U-index: A Universal Indexing Framework for Matching Long Patterns

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Joint work with
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Solon P. Pissis

The text indexing problem

- Given a string $T[0..n)$ over the alphabet Σ, pre-process T so that the following queries can be answered efficiently for any string $P[0..m)$:

  - $Locate(P, T)$: return all the positions where P occurs in T;
  - $Count(P, T)$: count the number of occurrences of P in T;
  - $Extract(i, j, T)$: report the substring $T[i..j]$.

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- **More about this on Friday: “25 years of compressed self-indexes” !**

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    1. **Compressed**: The text is replaced (is “self-indexed”) with a compressed representation.

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- Solutions in 1. are very space-efficient but generally slower to build and query than solutions in 2. which — on the other hand — are space-inefficient.

- **Example.** The (uncompressed) **suffix array** is much faster to query than the FM-index but requires $n \log n$ bits on top of the text.

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- **Main idea**: if we compute a **sketch** of the text T, say $S = Sketch(T)$, then $Index(S)$ will be smaller/faster than $Index(T)$ because S is **a lot smaller** than T, for any $Index$.

- At query time: we also compute $Q = Sketch(P)$ and match Q against S. Candidate matches (including *false positives*) are mapped back to T to be verified.

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- That is, we have a **universal framework** because:

  - **any index** can be used for S;

  - **any locally-consistent sampling algorithm** can be used to sketch the text and obtain S.

Intermezzo: sketching with minimizers

- Consider each window of w consecutive k-mers from a string T: sample one k-mer out of w and call it the "representative" of the window — or its *minimizer*.

- We would like to sample the **same minimizer** from consecutive windows so that the **set of distinct minimizers** forms a succinct sketch for T.

Example for $w = 4$ and $k = 7$.

```
ACGGTAGAACCGATTCAAATTCGAT…

ACGGTAGAAC
 CGGTAGAACC
  GGTAGAACCG
   GTAGAACCGA
    TAGAACCGAT
     AGAACCGATT
      GAACCGATTC
       AACCGATTCA
          …
```

Intermezzo: sketching with minimizers

- **Q.** How do we compare different sampling algorithms?

  A. We define the *density* of a sampling algorithm as the fraction between the number of (distinct) minimizers and the total number of k-mers of T.

  The lower the density, the better!

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  The lower the density, the better!

- Since the same k-mer cannot be a minimizer for more than w consecutive k-mers, we immediately have a **lower bound** of $1/w$ on the density of any sampling algorithm.

```
TAGAACCGAT
 AGAACCGATT
  GAACCGATTC
   AACCGATTCA
    ...
```

The “folklore”, random, minimizer

- Take the **leftmost smallest k-mer of the window** according to an order $\mathcal{O}_k$.
- We usually define the total order using a random hash function (*random* minimizer).
- In this case, the density is $2/(w+1)$: almost a factor of 2 away from the lower bound for large w.

function MINIMIZER$(W, w, k, \mathcal{O}_k)$

    $o_{min} = +\infty$

    $p = 0$

    for $i = 0;\ i < w;\ i = i + 1$ **do**

        $o = \mathcal{O}_k(W[i..i+k))$

        if $o < o_{min}$ **then**

            $o_{min} = o$

            $p = i$

    return p

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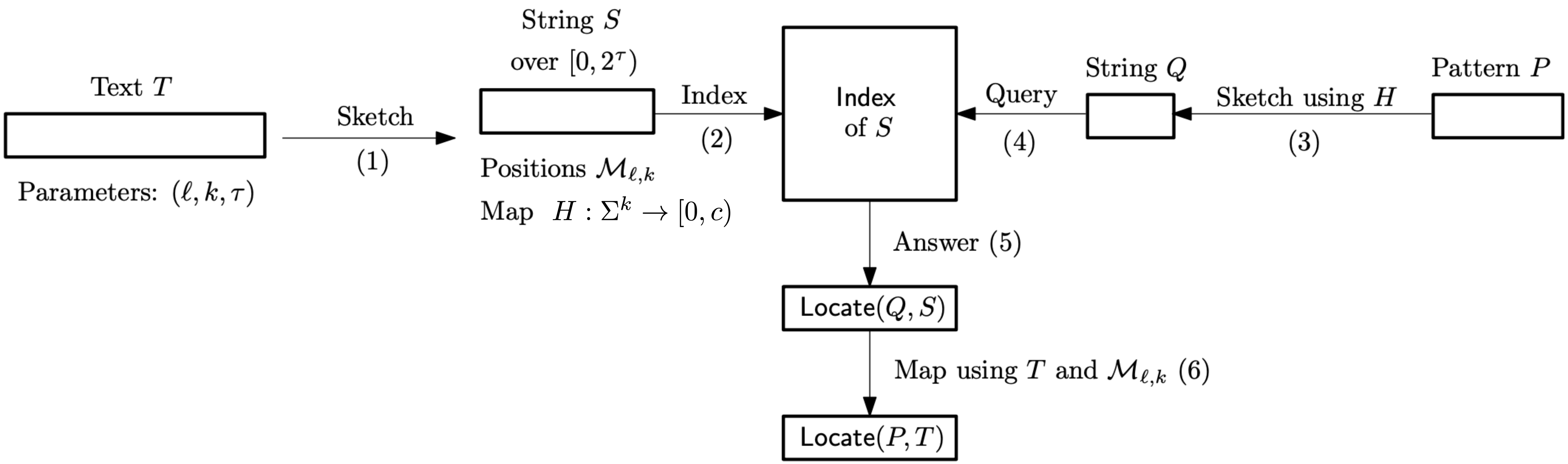
```

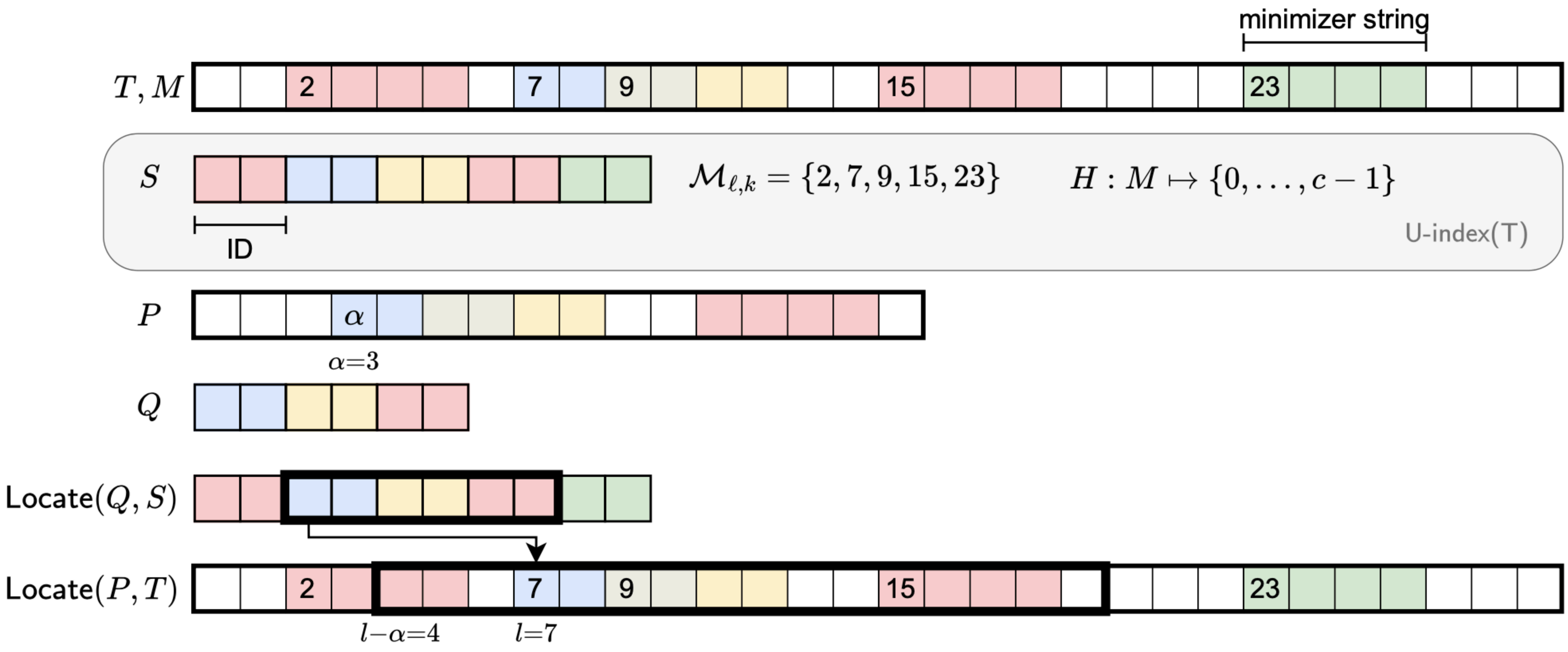
More about random minimizers on Thursday!

The U-index framework for matching long patterns

- We fix integers $k > 0$ and $\ell \geq k$ and let $w := \ell - k + 1$, so that any pattern P of length $m \geq \ell$ contains at least one minimizer.



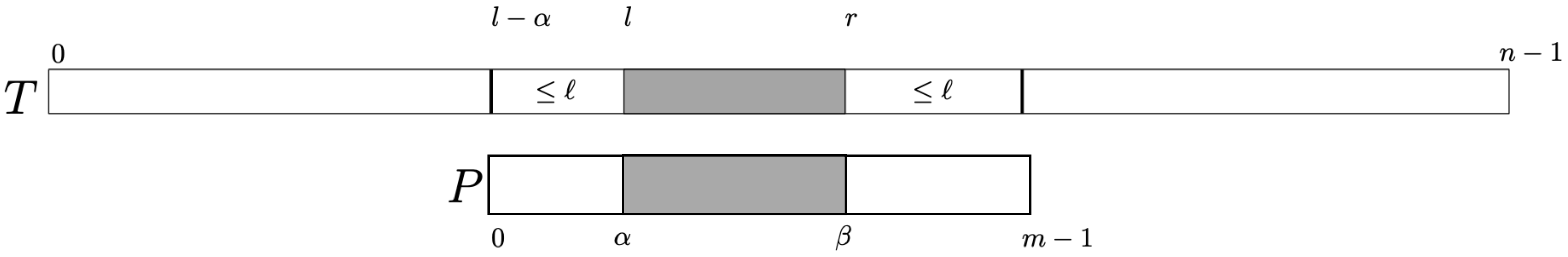
An example



minimizer string
T, M
2
7
9
15
23
S
ID
$\mathcal{M}_{\ell,k} = \{2, 7, 9, 15, 23\}$
$H : M \mapsto \{0, \ldots, c-1\}$
U-index(T)
P
α
α=3
Q
Locate(Q, S)
Locate(P, T)
2
7
9
15
23
$l - \alpha$=4
l=7

Theoretical guarantees

- Using some machinery, we guarantee that an occurrence in $Locate(Q, S)$ is verified in $O(1)$, rather than $O(m)$. This can be done in $O(z)$ space on top of the space of the text, where z is the number of minimizers of T.



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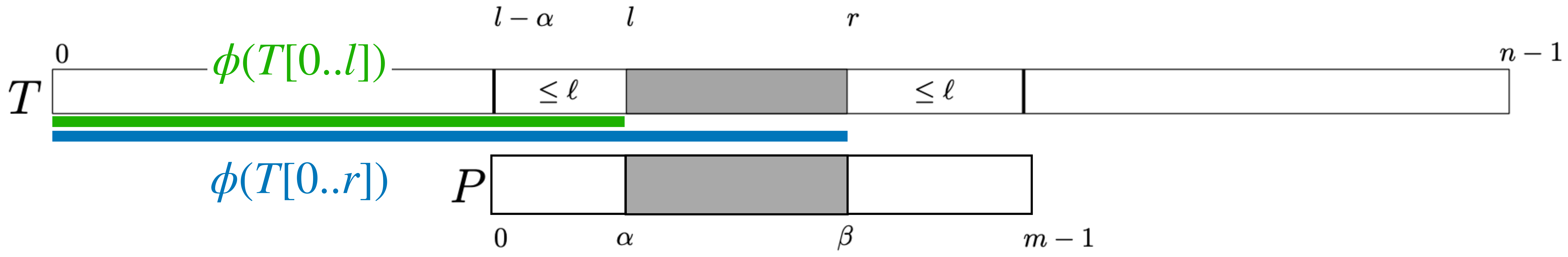

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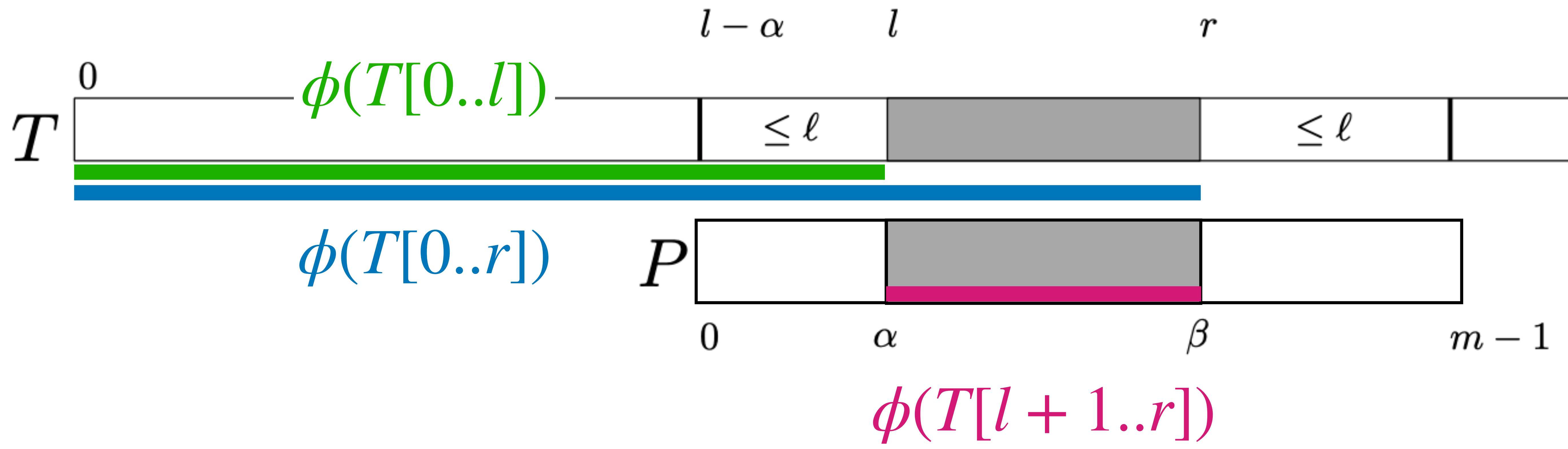

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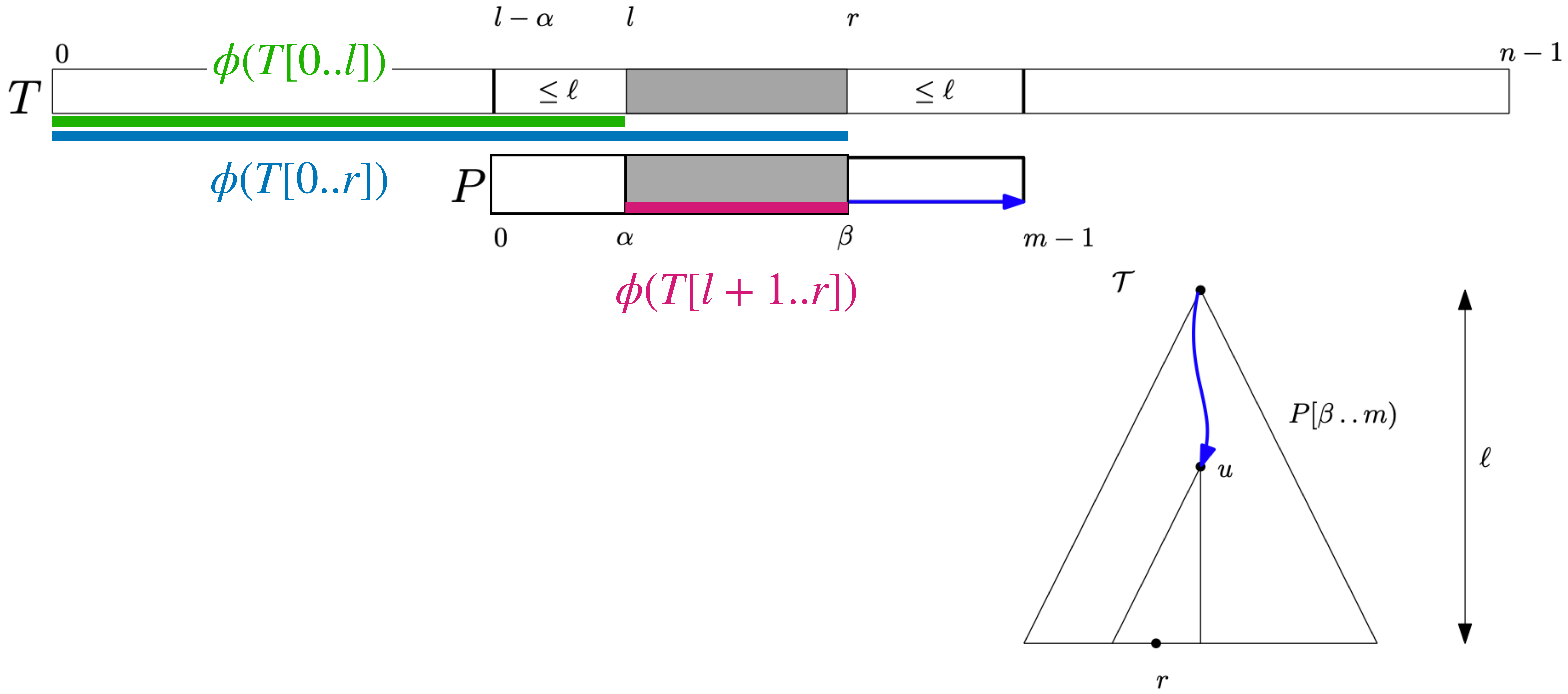

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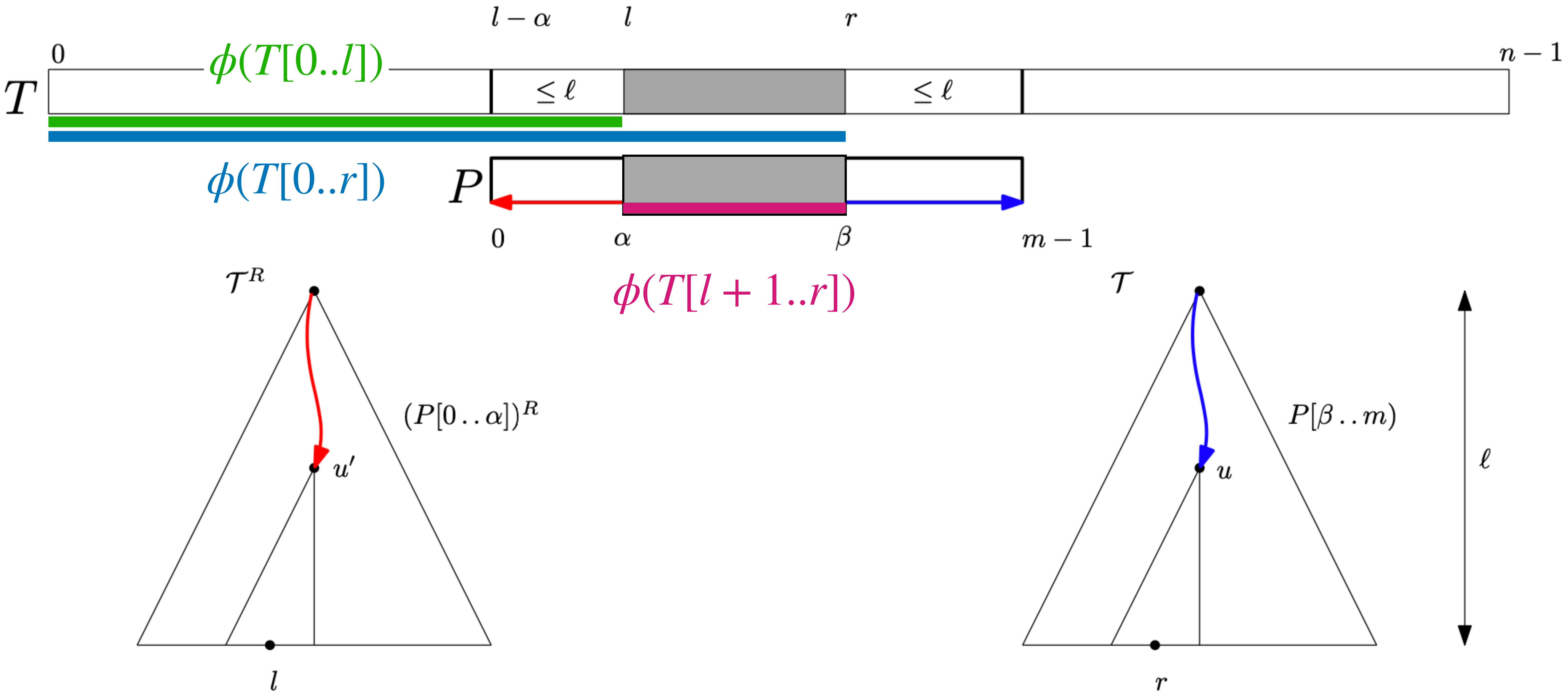
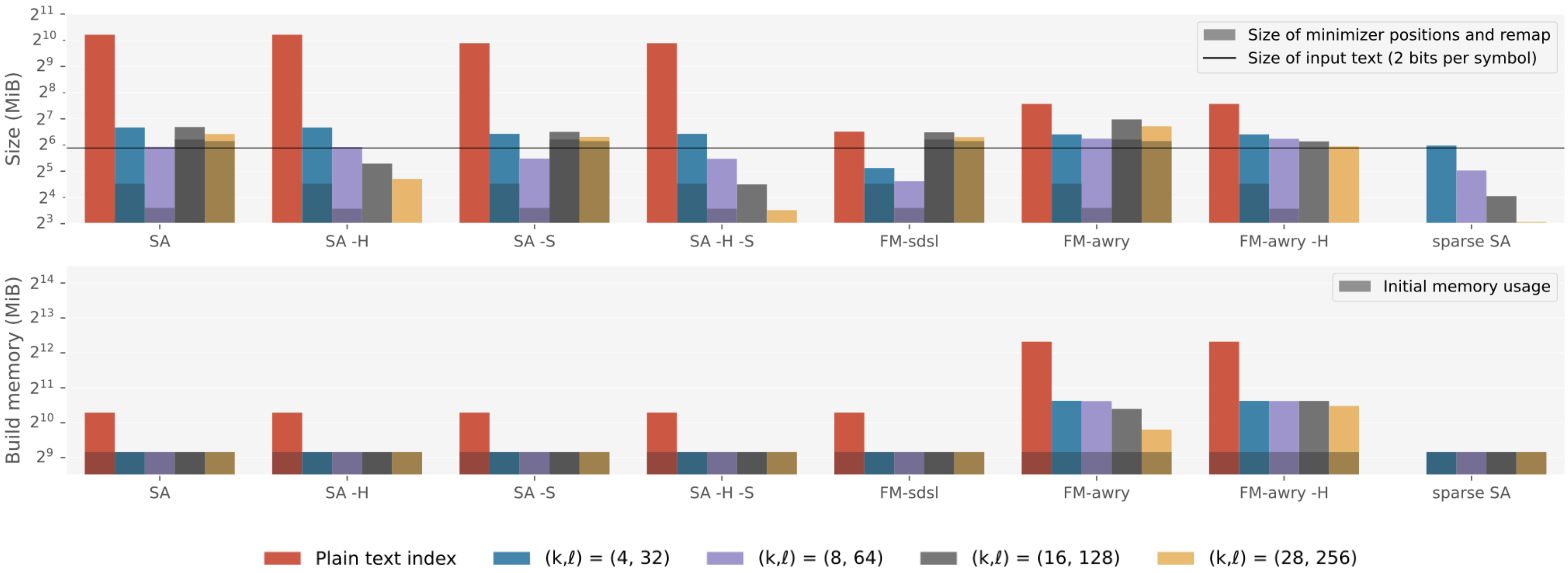
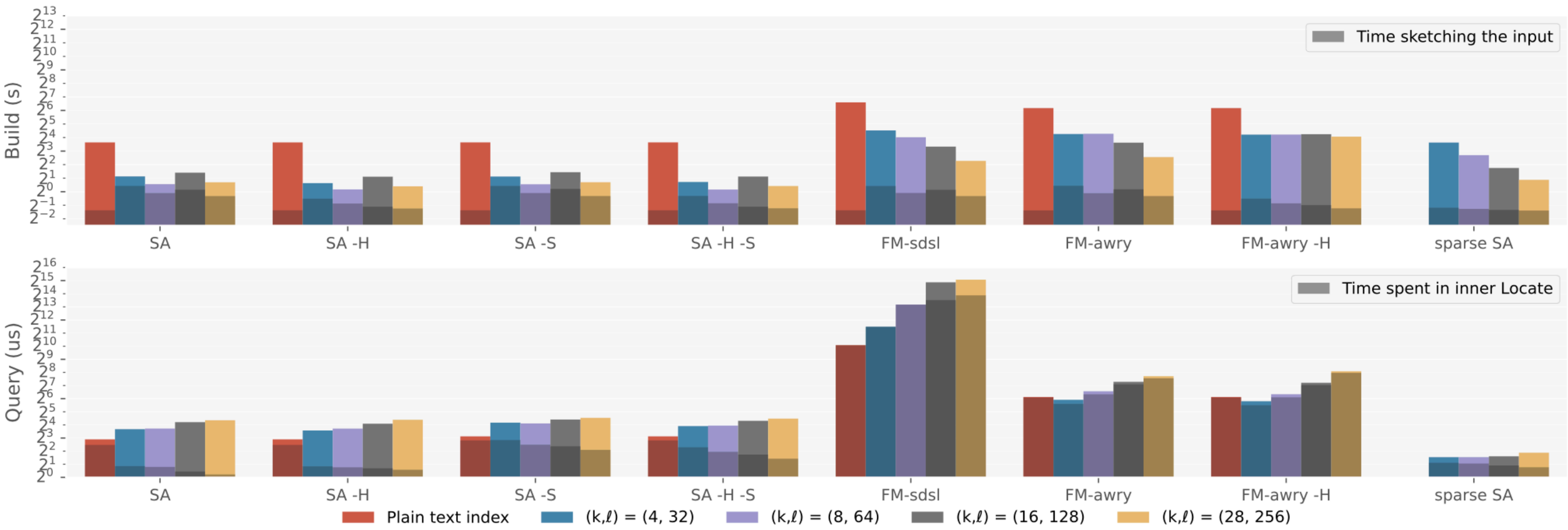


Results — Index size and build space for human chr 1



Results — Build and query time for human chr 1



Conclusions

- Main take-away: U-index is a framework to **enhance the performance of any off-the-shelf text index**, provided that the patterns to match are **reasonably long**.
- Example application: **long read mapping** to reference genomes.
- Bottleneck: verifying false positive matches.
- Rust code: https://github.com/u-index/u-index-rs

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Thank you for the attention!
A special thank to all my co-authors!

An example application

- We demonstrated that the U-index framework can be useful for **long read mapping**.
- A core problem in Computational Biology; it involves aligning long patterns to a reference genome.
- Experimental setting: we align 450 HiFi long reads (avg. length is 16 kbp) on a complete human reference genome. We use $k = 8$ and $\ell = 128$ and split each read in patterns of length $m = 256$.

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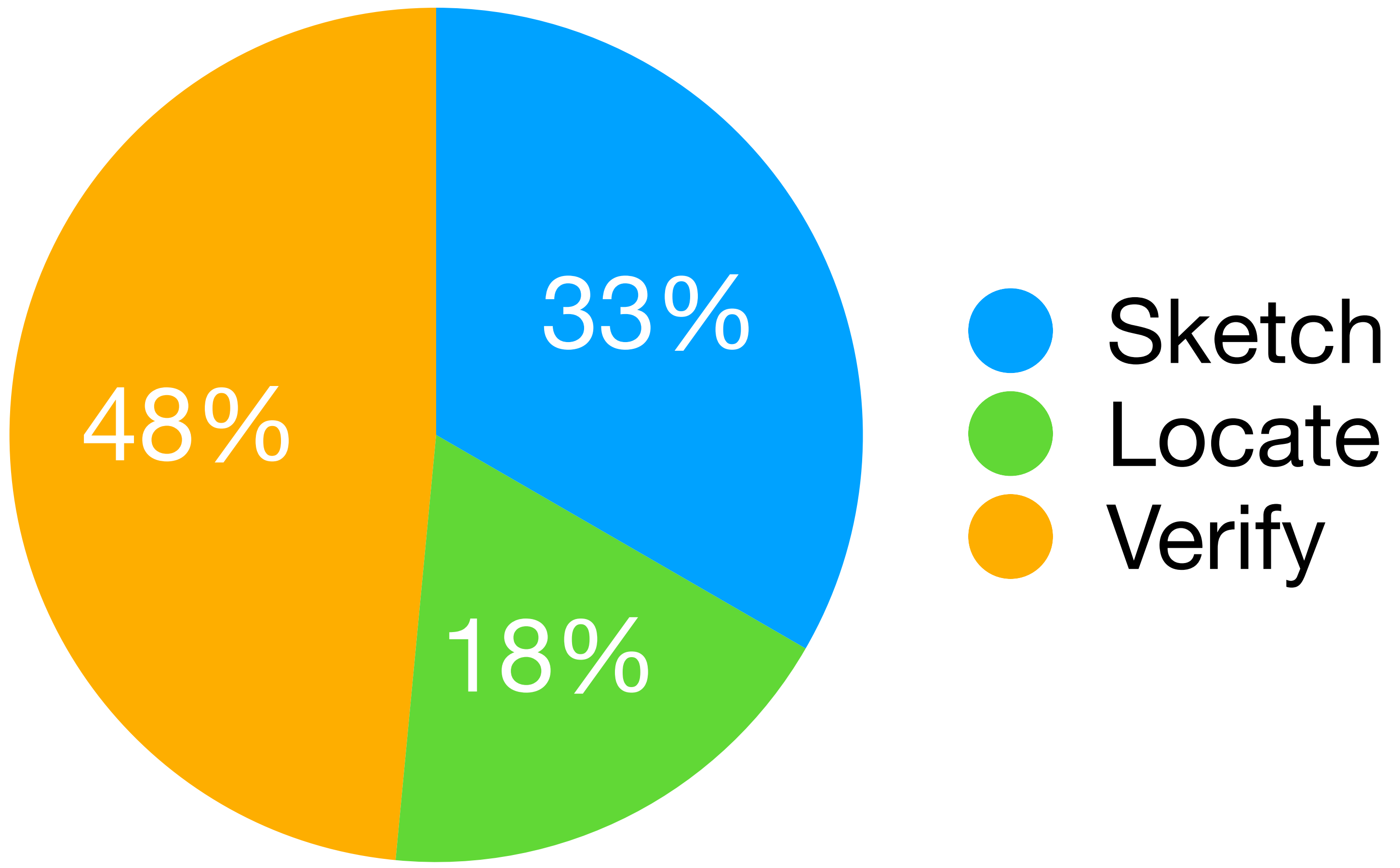
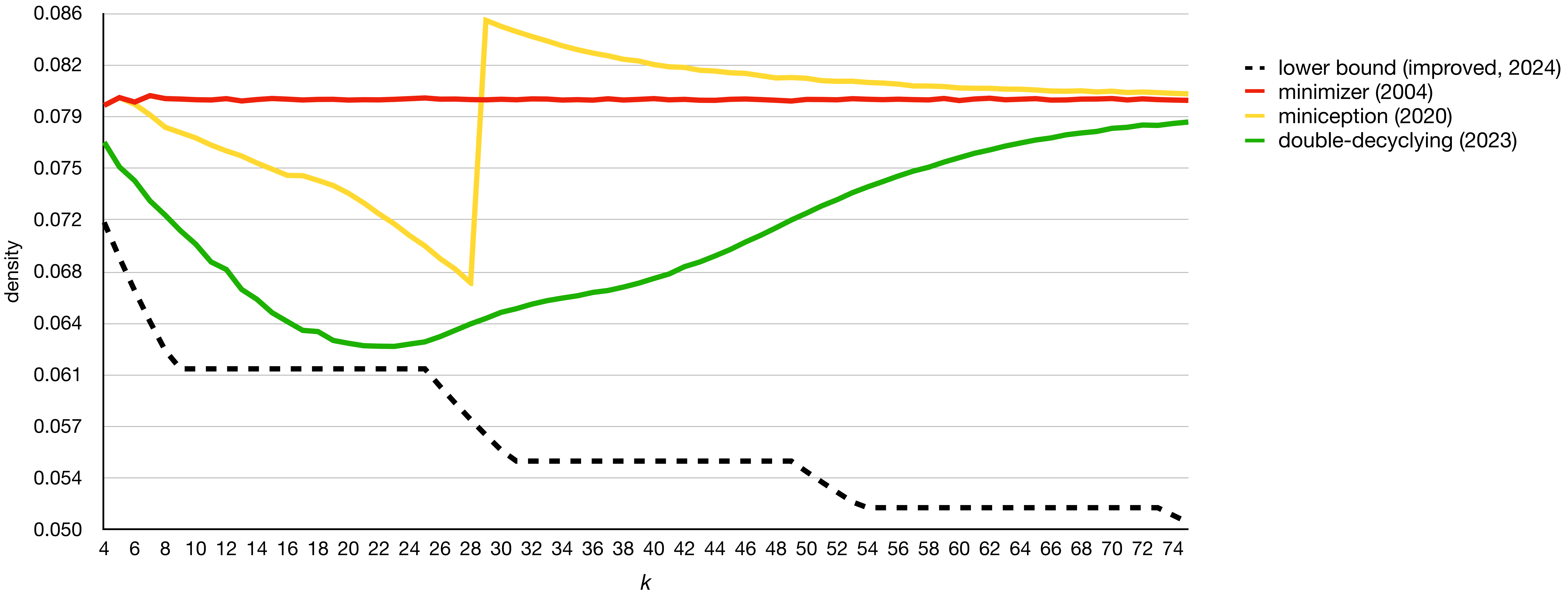
- Very practical numbers **using a suffix array** as index: the U-index is built in 12 seconds with $\approx 9\mu$s per pattern (23 avg. false positives per pattern).



Density by varying *k*



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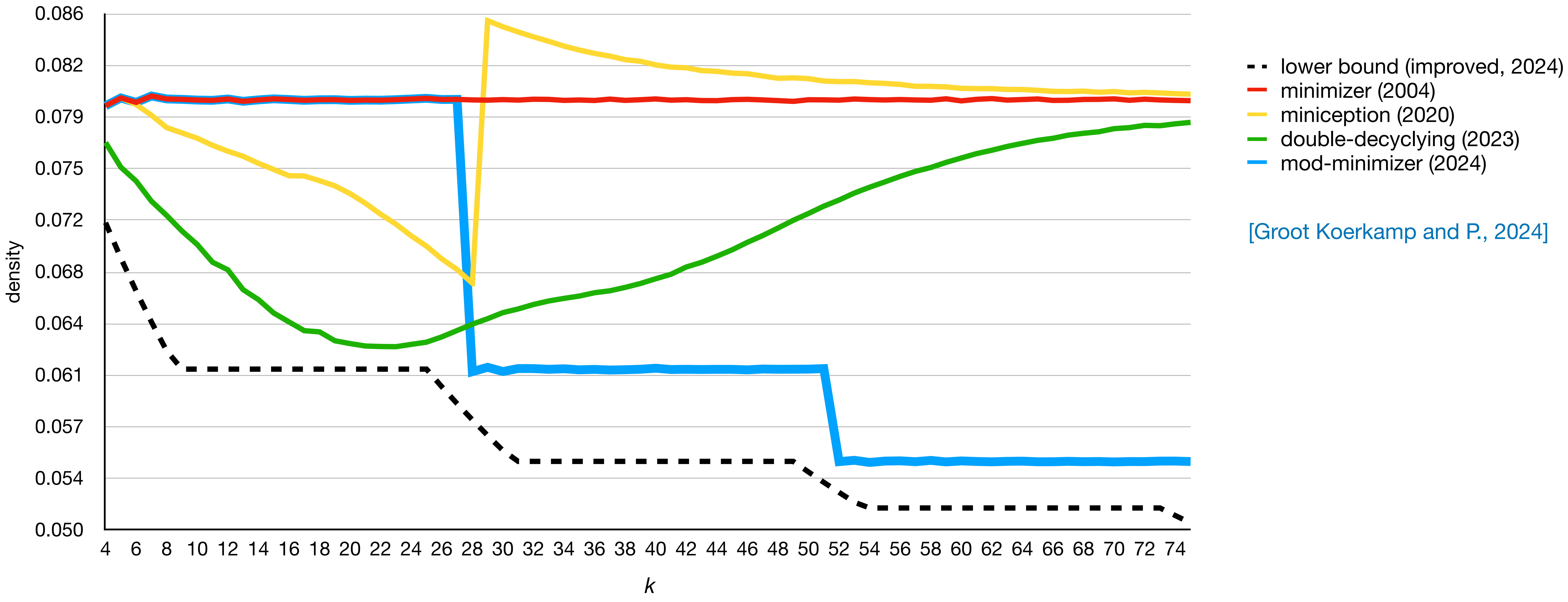

[Groot Koerkamp and P., 2024]

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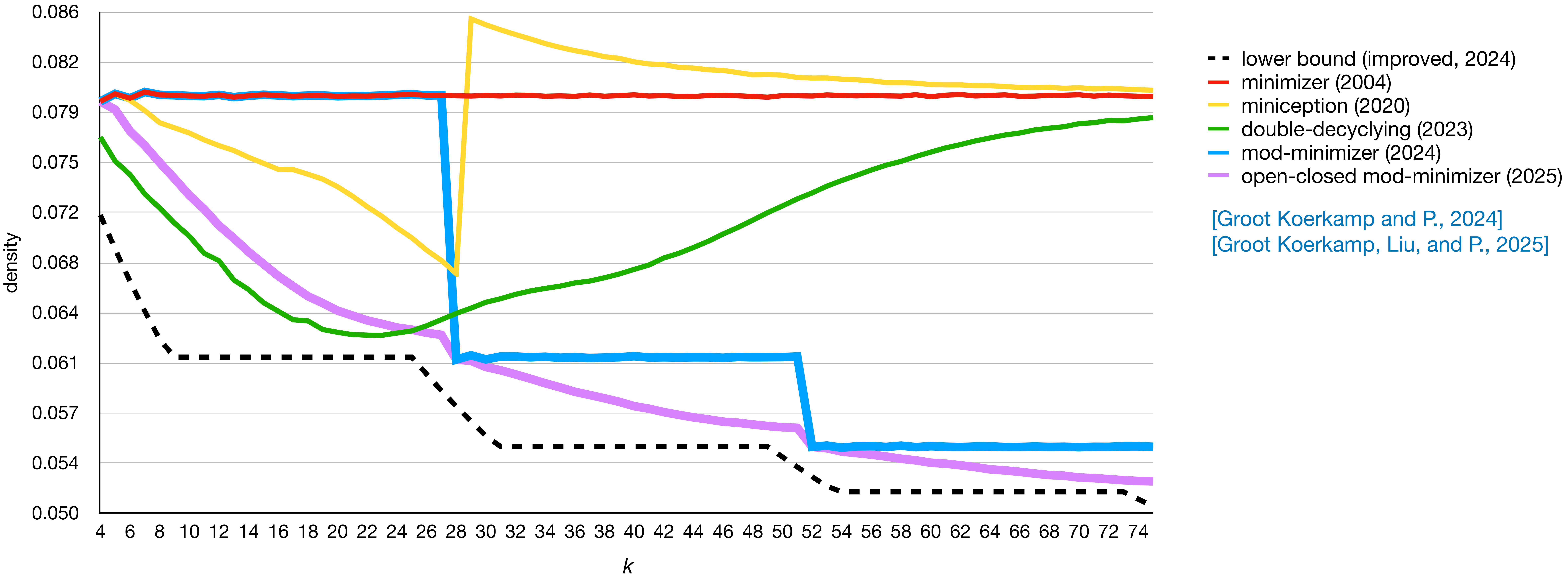

[Groot Koerkamp and P., 2024]
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