Parallel Computation for the All-Pairs Suffix-Prefix Problem

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Outline

1. Introduction
2. Preliminaries
3. Related work
4. Parallel Algorithm
5. Experiments
6. Conclusion

Introduction

All-pairs suffix-prefix matching problem (APSP):

- Given a collection of strings $\mathcal{S} = S^1, S^2, \ldots, S^m$, and a threshold τ.
- APSP is to find, for all pairs S^i and S^j, the longest suffix of S^i that overlaps S^j that is larger than τ.
- Suffix-prefix match (overlap):

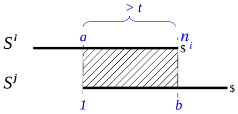

Figure: S^i overlaps S^j, the suffix $S^i[a, n_i - 1]$ is equal to the prefix $S^j[1, b]$

Motivation:

- DNA assembly (bottleneck stage).
- EST clustering.
- Approximating the shortest common superstring.

Introduction

Practical Algorithms:

- DNA assemblers provide fast solutions with non-optimal algorithms.
- SGA [Simpson and Durbin, 2010] and Readjoiner [Gonnella and Kurtz, 2012] have isolated overlap detection stage.
- [Rachid and Malluhi, 2015] presented SOF to solve the APSP for DNA sequences. SOF has a good performance with multiple threads[1].

Optimal Algorithms:

- [Gusfield et al., 1992] solved the APSP in optimal time $\rightarrow$ suffix trees and stacks.
- [Ohlebusch and Gog, 2010] improved memory usage and running time $\rightarrow$ enhanced suffix arrays and stacks.
- [Tustumi et al., 2016] proposed a different traversal of the enhanced suffix array and replaced stacks by linked lists to achieve a better practical running time.

[1] SGA, Readjoiner and SOF may be executed in multithreading environments.

Introduction

Our proposal:

- We showed how to parallelize the optimal algorithm by [Tustumi et al., 2016] to solve the APSP.
- Our parallel algorithm achieves a consistent speedup with a small memory footprint when compared with [Tustumi et al., 2016].
- Also, it is competitive with SOF when the threshold τ is small.

Workflow:

- Our algorithm is composed by three phases.
- We separated the computation of the local solution followed by the global solution and by the identical suffixes searching into independent phases.

Outline

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2. Preliminaries

3. Related work

4. Parallel Algorithm

5. Experiments

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Preliminaries:

Let $S[1,n]$ be a string of length $|S| = n$ over an ordered alphabet Σ.

- A prefix is a substring of the form $S[1,i]$.
- A suffix is a substring $S[i,n]$ that will be denoted by S_i.

The suffix array of $S[1,n]$, SA, is an array of integers in $[1,n]$ that gives the lexicographic order of all suffixes:

- $S_{\mathrm{SA}[1]} < S_{\mathrm{SA}[2]} < \ldots < S_{\mathrm{SA}[n]}$;
- We denote the position of S_i in SA as $\mathrm{pos}(S_i)$.

The LCP-array stores the length of the longest common prefix (*lcp*) of two consecutive suffixes in SA:

- $\mathrm{LCP}[i] = lcp(S_{\mathrm{SA}[i]}, S_{\mathrm{SA}[i-1]})$ for $1 < i \leq n$, and
- $\mathrm{LCP}[1] = 0$.

The range minimum query (*rmq*) on LCP gives the smallest *lcp* value in an interval of SA:

- $rmq(i,j) = \min_{i<k\leq j}\{\mathrm{LCP}[k]\}$.
- It is well known that $lcp(S_{\mathrm{SA}[i]}, S_{\mathrm{SA}[j]}) = rmq(i,j)$, with $1 \leq i < j \leq n$.

Preliminaries:

Let $\mathcal{S} = S^1, S^2, \ldots, S^m$ be a collection of strings of lengths $n_i = |S^i|$.

- $S^{cat} = S^1 \cdot \$_1 \cdot S^2 \cdot \$_2 \cdots S^m \cdot \$_m$ is the concatenated string of length $N = m + \Sigma_{i=1}^{m} n_i$.
- Each $\$_i$ is a distinct separator not in Σ that precedes $\forall \alpha \in \Sigma$, and $\$_i < \$_j$ if $i < j$.
- $S_k^{\$}$ denotes the prefix of S_k^{cat} that ends at the first separator $\$_j$.

The generalized suffix array of $\mathcal{S}$, GSA, is the SA of the concatenated string S^{cat}.

For a clearer notation, we introduce:

- STR indicates which string in $\mathcal{S}$ a suffix came from, $\mathrm{STR}[i] = j$ if $S_{\mathrm{SA}[i]}^{\$}$ ends with $\$_j$.
- SA′ holds the position of a suffix with respect to the string it came from (up to the separator), defined as $\mathrm{SA}'[i] = k$ if $S_{\mathrm{SA}[i]}^{\$} = S_k^j \$_j$.

GESA denotes the GSA enhanced with the arrays STR, SA′ and LCP.

Preliminaries:

Let S^k be the j-th (lexicographically) smallest string in $\mathcal{S}$.

- P is an array of $m+1$ integers that stores in $\mathrm{P}[j] = \mathrm{pos}(S^k[1, n_k])$.
- We define $\mathrm{P}[0] = m + 1$.

Let $B^j = (\mathrm{P}[j-1], \mathrm{P}[j]]$[2] be a block of GESA corresponding to S^k.

- GESA can be partitioned into m blocks $B^1, B^2, \ldots, B^m$, one for each string S^k in $\mathcal{S}$.

	i	SA	LCP	STR	SA′	$S^\$_{\mathrm{SA}[i]}$
	1	4	0	1	4	$\$_1$
	2	8	0	2	4	$\$_2$
	3	11	0	3	3	$\$_3$
	4	15	0	4	4	$\$_4$
P[0] →	5	7	0	2	3	a$\$_2$
	6	10	1	3	2	a$\$_3$
	7	14	1	4	3	a$\$_4$
P[1] →	8	9	1	3	1	aa$\$_3$
	9	13	2	4	2	aa$\$_4$
P[2] →	10	1	2	1	1	aac$\$_1$
	11	2	1	1	2	ac$\$_1$
P[3] →	12	5	2	2	1	aca$\$_2$
	13	3	0	1	3	c$\$_1$
	14	6	1	2	2	ca$\$_2$
P[4] →	15	12	2	4	1	caa$\$_4$

Figure: GESA of $\mathcal{S} = \{\mathrm{aac}, \mathrm{aca}, \mathrm{aa}, \mathrm{caa}\}$. Suffixes in block 1 are highlighted.

[2] open interval: $\mathrm{P}[j-1]+1$ stores the $lcp(S_{\mathrm{SA}[\mathrm{P}[j-1]+1]}, S_{\mathrm{SA}[\mathrm{P}[j-1]]})$

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2. Preliminaries

3. Related work

4. Parallel Algorithm

5. Experiments

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Related work:

The algorithm by [Tustumi et al., 2016] solves the APSP in optimal $O(N + m^2)$ time, based on the following remarks:

- All suffixes that overlap S^k are in positions prior to pos(S^k) or are identical to S^k and directly succeed pos(S^k).
- If two different suffixes of S^r are a prefix of S^k, the longest is closer to pos(S^k).
- Given two prefixes $S^t < S^k$, if a suffix of S^r, of length ℓ, overlap S^t and $\ell > lcp(S^t, S^k)$, then such suffix does not overlap S^k.

	i	SA	LCP	STR	SA′	$S^{\$}_{\mathrm{SA}[i]}$
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P[0] →	5	7	0	2	3	a$\$_2$
	6	10	1	3	2	a$\$_3$
	7	14	1	4	3	a$\$_4$
P[1] →	8	9	1	3	1	aa$\$_3$
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Figure: GESA of $\mathcal{S} = \{\mathrm{aac}, \mathrm{aca}, \mathrm{aa}, \mathrm{caa}\}$.

Related work:

Algorithm [Tustumi et al., 2016]:

- The blocks are processed in order, $B^1, B^2, \ldots, B^m$.
- For each B^j: suppose that $\text{pos}(S^k) = \text{P}[j]$ and $\text{pos}(S^t) = \text{P}[j-1]$.
  1. Local solution is found scanning B^j backwards;
  2. Global solution is obtained reusing the local solutions of the previous blocks.
  3. Identical suffixes are found scanning GESA forward from $\text{P}[j]+1$.
- The algorithm uses m local lists and m global lists to track all overlaps seen so far.

	i	SA	LCP	STR	SA′	$S^{\$}_{\text{SA}[i]}$
	1	4	0	1	4	$\$_1$
	2	8	0	2	4	$\$_2$
	3	11	0	3	3	$\$_3$
	4	15	0	4	4	$\$_4$
P[0] $\rightarrow$	5	7	0	2	3	a$\$_2$
	6	10	1	3	2	a$\$_3$
	7	14	1	4	3	a$\$_4$
P[1] $\rightarrow$	8	9	1	3	1	aa$\$_3$
	9	13	2	4	2	aa$\$_4$
P[$j-1$] $\rightarrow$	10	1	2	1	1	aac$\$_1$ $\leftarrow S^t$
	11	2	1	1	2	ac$\$_1$
P[j] $\rightarrow$	12	5	2	2	1	aca$\$_2$ $\leftarrow S^k$
	13	3	0	1	3	c$\$_1$
	14	6	1	2	2	ca$\$_2$
P[4] $\rightarrow$	15	12	2	4	1	caa$\$_4$

Figure: GESA of $\mathcal{S} = \{\text{aac}, \text{aca}, \text{aa}, \text{caa}\}$.

Related work:

Algorithm [Tustumi et al., 2016]:

- Local solution:
  - For block B^j:
  - GESA is scanned backwards, from $\mathsf{P}[j]$ to $\mathsf{P}[j-1]+1$.
  - $\ell = rmq(i, \mathsf{P}[j])$ is computed in $O(1)$ time during the scanning of B^j.
    - if $|S^{\mathsf{STR}[i]}_{\mathsf{SA}'[i]}| = \ell$ then $S^{\mathsf{STR}[i]}$ overlaps S^k in ℓ symbols, and $insert\_at\_end(L_{local}[\mathsf{STR}[i]], \ell)$.
    - At the end, the longest overlaps in B^j are at the front of each local list.

	i	SA	LCP	STR	SA′	$S^{\$}_{\mathsf{SA}[i]}$
	1	4	0	1	4	$\$_1$
	2	8	0	2	4	$\$_2$
	3	11	0	3	3	$\$_3$
	4	15	0	4	4	$\$_4$
P[0] →	5	7	0	2	3	a$\$_2$
	6	10	1	3	2	a$\$_3$
	7	14	1	4	3	a$\$_4$
P[1] →	8	9	1	3	1	aa$\$_3$
	9	13	2	4	2	aa$\$_4$
P[2] →	10	1	2	1	1	aac$\$_1$
	11	2	1	1	2	ac$\$_1$
P[3] →	12	5	2	2	1	aca$\$_2$
	13	3	0	1	3	c$\$_1$
	14	6	1	2	2	ca$\$_2$
P[4] →	15	12	2	4	1	caa$\$_4$

i	$L_{local}[1]$	$L_{local}[2]$	$L_{local}[3]$	$L_{local}[4]$
8	[ ]	[ ]	[ ]	[ ]
7	[ ]	[ ]	[ ]	[1]
6	[ ]	[ ]	[1]	[1]
5	[ ]	[1]	[1]	[1]

Figure: GESA of $\mathcal{S} = \{\mathrm{aac}, \mathrm{aca}, \mathrm{aa}, \mathrm{caa}\}$.

Related work:

Algorithm [Tustumi et al., 2016]:

- Global solution:
  - The longest suffix of S^r that overlaps S^k may be positioned in a previous block.
  - The global lists store these overlaps.
  - Each $L_{global}[r]$ is updated as each block is processed.
    - First, we remove suffixes larger than $lcp(S^t, S^k)$ from local lists.
    - $L_{local}[r]$ is prepended in the global list $L_{global}[r]$.
    - The first element of each $L_{global}[r]$ is the longest overlap of S^r to S^k, that is Ov$[k, r]$.

	i	SA	LCP	STR	SA′	$S^{\$}_{\mathrm{SA}[i]}$
	1	4	0	1	4	$\$_1$
	2	8	0	2	4	$\$_2$
	3	11	0	3	3	$\$_3$
	4	15	0	4	4	$\$_4$
P[0] →	5	7	0	2	3	a$\$_2$
	6	10	1	3	2	a$\$_3$
	7	14	1	4	3	a$\$_4$
P[1] →	8	9	1	3	1	aa$\$_3$
	9	13	2	4	2	aa$\$_4$
P[2] →	10	1	2	1	1	aac$\$_1$
	11	2	1	1	2	ac$\$_1$
P[3] →	12	5	2	2	1	aca$\$_2$
	13	3	0	1	3	c$\$_1$
	14	6	1	2	2	ca$\$_2$
P[4] →	15	12	2	4	1	caa$\$_4$

i	$L_{local}[1]$	$L_{local}[2]$	$L_{local}[3]$	$L_{local}[4]$
12	[ ]	[ ]	[ ]	[ ]
11	[2]	[ ]	[ ]	[ ]
10	[2]	[ ]	[ ]	[ ]

$P[j-1]$	$L_{global}[1]$	$L_{global}[2]$	$L_{global}[3]$	$L_{global}[4]$
5	[ ]	[1]	[1]	[1]
8	[ ]	[1]	[2,1]	[2,1]
10	[2]	[1]	[1]	[1]

Figure: GESA of $\mathcal{S} = \{\mathrm{aac}, \mathrm{aca}, \mathrm{aa}, \mathrm{caa}\}$.

Related work:

Algorithm [Tustumi et al., 2016]:

- Identical suffixes:
  - We scan GESA forward from $i = \mathrm{P}[j] + 1$ to q, while $\mathrm{LCP}[q] = n_k$.
  - The length of these suffixes are inserted in Ov, possibly overwriting the results in $L_{global}[r]$, which is correct as such overlaps are larger.

	i	SA	LCP	STR	SA′	$S^{\$}_{\mathrm{SA}[i]}$
	1	4	0	1	4	$1
	2	8	0	2	4	$2
	3	11	0	3	3	$3
	4	15	0	4	4	$4
P[0] →	5	7	0	2	3	a$2
	6	10	1	3	2	a$3
	7	14	1	4	3	a$4
P[1] →	8	9	1	3	1	aa$3
	9	13	2	4	2	aa$4
P[2] →	10	1	2	1	1	aac$1
	11	2	1	1	2	ac$1
P[3] →	12	5	2	2	1	aca$2
	13	3	0	1	3	c$1
	14	6	1	2	2	ca$2
P[4] →	15	12	2	4	1	caa$4

$$Ov[m, m]^3 = \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & & 1 & 2 & 2 \\ 2 & 2 & & 1 & 1 \\ 3 & & 1 & & 2 \\ 4 & 1 & 2 & & \end{array}$$

Figure: GESA of $\mathcal{S} = \{\mathrm{aac}, \mathrm{aca}, \mathrm{aa}, \mathrm{caa}\}$.

[3] $\mathrm{Ov}[k, r]$ the length of the longest suffix of S^r that overlaps S^k.

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3. Related work

4. Parallel Algorithm

5. Experiments

6. Conclusion

Parallel Algorithm:

We split the computation of all overlaps to solve the APSP in parallel:

At a glance, our algorithm is composed by:

1. Compute all local solutions scanning the blocks B^j concurrently.
2. Compute all global solutions accessing the local lists in parallel.
3. Compute all identical suffixes of all strings scanning the GESA in parallel.

Algorithm: Suppose that for each block B^j, $pos(S^k) = \mathrm{P}[j]$ and $\mathrm{pos}(S^t) = \mathrm{P}[j-1]$.

	i	SA	LCP	STR	SA′	$S^{\$}_{\mathrm{SA}[i]}$
	1	4	0	1	4	$\$_1$
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P[$j-1$] →	10	1	2	1	1	aac$\$_1$ ← S^t
	11	2	1	1	2	ac$\$_1$
P[j] →	12	5	2	2	1	aca$\$_2$ ← S^k
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Figure: GESA of $\mathcal{S} = \{\mathtt{aac}, \mathtt{aca}, \mathtt{aa}, \mathtt{caa}\}$.

Parallel Algorithm:

1. Local solutions:
    - Scan all the m blocks in parallel.
        - Each block B^j is scanned backwards.
        - Whenever $|S^{r=\mathrm{STR}[i]}_{\mathrm{SA}'[i]}| = rmq(\mathrm{P}[j], i)$[4] then a suffix of S^r overlaps S^k.
    - We store the overlaps at a squared matrix of local lists:
        - $L_{local}[r][j]$ stores the length of a suffix of S^r that overlaps S^k.
        - The overlaps are ordered decreasingly by their lengths due to the backward scan.
    - We compute $\mathrm{Min}[j] = rmq(\mathrm{P}[j-1], \mathrm{P}[j]) = lcp(S^k, S^t)$
    - At the end, all local solutions have been computed and are stored into the local lists.

	i	SA	LCP	STR	SA′	$S^{\$}_{\mathrm{SA}[i]}$	
	1	4	0	1	4	$\$_1$	
	2	8	0	2	4	$\$_2$	
	3	11	0	3	3	$\$_3$	
	4	15	0	4	4	$\$_4$	
P[0] →	5	7	0	2	3	a$\$_2$	
	6	10	1	3	2	a$\$_3$	
	7	14	1	4	3	a$\$_4$	
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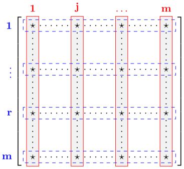
$\mathrm{P}[j-1]$ →	10	1	2	1	1	aac$\$_1$	$\leftarrow S^t$
	11	2	1	1	2	ac$\$_1$	
$\mathrm{P}[j]$ →	12	5	2	2	1	aca$\$_2$	$\leftarrow S^k$
	13	3	0	1	3	c$\$_1$	
	14	6	1	2	2	ca$\$_2$	
P[4] →	15	12	2	4	1	caa$\$_4$	

	1	2	3	4
Min =	0	2	1	0



Local lists, columns are being accessed in parallel

[4] The *rmqs* are solved as LCP is scanned, ℓ starts with ∞ and $\ell = min(\ell, \mathrm{LCP}[i+1])$;.

Parallel Algorithm:

2. Global solutions:
   - We process the m lines of matrix L_{local} in parallel.
     - Each local list $L_{local}[r][j]$ corresponds to the suffixes of S^r that overlap S^k in B^j.
   - For each line r (in parallel):
     - We process lists $L_{local}[r][j]$ in order $j = 1, 2, \ldots, m$.
     - We use a global list L_{Global} that is updated according to $\text{Min}[j] = lcp(S^t, S^k)$.
     - L_{global} is initially empty and for each $j = 1, 2, \ldots, m$, all suffixes larger than $\text{Min}[j]$ are removed, these suffixes are no longer overlaps for the next blocks.
     - $L_{local}[r][j]$ is prepended to L_{global}
     - $\text{Ov}[r, k] \leftarrow first(L_{global})$[5].

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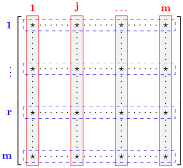
	1	2	3	4
Min =	0	2	1	0



Local lists, lines are being accessed in parallel

[5] The longest suffix of S^r that overlaps S^k will be the first element of L_{global}.

Parallel Algorithm:

3. Identical suffixes:
   - Scan all the end of blocks B^j concurrently.
   - For each block B^j and its corresponding string S^k:
     - All suffixes of S^r identical to S^k appear directly after pos(S^k).
     - We scan from $P[j]+1$ while the next suffixes have the same length of S^k.
     - $Ov[r,k] \leftarrow LCP[i]$[6].

	i	SA	LCP	STR	SA′	$S^{\$}_{SA[i]}$
	1	4	0	1	4	$\$_1$
	2	8	0	2	4	$\$_2$
	3	11	0	3	3	$\$_3$
	4	15	0	4	4	$\$_4$
P[0] →	5	7	0	2	3	a$\$_2$
	6	10	1	3	2	a$\$_3$
	7	14	1	4	3	a$\$_4$
P[1] →	8	9	1	3	1	aa$\$_3$
	9	13	2	4	2	aa$\$_4$
P[2] →	10	1	2	1	1	aac$\$_1$
	11	2	1	1	2	ac$\$_1$
P[3] →	12	5	2	2	1	aca$\$_2$
	13	3	0	1	3	c$\$_1$
	14	6	1	2	2	ca$\$_2$
P[4] →	15	12	2	4	1	caa$\$_4$

[6]Different from [Tustumi et al., 2016] $Ov[r,k]$ the length of the longest suffix of S^r that overlaps S^k.

Parallel Algorithm:

Theoretical costs:

- Time:
  - Our algorithm runs in $O(N + m^2/t)$ time, where t is the number of threads.
    - Local solution: $O(\max_{1 \leq j \leq m} |B^j|)$ to scan all blocks.
    - Global solution: $O(m^2/t)$ to access all local lists.
    - Identical suffixes: $O(N)$, since it reads at most N elements of GESA.
  - The worst case happens only when the string lengths are very unbalanced.
  - In realistic cases ($m \gg t$ and all strings with about the same size) the parallel time is close to $N/t + m^2/t$.
- Space:
  - Our algorithm uses $O(N + m^2)$ of space.
    - which is equal to the sequential algorithm by [Tustumi et al., 2016].
  - The space is given by the $O(N)$ space of the GESA, and by the $O(m^2 + N)$ space of the matrix of local lists, where each list stores at most N overlaps.

Outline

1. Introduction

2. Preliminaries

3. Related work

4. Parallel Algorithm

5. Experiments

6. Conclusion

Experiments:

Implementation:

- C++ using OpenMP.
- sdls-lite v.2 to construct the GESA.
- Source code: `https://github.com/felipelouza/p-apsp`.

Comparison:

- p-apsp: our parallel algorithm.
- apsp: sequential optimal algorithm by [Tustumi et al., 2016].
- SOF: practical (non-optimal) solution by [Rachid and Malluhi, 2015].

Number of threads:

- $t = \{1, 2, 4, 8, 16, 32\}$
- set by `omp_set_num_threads()` for p-apsp and SOF

Configuration:

- 64 bits Debian GNU/Linux 8 (kernel 3.16.0-4)
- Intel Xeon Processor E5-2630 v3 20M Cache 2.40-GH
- 384 GB of RAM.

Experiments:

Dataset:

- We used $m = 300.000$ strings from EST database of *C. elegans*[7].

Minimum overlap length (τ):

- We limited the number of overlaps by $\tau = \{5, 10, 15, 20\}$

Table: Number of overlaps found with 100.000, 200.000 and 300.000 ESTs varying τ.

m/τ	5	10	15	20
100.000	18,853,491	206,154	88,725	82,427
200.000	71,451,170	2,675,759	2,139,431	2,077,125
300.000	162,135,112	7,044,274	5,800,397	5,617,779

Observation:

- The number of overlaps decreases as τ increases.
- For 300.000, when $\tau = 5$ the number of overlaps is 23 times larger than when $\tau = 10$.
- Such variation impacts the performance of all algorithms.

[7] `http://www.uni-ulm.de/in/theo/research/seqana.html`

Experiments:

Running Time[8]:

- SOF was the fastest in all experiments.
- p-apsp has shown a good performance for small threshold τ.
- There is an overhead with $\tau = 5$ when comparing p-apsp$_1$ to apsp.

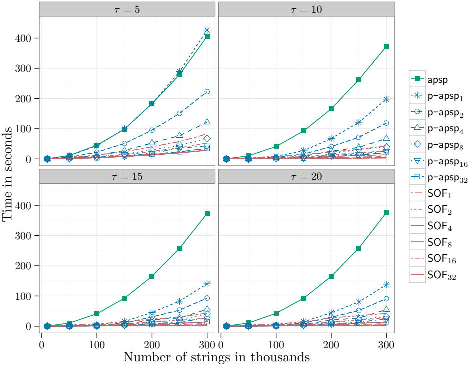


Figure: Running time for varying values of τ (`omp_get_wtime()`).

[8] not accounting for the time to build the GESA for apsp and p-apsp, and compact prefix tree for SOF.

Experiments:

Speedup:

- We evaluated the speedup of p−apsp and SOF over its serial versions.
- p−apsp and SOF improve as the number of threads increases.
- p−apsp achieved a better speedup with the increasing number of threads.

Table: Experiments with 300.000 ESTs with $\tau = 5$. The table shows the running time in seconds.

	apsp	p−apsp		SOF	
n. threads	time	time	speedup	time	speedup
1	397.17	463.33		**82.80**	
2		222.78	**1.91**	**52.49**	1.58
4		121.35	**3.51**	**29.50**	2.81
8		68.11	**6.26**	**28.30**	2.93
16		43.41	**9.82**	**28.64**	2.89
32		34.65	**12.31**	**23.62**	3.50

Experiments:

Peak Memory:

- The memory usage decreases as τ increases (number of overlaps).
- SOF uses less memory in all experiments.
- p–apsp memory usage is very similar to apsp, differing only by a constant factor.

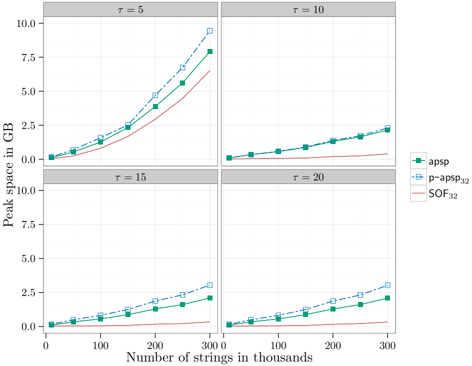


Figure: Running time for varying values of τ (`malloc_count library`).

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6. Conclusion

Conclusion:

Future works:

- Semi-external memory: The GESA can be constructed in external memory and its blocks can be accessed as necessary, reducing the peak memory.
- Different architecture model: such as cloud distributed computing, possibly enabling the usage of hundreds of threads.

Thank you!

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