A space-efficient, locality-preserving and dynamic data structure for indexing k-mers

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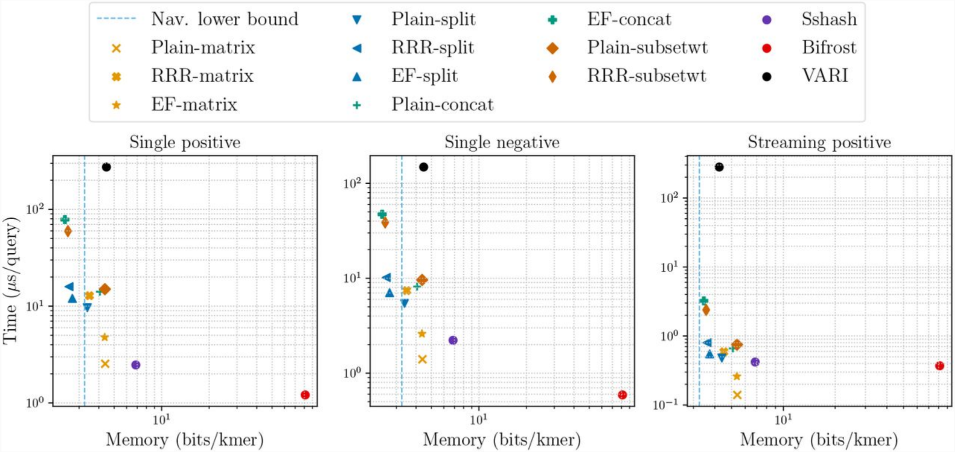
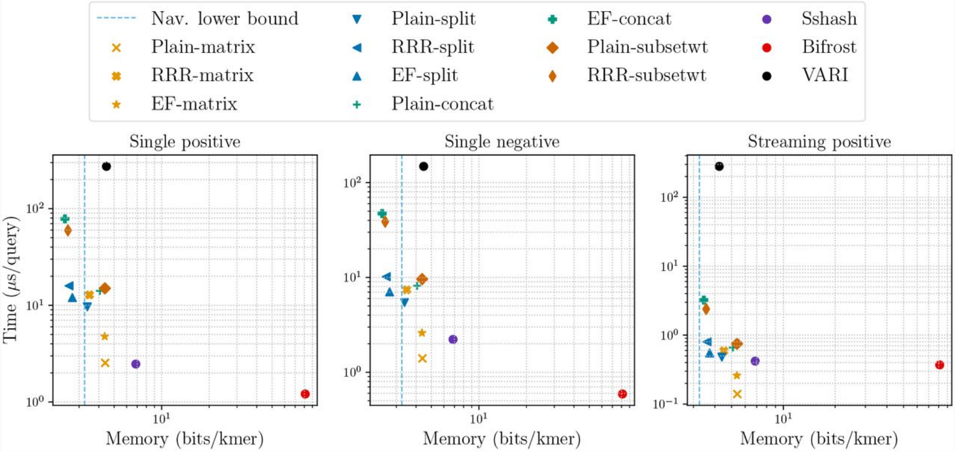
Plenty of compact data structures for storing *k*-mers



Query time and memory usage of some efficient data structures, taken from [Alanko et al. 22]

Motivation

Plenty of compact data structures for storing k-mers ...but most of them are static



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Revisiting a simple idea: k-mers as a sparse set of integers

[Conway & Bromage 11]

- we can see k-mers as integers in $[\![4^k]\!]$
  `A` $\rightarrow$ `00`   `C` $\rightarrow$ `01`   `G` $\rightarrow$ `10`   `T` $\rightarrow$ `11`
- since they're usually very sparse, we can use a sparse bitvector to store them

Limitations

- it's not really dynamic
- it's not cache-efficient
  - index(`ATAACGCCA`) = 49,556
  - index(`TAACGCCAT`) = 198,227

$\rightarrow$ average distance of $4^k/2$

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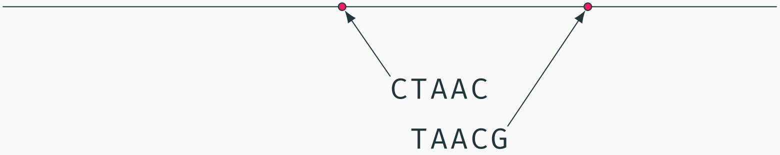
How can we improve this approach?

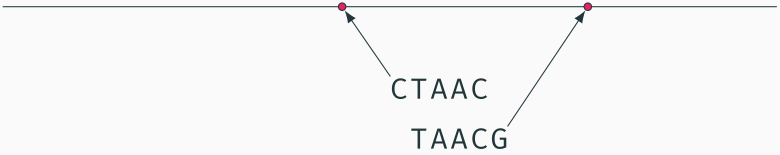
Wish list for an ideal data structure

- space-efficient: few bits / k-mer
- dynamic: support insertion and deletion after construction
- efficient queries:
  - membership
  - enumeration
  - insertion
  - (deletion)
- locality-preserving: reduce cache misses when querying consecutive k-mers

Preserving k-mer locality

A LOCALITY-PRESERVING ENCODING OF *K*-MERS

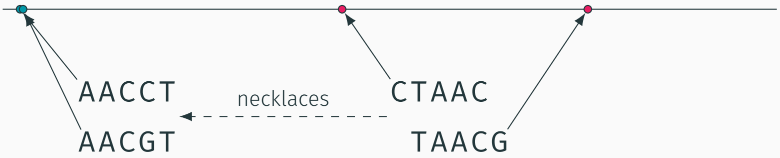




Alternative encoding based on necklaces

The necklace of x is its smallest cyclic rotation $\langle x \rangle = \min_{0 \leqslant i < k} x^{(i)}$

A locality-preserving encoding of k-mers



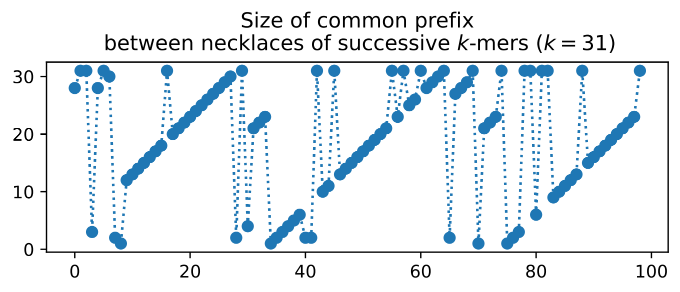
Alternative encoding based on necklaces

The necklace of x is its smallest cyclic rotation $\langle x \rangle = \min_{0 \leqslant i < k} x^{(i)}$

- $x \mapsto (\langle x \rangle,$ rotation index) is a bijective transformation
- necklaces of consecutive k-mers share long prefixes

A closer look at the locality of necklaces

AACGTCATCTCTCATTCTGGTCGTTCTTCCT
AACGTCATCTCTCATTCTGTTCGTTCTTCCT
AACGTCATCTCTCATTCTGTGCGTTCTTCCT
AACGTCATCTCTCATTCTGTGAGTTCTTCCT
AACGTCATCTCTCATTCTGTGACTTCTTCCT
AACGTCATCTCTCATTCTGTGACATCTTCCT
AACGTCATCTCTCATTCTGTGACACCTTCCT
AACGTCATCTCTCATTCTGTGACACGTTCCT
AACGTCATCTCTCATTCTGTGACACGCTCCT
AACGTCATCTCTCATTCTGTGACACGCACCT
AACGTCATCTCTCATTCTGTGACACGCAGCT
AACGTCATCTCTCATTCTGTGACACGCAGGT
AACGTCATCTCTCATTCTGTGACACGCAGGG
ACACGCAGGGTACGTCATCTCTCATTCTGTG



Ranking necklaces to improve compression

The number of necklaces of size k on an alphabet with σ letters is $\sim \frac{\sigma^k}{k}$

so only a fraction $\frac{1}{k}$ of the universe is actually used

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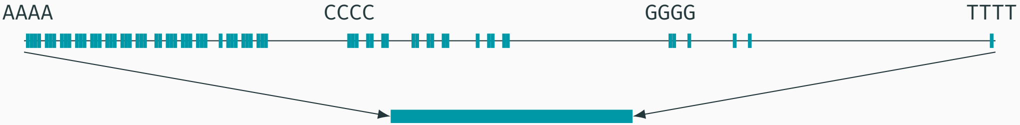


Ranking: given a necklace $\langle x \rangle$, find i s.t. $\langle x \rangle$ is the i-th smallest necklace of size k

We can compute the rank in $\mathcal{O}(k^2)$ time [Sawada & Williams 17]

(Can we do better? for batch queries maybe?)

Tradeoff: better compression + locality vs $\mathcal{O}(k^2)$ queries

Compressing sparse integer sets

[Elias 74, Fano 71]

- separate the high bits and low bits
- compress them with different methods

We choose the size of the low bits as $l = \left\lceil \lg \frac{u}{n} \right\rceil$

- n is the number of elements
- u is the size of the universe
  e.g. $u = 4^k$ for k-mers

$\{2, 3, 210, 216, 231, 265, 491, 499\}$

high bits (slowly increasing)	low bits (l)
000	000010
000	000011
011	010010
011	011000
011	100111
100	001001
111	101011
111	110011

Space usage of Elias-Fano

$$EF(n, u) = 2n + n\left\lceil \lg \frac{u}{n} \right\rceil$$

e.g. for $n = 10^{10}$ and $u = 4^{31}$, EF uses 31 bits / item

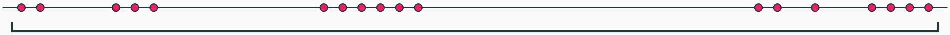
Information theoretic lower bound

$$\lg \binom{u}{n} \approx n \lg e + n \lg \frac{u}{n}$$
$$\approx 1.44n + n \lg \frac{u}{n}$$

Note that the bound can get lower if we have additional knowledge about the distribution.

Partitioning sparse integer sets

Partitioning sparse integer sets [Ottaviano & Venturini 14]



lot of empty regions

Partitioning sparse integer sets [Ottaviano & Venturini 14]

Split the sequence into smaller blocks

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Split the sequence into smaller blocks, choose the best encoding:

- for sparse blocks: Elias-Fano ; $2n + n\left\lceil \lg \frac{u}{n} \right\rceil$ bits
- for dense blocks: plain bitset ; u bits
- for full blocks: lower bound + size is enough

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Computing the optimal partition

- optimal solution in $\mathcal{O}(n^2)$ using dynamic programming
- $(1+\varepsilon)$-approximation in $\mathcal{O}(n \cdot \frac{1}{\varepsilon} \ln \frac{1}{\varepsilon})$

Dynamic version & complexity recap [Pibiri & Venturini 17]

[Pibiri & Venturini 17] presents an approach to make the partitions dynamic using $o(n)$ extra space

$\rightarrow$ WIP, *no practical implementation available yet*

Query complexity

- membership and successor in $\mathcal{O}(\lg \lg n)$
- insertion and deletion in $\mathcal{O}(\lg n \,/\, \lg \lg n)$

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- ranking saves $\lg k$ bits / k-mer but costs $\mathcal{O}(k^2)$ / query
- partitioning typically saves $\frac{1}{2} \lg k$ bits / k-mer

Conclusion

Take-home messages

Using necklaces to represent k-mers

- preserves locality
- improves compression

Partitioned sparse sets

- fit in well with necklace locality
- can support dynamic operations

Future steps

- efficient implementation of the dynamic partitions
- batch necklace computation
- batch rank computation
- subquadratic ranking?
- bound on the necklace distance

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Thank you!

Appendix

- Alanko, Jarno N, Simon J Puglisi & Jaakko Vuohtoniemi (2022). **“Succinct k-mer sets using subset rank queries on the spectral burrows-wheeler transform”.** In: *bioRxiv*, pp. 2022–05.
- Conway, Thomas C & Andrew J Bromage (2011). **“Succinct data structures for assembling large genomes”.** In: *Bioinformatics* 27.4, pp. 479–486.
- Elias, Peter (1974). **“Efficient storage and retrieval by content and address of static files”.** In: *Journal of the ACM (JACM)* 21.2, pp. 246–260.
- Fano, Robert Mario (1971). ***On the number of bits required to implement an associative memory.*** Massachusetts Institute of Technology, Project MAC.
- Ferragina, Paolo, Igor Nitto & Rossano Venturini (2011). **“On optimally partitioning a text to improve its compression”.** In: *Algorithmica* 61, pp. 51–74.

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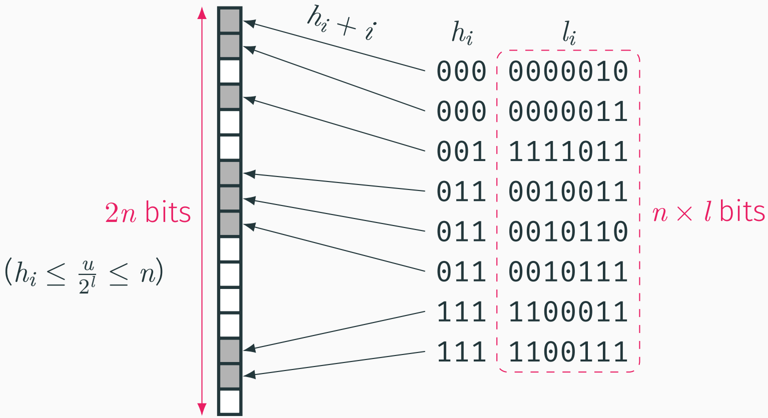
- Ottaviano, Giuseppe & Rossano Venturini (2014). **"Partitioned elias-fano indexes".** In: *Proceedings of the 37th international ACM SIGIR conference on Research & development in information retrieval*, pp. 273–282.
- Pibiri, Giulio Ermanno & Rossano Venturini (2017). **"Dynamic elias-fano representation".** In: *28th Annual symposium on combinatorial pattern matching (CPM 2017)*. Schloss Dagstuhl-Leibniz-Zentrum fuer Informatik.
- Sawada, Joe & Aaron Williams (2017). **"Practical algorithms to rank necklaces, Lyndon words, and de Bruijn sequences".** In: *Journal of Discrete Algorithms* 43, pp. 95–110.

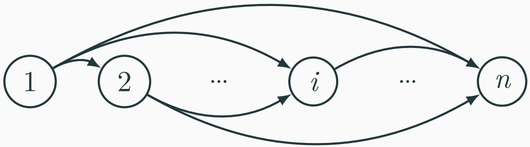
A closer look at Elias-Fano encoding [Elias 74, Fano 71]

$S = \{2, 3, 251, 403, 406, 407, 995, 999\}$ $n = 8$ $u = 1000$ $l = \lceil \lg \frac{u}{n} \rceil = 7$ bits



Optimal partition as a shortest path [Ferragina et al. 11]

- $V = [\![1, n]\!] \quad E = \{i < j\,;\, i, j \in V\}$
- $w_{i,j} =$ cost to encode $S[i, j]$



Computing the optimal partition

- optimal solution in $\mathcal{O}(|V| + |E|) = \mathcal{O}(n^2)$ using dynamic programming
- $(1 + \varepsilon)$-approximation in $\mathcal{O}(n \cdot \frac{1}{\varepsilon} \ln \frac{1}{\varepsilon})$ by sparsifying the graph