LOWER AND UPPER BOUNDS FOR STRING MATCHING IN LABELLED GRAPHS

Massimo Equi

Supervisor: Veli Mäkinen Co-supervisor: Alexandru I. Tomescu Opponent: Nicola Prezza



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String Matching in Plain Text

\mathcal{T} = A C G C G T C G G A A T G T C A G C T A T A A G

P = A A T G T C



String Matching in Plain Text

T = A C G C G T C G G A A T G T C A G C T A T A A G

P = A A T G T C

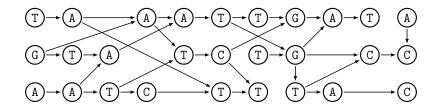


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String Matching in Labelled Graphs

String Matching in Labelled Graphs (SMLG)

SMLG for graph $G = (V, E, \ell)$ and pattern string P

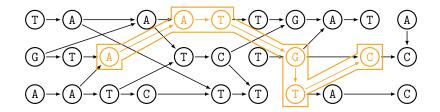


P = A A T G T C



String Matching in Labelled Graphs (SMLG)

SMLG for graph $G = (V, E, \ell)$ and pattern string P



P = A A T G T C



• Lower bound: **minimum** number of operations needed by an algorithm to solve the problem



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- E.g. $\Omega(|V|)$, checking at least all nodes in the graph



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- E.g. $\Omega(|V|)$, checking at least all nodes in the graph
- Upper bound: **maximum** number of operations needed by an algorithm to solve the problem
- E.g. $O(|V|^{|P|})$, checking all possible paths of length |P|





Ideally, we want to make them match

•
$$\Omega(|V|) \rightarrow ? \leftarrow O(|V|^{|P|})$$



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If they match, the algorithm is **optimal**



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• $\Omega(|V|) \rightarrow ? \leftarrow O(|V|^{|P|})$

If they match, the algorithm is optimal

There are many possibilities in between:

• $O(|E| + |V|), O(|E| \log |E|), O((|E||V|)^c)$



Back in the 90s: querying the Web



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Nowadays: bioinformatics, graph databases, graph mining for network analysis



Back in the 90s: querying the Web

Nowadays: bioinformatics, graph databases, graph mining for network analysis

Main focus for us: Bioinformatics

- Pangenomics
- Sequence Alignment in Variation Graphs



State of the art for SMLG				
Year	Authors	Graph	Exact/	Time
			Approximate	
1992	Manber, Wu	DAG	approximate	$O(E P + occ \log \log P)$
1993	Akutsu	Tree	exact	<i>O</i> (<i>N</i>)
1995	Park, Kim	DAG	exact ⁽²⁾	O(N+ E P)
1997	Amir et al.	general	exact	O(N + E P)
1997	Amir et al.	general	approximate ⁽¹⁾	NP-Hard
1997	Amir et al.	general	approximate	$O(N P \log N + E P)$
1998	Navarro	general	approximate	O(N P + E P)
2017	Vadaddi et al.	general	approximate	O((V +1) E P)
2017	Rautiainen,	general	approximate	O(N + E P)
	Marschall			

Table: (1) errors in the graph, (2) matches span only one edge.





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String Matching in Labelled Graphs

Four publications



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String Matching in Labelled Graphs

Four publications

Paper I

On the Complexity of String Matching for Graphs Massimo Equi, Roberto Grossi, Veli Mäkinen, Alexandru I. Tomescu ICALP 2019

Paper II

Graphs Cannot Be Indexed in Polynomial Time for Sub-quadratic Time String Matching, Unless SETH Fails Massimo Equi, Veli Mäkinen, Alexandru I. Tomescu SOFSEM 2021



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They provide quadratic conditional lower bounds based on SETH

- Paper I deals with the **online** case
- Paper II deals with the indexed case



Four publications



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Four publications

Paper III

Linear Time Construction of Indexable Founder Block Graphs Veli Mäkinen, Bastien Cazaux, **Massimo Equi**, Tuukka Norri, Alexandru I. Tomescu

WABI 2020

Paper IV

Algorithms and Complexity on Indexing Elastic Founder Graphs Massimo Equi, Tuukka Norri, Jarno Alanko, Bastien Cazaux, Alexandru I. Tomescu, Veli Mäkinen

ISAAC 2021



Four publications

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ISAAC 2021

They provide efficient algorithms for a special class of graphs

- Paper III introduces the techniques for Founder Block Graphs
- Paper IV extends Paper III to Elastic Founder Graphs



Quick Complexity Background



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Let $X, Y \subseteq \{0,1\}^d$ be two sets of *n* binary vectors of length *d*.

Determine whether there exist $x \in X, y \in Y$ such that $x \cdot y = 0$



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$$X = \begin{pmatrix} 001 \\ 010 \\ 011 \\ 101 \end{pmatrix} \qquad \begin{pmatrix} 010 \\ 011 \\ 100 \\ 111 \end{pmatrix} = Y$$



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Orthogonal Vectors Hypothesis (OVH)

No algorithm can solve Orthogonal Vectors in time $O(n^{\alpha} \operatorname{poly}(d))$, $\alpha < 2$



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Orthogonal Vectors Hypothesis (OVH)

No algorithm can solve *Orthogonal Vectors* in time $O(n^{\alpha} \operatorname{poly}(d))$, $\alpha < 2$

CNF-SAT can be reduced to OV, thus SETH \Rightarrow OVH



Paper I



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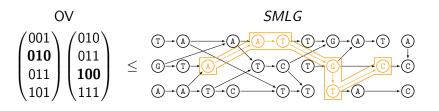
Theorem

For any $\epsilon > 0$ and any DAG G, the exact SMLG problem on G cannot be solved in either $O(|E|^{1-\epsilon}|P|)$ or $O(|E||P|^{1-\epsilon})$ time unless OVH is false.



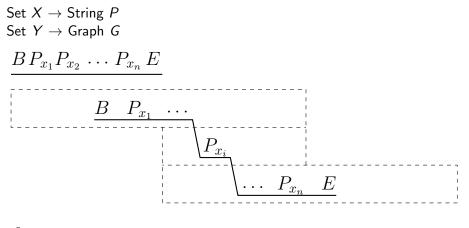
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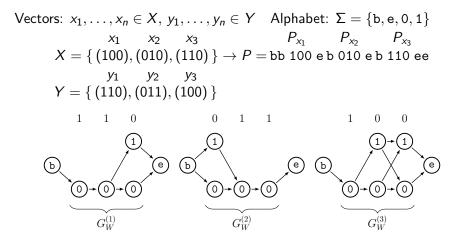
String Matching in Labelled Graphs





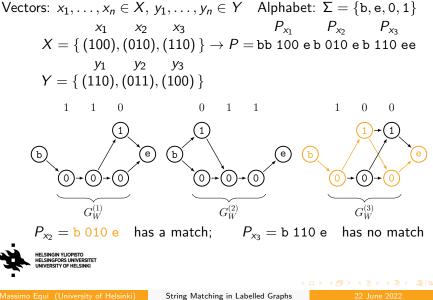
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Paper I





Paper I



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Paper II



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Theorem

For any $\alpha, \beta, \delta > 0$, with $\beta < 1$ or $\delta < 1$, there is no algorithm preprocessing a labeled graph $G = (V, E, \ell)$ in time $O(|E|^{\alpha})$ such that for any pattern string P we can solve the SMLG problem on G and P in time $O(|P| + |E|^{\delta}|P|^{\beta})$, unless OVH is false.



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Linear independent-components (lic) reduction

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Linear independent-components (lic) reduction

$$\begin{pmatrix} X & Y \\ 001 \\ 010 \\ 011 \\ 101 \end{pmatrix} \begin{pmatrix} 010 \\ 011 \\ 100 \\ 111 \end{pmatrix} \leq_{lic} \text{ Any problem respecting a lic reduction}$$

lic reduction: P depends only on X, G depends only on Y





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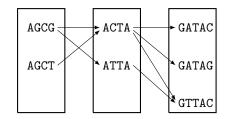
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From an MSA[m, n] we can build a Founder Block Graph (FBG)

 $\begin{array}{l} A \ G \ C \ G \ A \ C \ T \ A \ G \ A \ T \ A \ C \\ A \ G \ C \ T \ A \ C \ T \ A \ G \ A \ T \ A \ G \\ \end{array} \xrightarrow{} \\ A \ G \ C \ G \ A \ T \ A \ G \ T \ A \ C \\ \end{array} \xrightarrow{} \\ \begin{array}{l} A \ G \ C \ T \ A \ C \ T \ A \ G \ T \ A \ C \\ \end{array} \xrightarrow{} \end{array}$

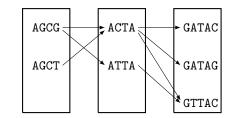




From an MSA[m, n] we can build a Founder Block Graph (FBG)

 \rightarrow

A G C G A C T A G A T A C A G C T A C T A G A T A G A G C G A T T A G T T A C A G C T A C T A G T T A C



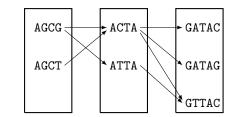
(v, w) ∈ E ⇔ ℓ(v)ℓ(w) matches an MSA row at the corresponding segments



From an MSA[m, n] we can build a Founder Block Graph (FBG)

 \rightarrow

A G C G A C T A G A T A C A G C T A C T A G A T A G A G C G A T T A G T T A C A G C T A C T A G T T A C



- (v, w) ∈ E ⇔ ℓ(v)ℓ(w) matches an MSA row at the corresponding segments
- Repeat-free property: every node label l(v) appears nowhere else in the graph



Repeat-free Founder Block Graphs



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Repeat-free Founder Block Graphs

• Can be constructed from an MSA optimising different functions



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Repeat-free Founder Block Graphs

- Can be constructed from an MSA optimising different functions
- Allow indexing in polynomial time
- Allow queries in time $O(|P| \log \sigma)$



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• Key property: a match spanning at least three nodes is "unique"



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- Key property: a match spanning at least three nodes is "unique"
- The Aho-Corasick automaton locates a matching node



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Querying algorithm

- Key property: a match spanning at least three nodes is "unique"
- The Aho-Corasick automaton locates a matching node
- Extend such match using the tries



Paper IV



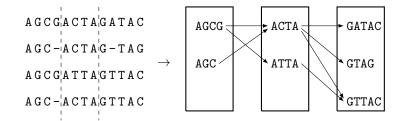
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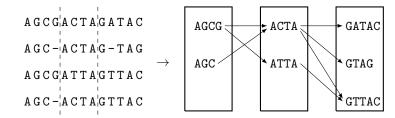
Paper IV

From an MSA[m, n] we can build an EFG $G = (\ell, V, E)$





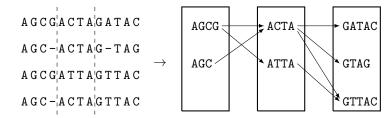
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(v, w) ∈ E ⇔ ℓ(v)ℓ(w) matches an MSA row at the corresponding segments



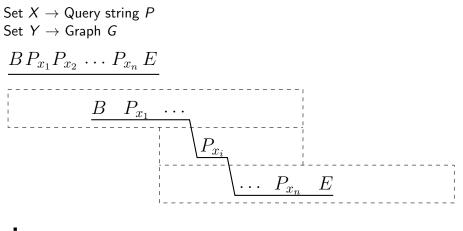
From an MSA[m, n] we can build an EFG $G = (\ell, V, E)$



- (v, w) ∈ E ⇔ ℓ(v)ℓ(w) matches an MSA row at the corresponding segments
- Semi-repeat-free property: every $\ell(v)$ can appear only as a prefix of $\ell(w)$, where v and w belong to the same block



Paper IV



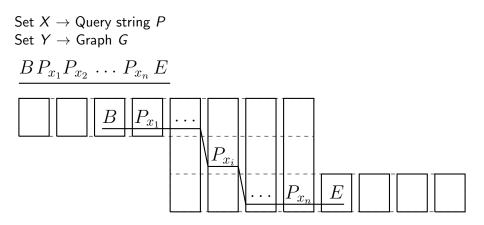


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We refine the previous techniques to achieve the same results also for the gapped case



We refine the previous techniques to achieve the same results also for the gapped case

Semi-repeat-free EFGs

• Can be constructed from a **gapped** MSA optimising different functions



We refine the previous techniques to achieve the same results also for the gapped case

Semi-repeat-free EFGs

- Can be constructed from a **gapped** MSA optimising different functions
- Allow indexing in polynomial time
- Allow querying in time $O(|P| \log \sigma)$



Conclusions and Open Questions

This thesis

- Paper I: SMLG cannot be solved in less than O(|E||P|) time
- **Paper II**: SMLG cannot be solved in less than O(|E||P|) time even after polynomial indexing
- **Paper III**: SMLG on FBGs can be solved with query time O(|P|), after polynomial time indexing
- **Paper IV**: SMLG on general EFGs respects the lower bound, (semi)-repeat-free EFGs give similar guarantees of FBG



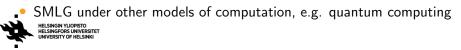
Conclusions and Open Questions

This thesis

- Paper I: SMLG cannot be solved in less than O(|E||P|) time
- **Paper II**: SMLG cannot be solved in less than O(|E||P|) time even after polynomial indexing
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Open Questions

- Non-repeat-free FBGs
- Trade-offs for a more general class of graphs, e.g. $O(|E|^2)$ indexing, $O(|P| \log |P|)$ queries





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OV Indexing Lower Bound

(N, M)-OV

OV over sets X and Y , wh	ere $ X = N$
and $ Y = M$	

We reduce OV to
$$(N, M)$$
-OV

•
$$(X_i, Y_j)$$
 is a (N, M) -OV instance

• Time to index:
$$O\left(d^{O(1)}|X_i|^lpha
ight)$$

• Time to query:
$$O\left(d^{O(1)}|X_i|^{\delta}|Y_j|^{eta}
ight)$$

•
$$O\left(d^{O(1)}\left(N^{\alpha-1}n+N^{\delta-1}M^{\beta-1}n^{2}\right)\right)$$

There exist α , β , δ that lead to time $O(n^{2-\epsilon})$ for OV

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X

 $X_1 \begin{cases} x_1 \\ \vdots \\ x_N \\ X_2 \end{cases} X_{N+1} \\ X_2 \begin{cases} x_{N+1} \\ \vdots \\ x_N \end{cases}$

 $X_{\lceil \frac{n}{N}\rceil} \begin{cases} x_{n-N+1} \\ \vdots \\ x \end{cases}$

1/-

Y y_1

 y_M

 y_{2M}

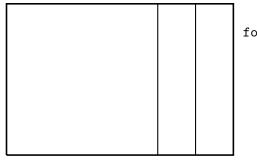
 $\begin{pmatrix} y_{M+1} \\ \vdots \\ y_{2} \end{pmatrix}$

 $\begin{pmatrix} y_{n-M+1} \\ \vdots \\ y_{\lceil \frac{n}{M} \rceil} \end{pmatrix}$

 Y_1

Construction of EFG from MSA

j = j + 1



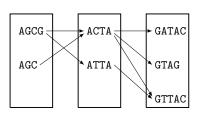
or every j:
while
$$j = f(j_x)$$
:
score $\leftarrow \max(\text{score}, \\ \# blocks(j_x) + 1);$
 $x \leftarrow x + 1;$
 $\# blocks(j) \leftarrow \text{score};$

 j_1

 $\begin{array}{ccc} f(j_1) & \#block(j_1) + 1 \\ j_2 & f(j_2) & \#block(j_2) + 1 \\ f(j_3) & \#block(j_3) + 1 \end{array}$



Construct string $D = \prod_{i \in \{1, 2, ..., b\}} \prod_{v \in V^i, (v, w) \in E} \ell^{-1}(w) \ell^{-1}(v)$



D =ATCAGCGA\$ ATTAGCGA\$ ATCACGA\$ CATAGATCA\$ GATGATCA\$ CATTGATCA\$ CATTGATTA\$

Build the suffix tree of D

Polynomial time in |D|, $O(|D| \log |D|)$ bits of space



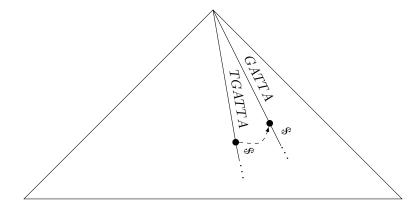
Index Elastic Founder Graphs

Query string Q = CGATTAGTTGATTA Ð

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Index Elastic Founder Graphs

Query string Q = CGATTAGT





Index Elastic Founder Graphs

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