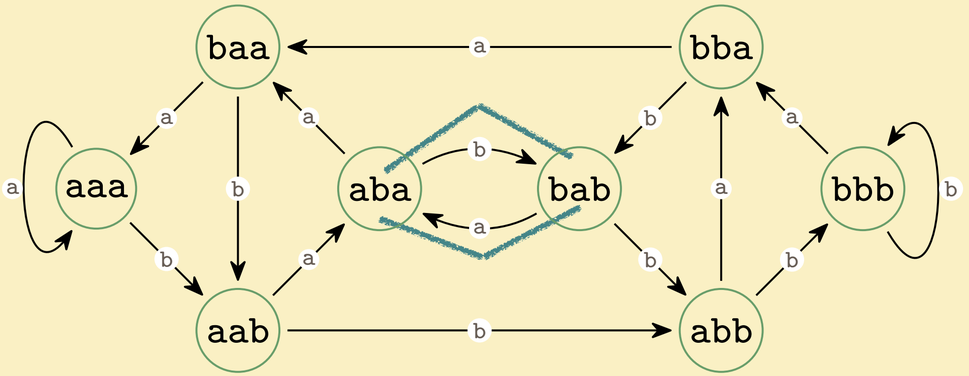

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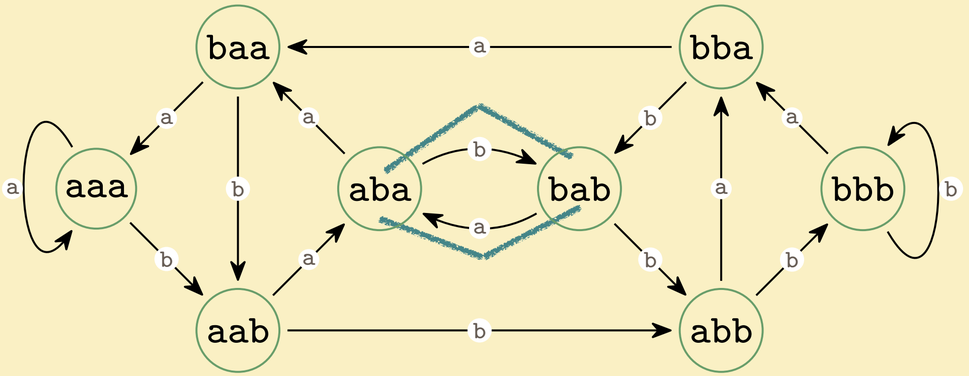

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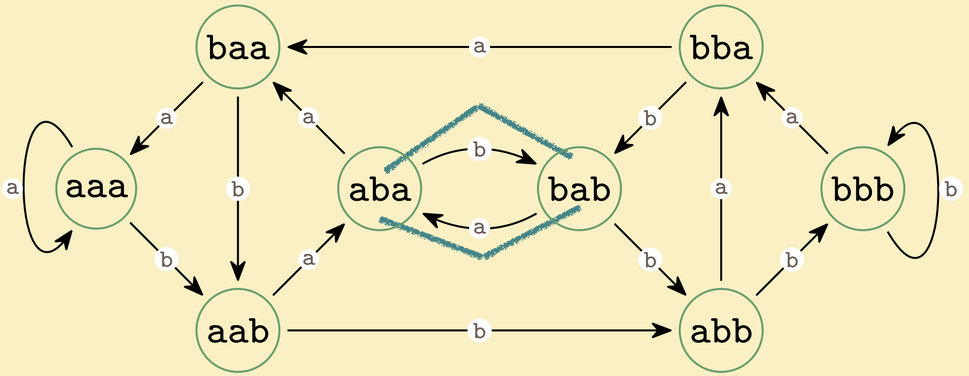

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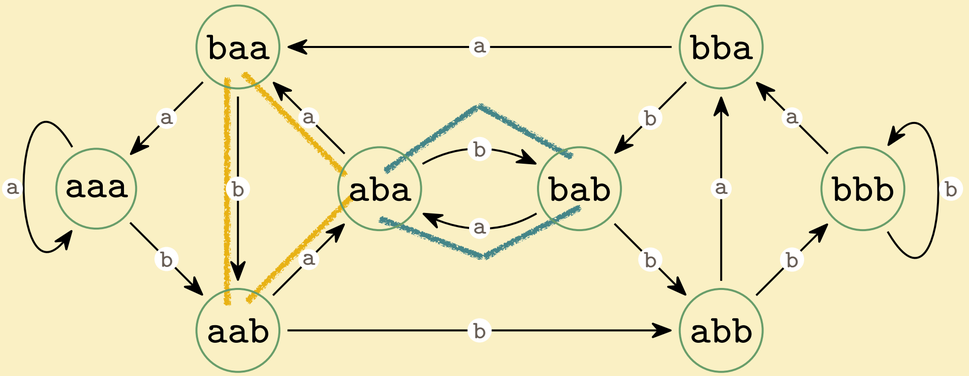

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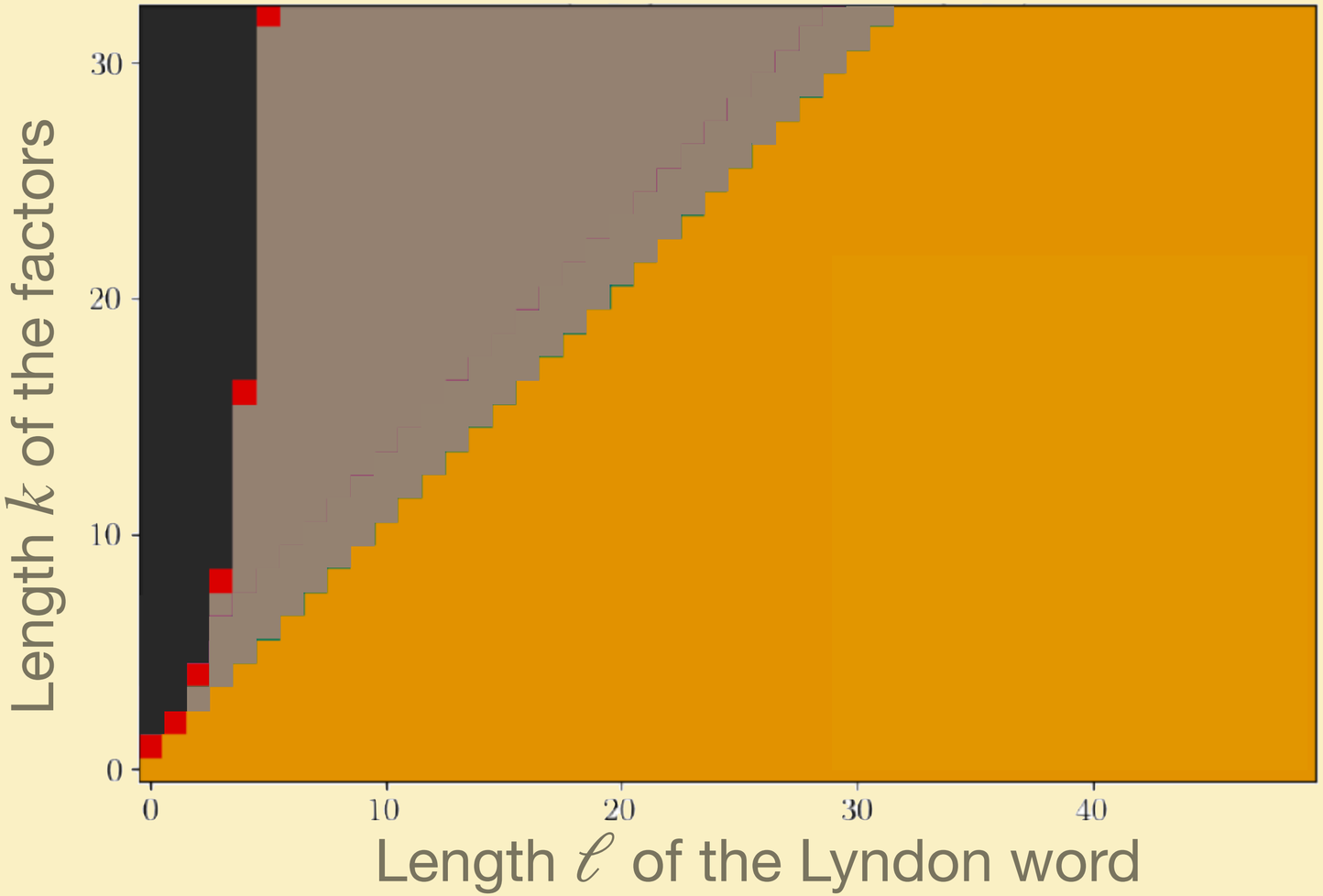
Question. How many k-perfect Lyndon words of length ℓ are there?

Counting simple cycles

State of knowledge



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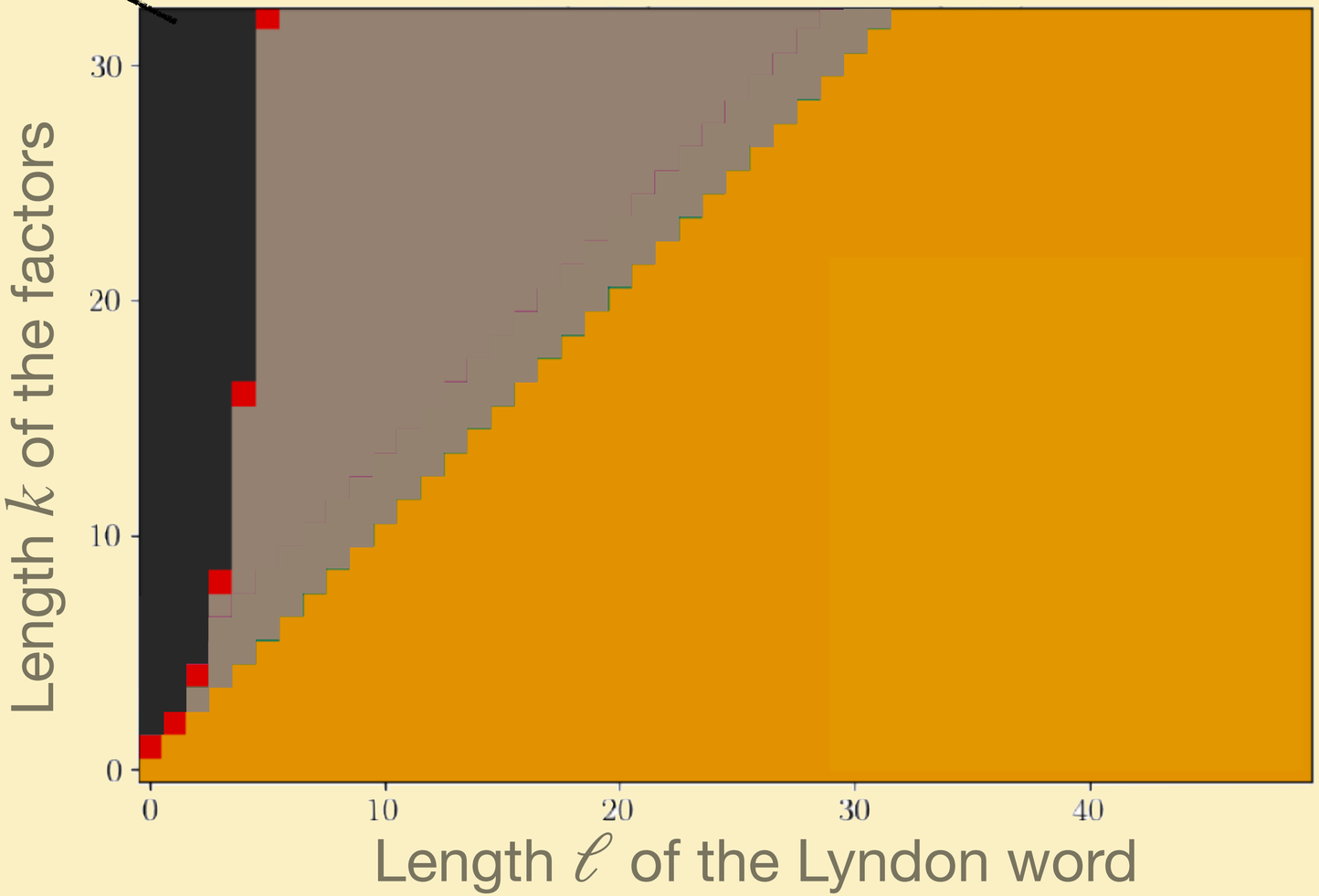
No such words (pigeonhole principle)



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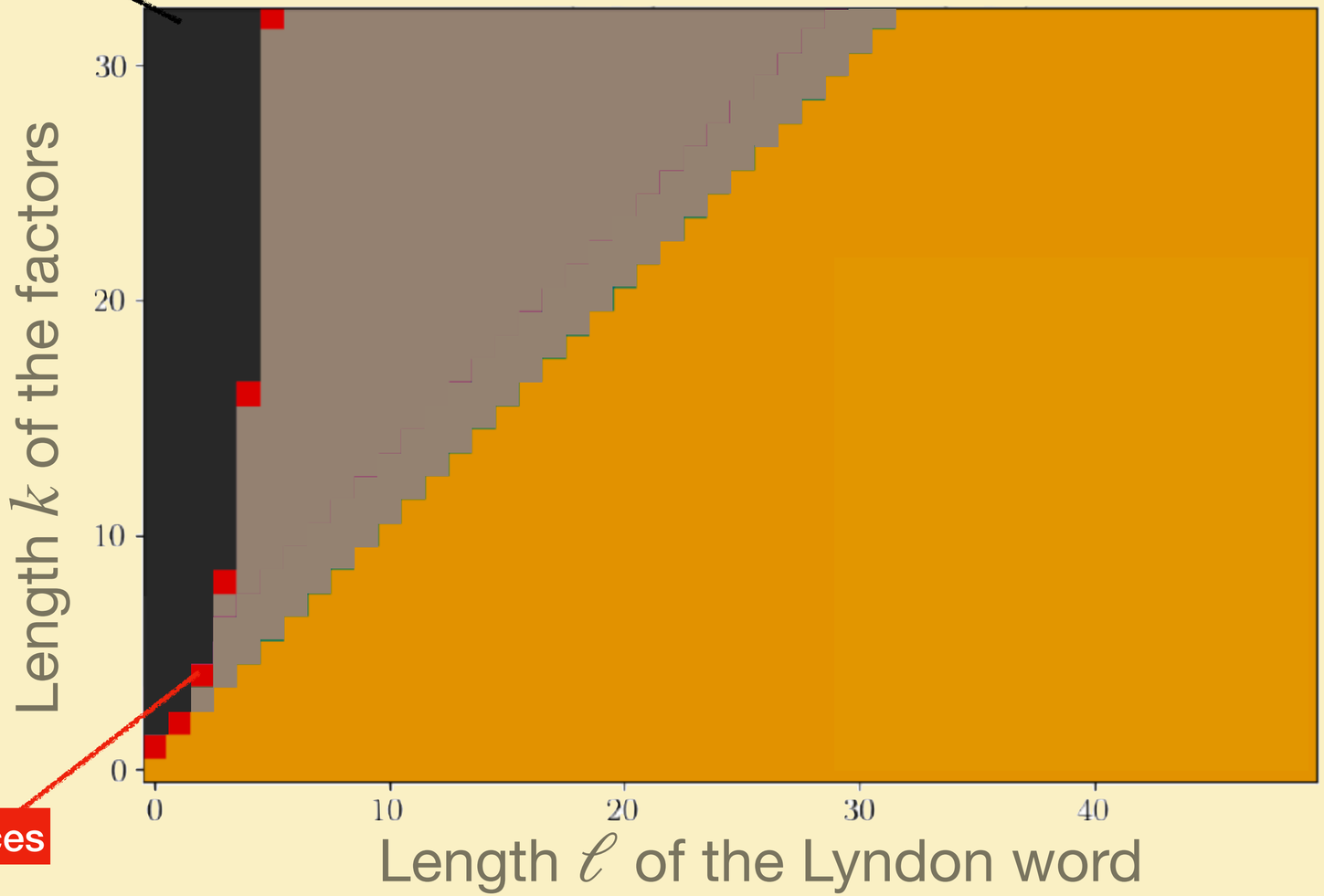

De Bruijn sequences

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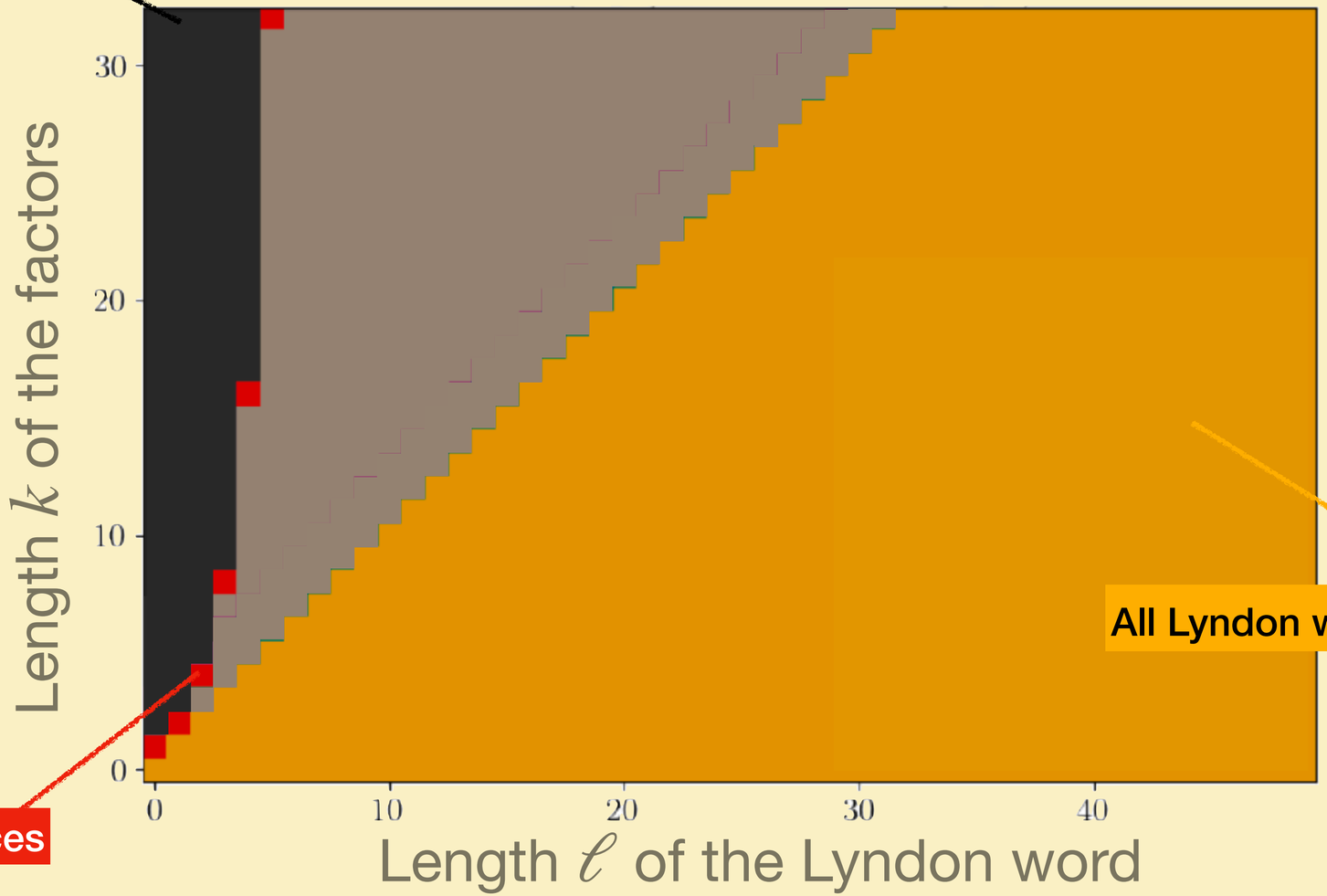

All Lyndon words are k-perfect ($k \geq \ell$)

De Bruijn sequences

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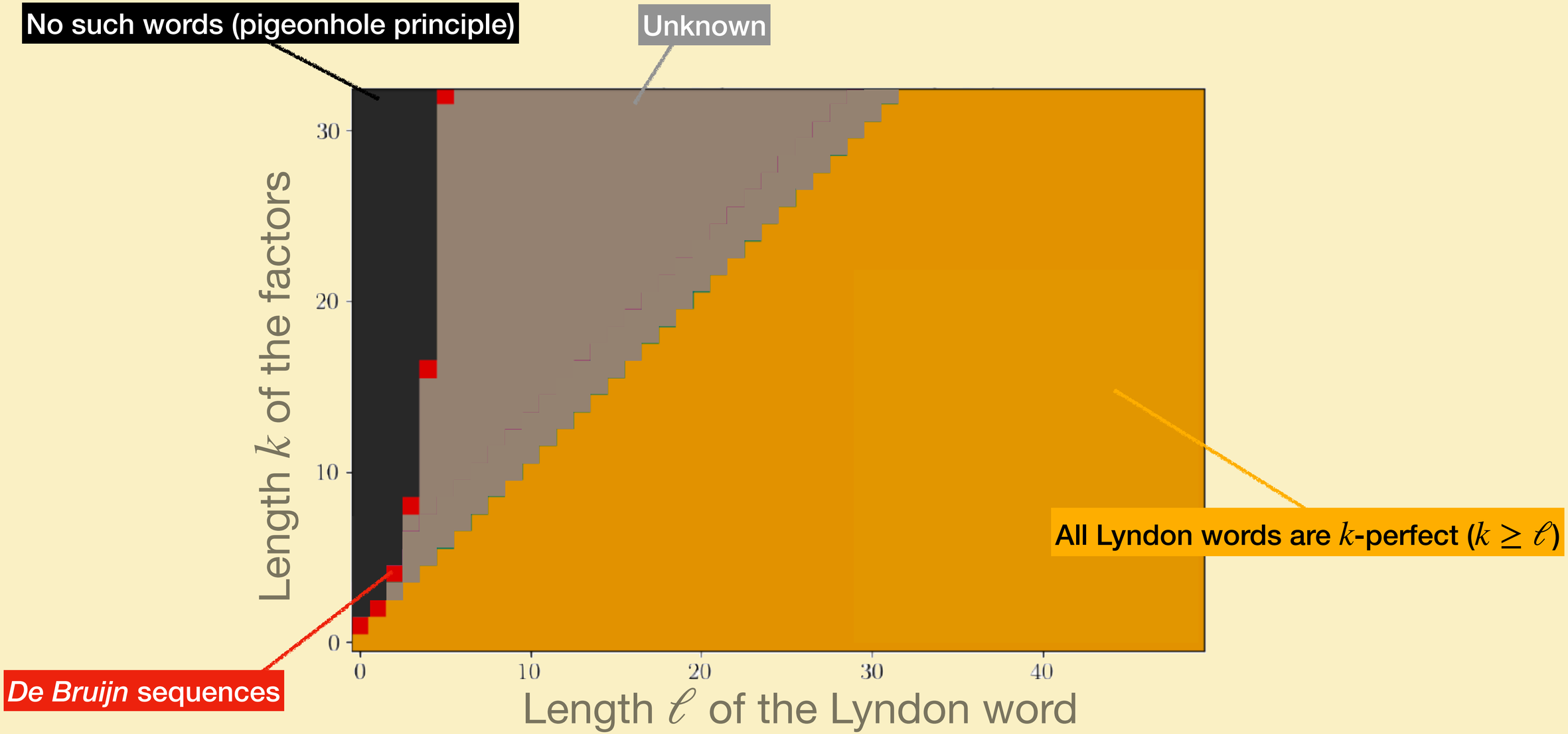

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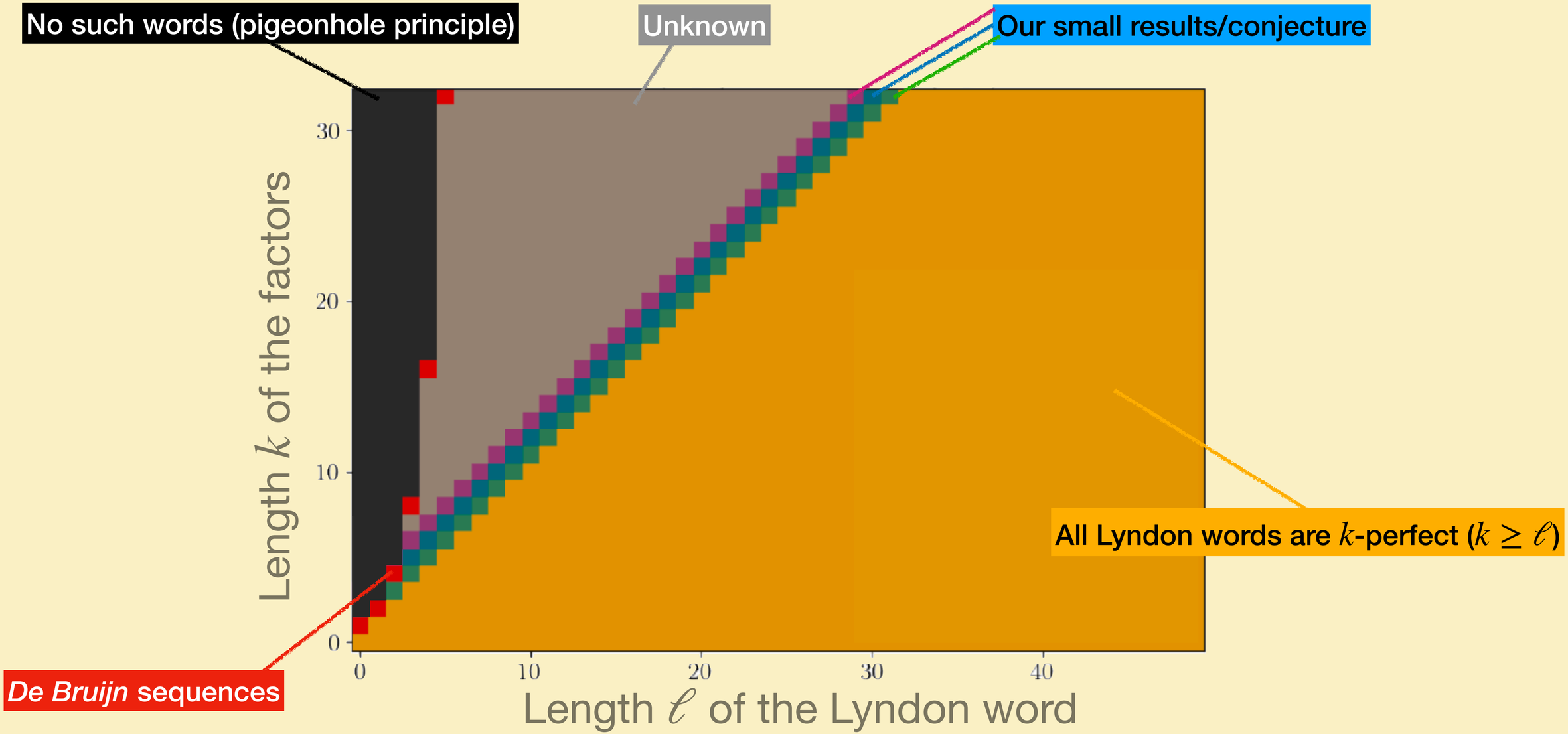

Establishing $\pi_\sigma(k, \ell = k+1)$

Proposition. A word w of length $k+1$ that admits a (circular) repeating factor of length k, necessarily **has a border**.

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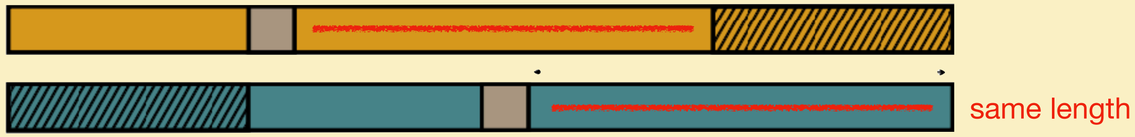

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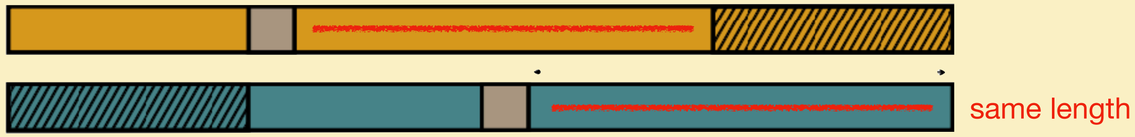

Consequently, such a word cannot be Lyndon.

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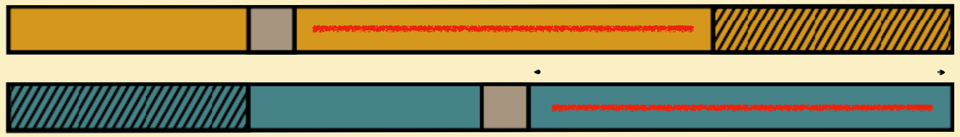


Consequently, such a word cannot be Lyndon.

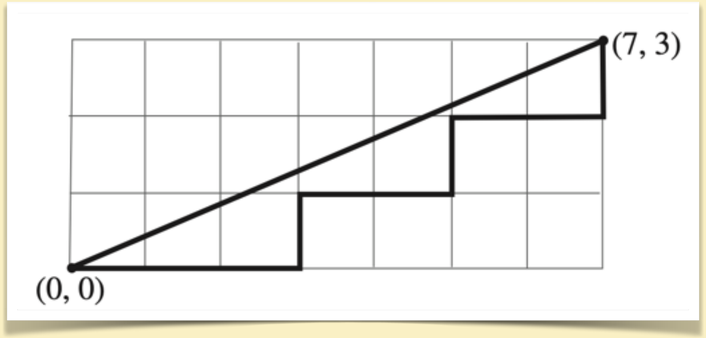
Corollary. All ℓ-long Lyndon words are k-perfect.

$$\pi_\sigma(k, \ell = k+1) = \lambda_\sigma(\ell)$$

Explicit formula exists

Establishing $\pi_\sigma(k, \ell = k+2)$

Definition *(Christoffel word)*. A word on a two-letter alphabet is a (lower) Christoffel word if it is obtained by discretizing a segment in the plane.



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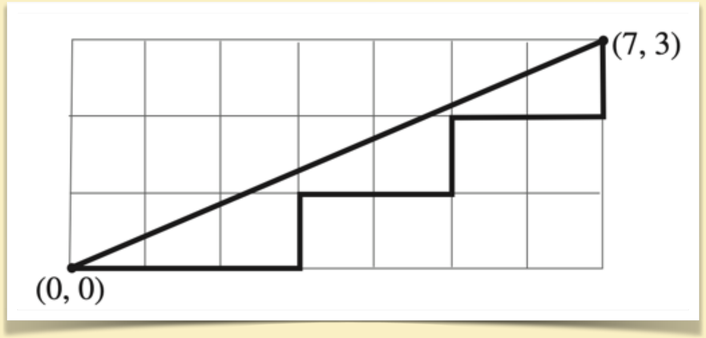

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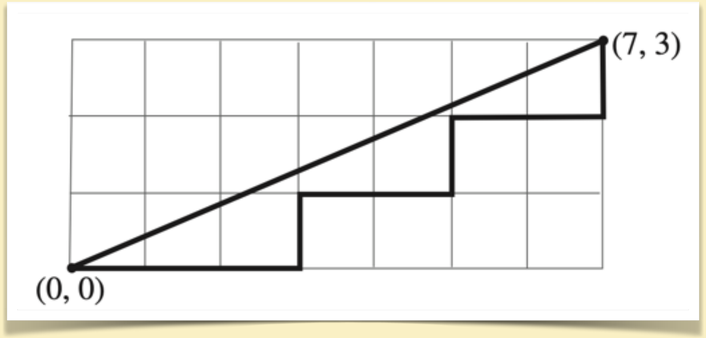

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$$\pi_\sigma(k, \ell = k+2) = \lambda_\sigma(\ell) - \varphi(\ell) \cdot \binom{\sigma}{2}$$

(number of Christoffel words) x (choice of two letters)

Conjecturing $\pi_\sigma(k, \ell = k + 3)$

Let ψ be the function: $n \mapsto 3/2 \cdot \varphi(n)$ if $n \equiv 0 \mod 4$,
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$$\pi_\sigma(k, \ell = k + 3) = \lambda_\sigma(k, \ell) - \binom{\sigma}{2}(\sigma \cdot \psi(\ell) - 2)$$ (?)

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Process.

1. We found out that $(\bar{\pi}_2(k, l = k+3))_k = 2 \cdot \text{OEIS}_{\text{A126246}} - 2$ using OEIS,

2. Guessing a small impact of σ on the formula, we found that
$\bar{\pi}_3 = 6 \cdot \text{OEIS}_{\text{A126246}} - 9$, $\bar{\pi}_4 = 24 \cdot \text{OEIS}_{\text{A126246}} - 12$, $\bar{\pi}_5 = 50 \cdot \text{OEIS}_{\text{A126246}} - 20$ and $\bar{\pi}_6 = 90 \cdot \text{OEIS}_{\text{A126246}} - 30$,

3. We derive the formula, and verify it on tractable instances.

A small Rust library

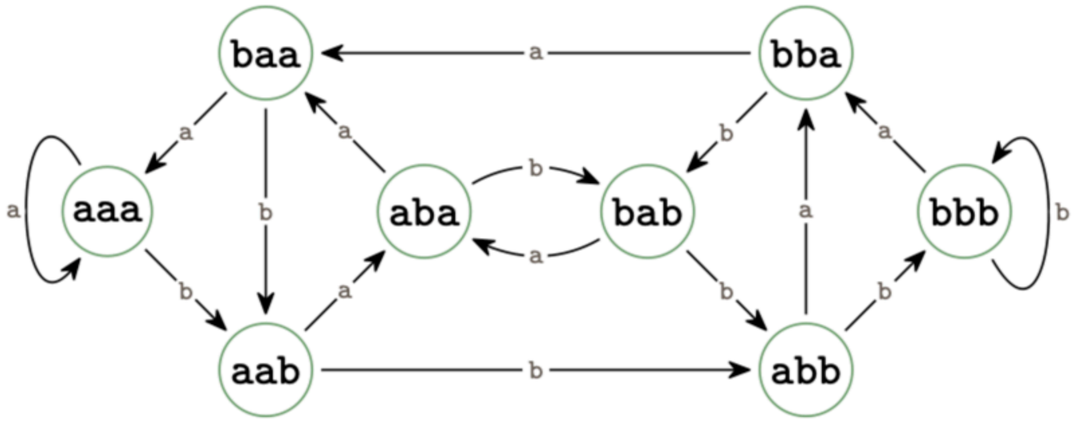
The dbg_cycles library

Objective. Make this counting as accessible as possible.

README

🔁 dBG_cycles: counting and enumerating simple cycles in the de Bruijn graph

`dBG_cycles` is a Rust library and a tool for counting and enumerating simple cycles in the (full) de Bruijn graph.



Under the hood, it relies on a bijection between those simple cycles and a restricted family of Lyndon words, that can be efficiently enumerated using Duval's algorithm. We hope it will help to further investigation on the cycle structure of de Bruijn graph.

⌨ A simple command line interface

Here are the commands available from the command line.

```
# Enumerate all the simple cycles of length 7 in the de Bruijn graph
./dbg_cycles enum --order 4 --length 7 --sigma 4
# Enumerate all the simple cycles in the de Bruijn graph of order 4
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# Count all the simple cycles of length 7 in the de Bruijn graph of
# Highlight whether it has been deduced from a direct formula or by
./dbg_cycles count --order 3 --length 5
# Count all the simple cycles in the de Bruijn graph of order 4 on a
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# Bring our conjecture in face of the enumerate-then-count approach.
# Couples of parameters that are less computationally demandant are
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It implements the Duval's algorithms (Lyndon word enumeration) and the bijection between Lyndon words and dBG simple cycles.

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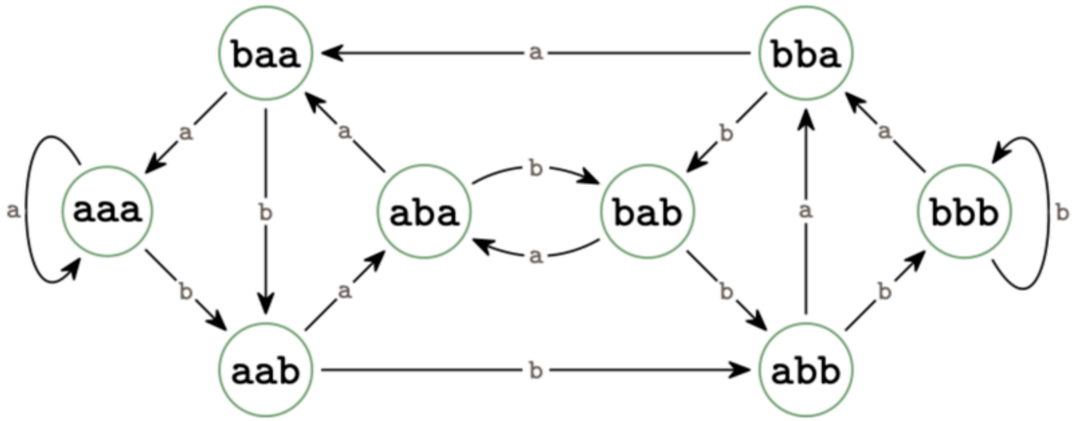

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Limitation. very slow for enumerating cycles larger than the order of the graph (filtering step, that discards most candidates).

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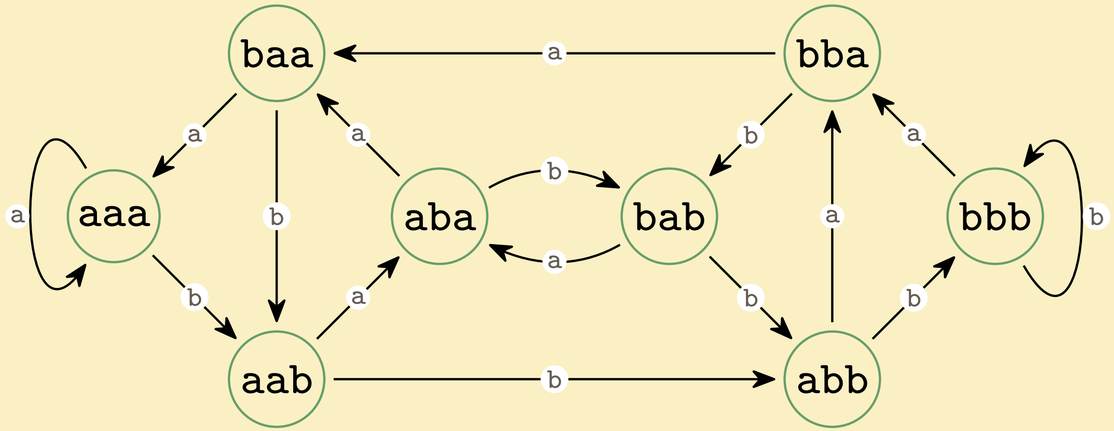

Interest for bioinformatics. Sliding windows (minimizers, compression schemes)

Their topology is still not fully understood. Eg. their simple cycles

- we collected the state of knowledge
- we slightly extended it
- we made these results as accessible as possible

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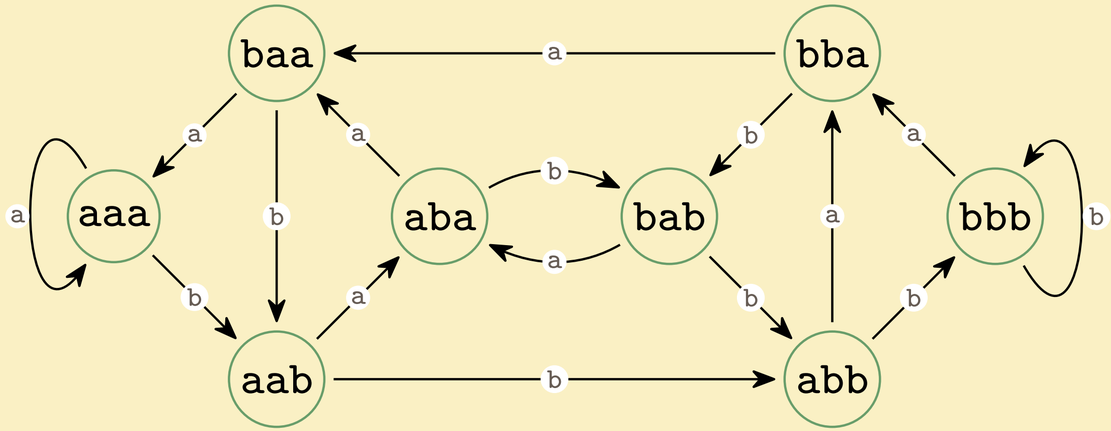

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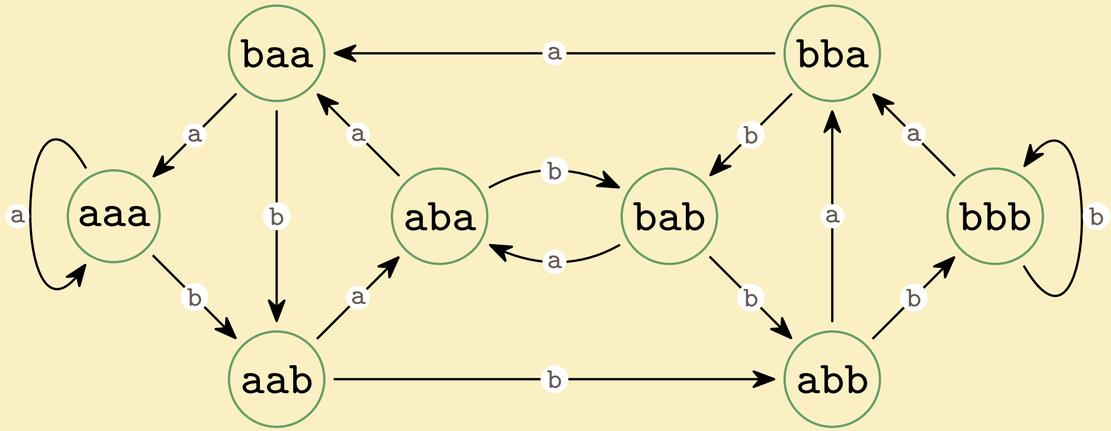

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Open question 2. Can we adapt Duval's algorithms to enumerate k-perfect Lyndon words directly? in optimal space and time?

Thoughts

- History of dBG and Lyndon words is long ⇒ hard to navigate between equivalent/close notions and "folklore" results when non-specialist.
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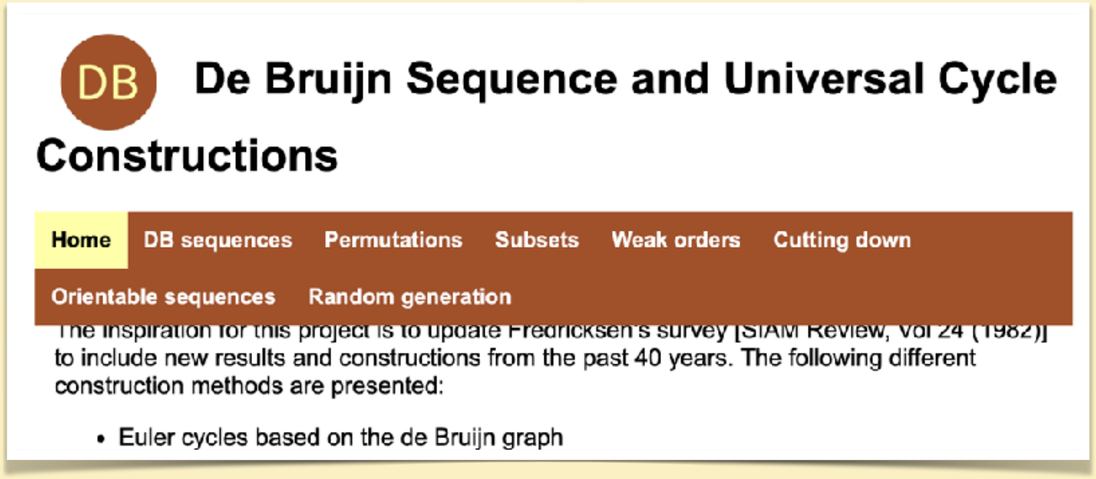

Open question 3. Should we start a collective effort and launch debruijngraph.org?

Counting simple cycles

in the *de Bruijn* graph

Léo Ackermann, Pierre Peterlongo