Semi-local string comparison: Algorithmic techniques and applications

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Abstract

The longest common subsequence (LCS) problem is a classical problem in computer science. The semi-local LCS problem is a generalisation of the LCS problem, arising naturally in the context of string comparison. In this work, we present a number of algorithmic techniques related to the semi-local LCS problem, and give a number of algorithmic applications of these techniques. Summarising the presented results, we conclude that semi-local string comparison turns out to be a useful algorithmic plug-in, which unifies, and often improves on, a number of previous approaches to various substring- and subsequence-related problems.

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Chapter 1

Introduction

1.1 Overview

The longest common subsequence (LCS) problem is a classical problem in computer science. Given two strings a, b of lengths m, n respectively, the LCS problem asks for the length of the longest string that is a subsequence of both a and b. This length is called the strings' LCS score. We refer the reader to monographs [29, 45] for the background and further references.

The semi-local LCS problem is a generalisation of the LCS problem, arising naturally in the context of string comparison. Given two strings a, b as before, the semi-local LCS problem asks for the LCS score of each string against all substrings of the other string, and of all prefixes of each string against all suffixes of the other string. In this work, we survey a number of algorithmic techniques related to the semi-local LCS problem, and present some algorithmic applications of these techniques.

The rest of this chapter contains the necessary preliminaries. In Section 1.2, we introduce basic terminology and notation. In Section 1.3, we describe our main algorithmic tool: a special class of integer matrices, called simple unit-Monge matrices, which are obtained as dominance counts of permutation matrices, and can be represented implicitly by a range tree data structure. In Section 1.4, we study the algebraic properties of simple unit-Monge matrices, and in Section 1.5 we give an efficient algorithm for distance multiplication in this matrix class.

In Chapter 2, we describe our main algorithmic techniques for the semi-local LCS problem. In Section 2.1, we formally define the semi-local LCS problem and related concepts. In Section 2.2, we introduce alignment dags and highest-score matrices. Exploiting the algebraic framework of unit-Monge matrices, in Section 2.3 we obtain an efficient algorithm for highest-score matrix composition. In Section 2.4, we generalise our techniques from LCS scores to arbitrary rational-weighted alignment scores and edit distances.

In Chapter 3, we introduce a conceptually simple algorithm for the semi-local LCS problem, called the seaweed algorithm, and show a number of its applications. In Section 3.1, we describe the seaweed algorithm itself, and in Sections 3.2 and 3.3, we apply it to solving the incremental and the common-substring versions of the LCS and semi-local LCS problems. Our algorithms match, improve on, or generalise existing algorithms for these problems.

In Chapter 4, we give a block version of the seaweed algorithm, which is slightly faster than the plain seaweed algorithm, and gives rise to further applications. In Section 4.1, we describe the block seaweed algorithm itself. In the case of an unbounded alphabet, the running time of the block seaweed algorithm matches the running time of the best known global LCS algorithm, while improving on it in functionality. By direct application of the block seaweed algorithm, in Section 4.2 we obtain an improved algorithm for the cyclic LCS problem, and in Section 4.3 for the longest repeating subsequence problem. In Section 4.4, we consider the approximate pattern matching problem, and apply the block seaweed algorithm to obtain an algorithm for this problem, matching the best known algorithm in running time.

In Chapter 5, we describe an extension of the seaweed algorithm that allows efficient semi-local comparison of two input strings, one of which is periodic. In Section 5.1, we describe the periodic seaweed algorithm itself. By application of the periodic seaweed algorithm, in Section 5.2 we obtain new algorithms for the tandem LCS problem and the tandem cyclic alignment problem, improving on existing algorithms in running time.

In Chapter 6, we consider the semi-local LCS problem restricted to permutation strings of length n. In particular, Section 6.1 gives an algorithm for the semi-local LCS problem on permutation strings. By direct application of this algorithm, in Section 6.2 we obtain an improved algorithm for the cyclic LCS problem on permutations. Further applications include improved algorithms for the problem of longest pattern-avoiding subsequence, given in Section 6.3, and for longest k-piece increasing and k-modal subsequence, given in Section 6.4. In Section 6.5, we consider the maximum clique problem in a circle graph represented by an interval model of size n. By application our semi-local LCS algorithm on permutations, we obtain new algorithms for this problem, both for general and sparse circle graphs, achieving a substantial improvement on existing algorithms in running time. In Section 6.6, we describe an application of these algorithms to the problem of finding exact and approximate commonly structured patterns in linear graphs.

In Chapter 7, we apply the semi-local LCS problem to compressed string comparison. Our goal is to obtain efficient algorithms that work on compressed strings without first decompressing them. In Section 7.1, we introduce the grammar compression (GC) framework, that generalises the classical LZ78 and LZW methods. In Section 7.2, we give an efficient algorithm for the three-way semi-local LCS problem on GC-strings. By application

of this algorithm, in Section 7.3 we obtain an algorithm for subsequence recognition in GC-strings, which improves on existing algorithms in running time.

In Chapter 8, we consider applications of our techniques that aim to reach beyond semi-local string comparison, with the ultimate goal of efficient fully-local comparison. In Section 8.1, we introduce the window-substring and window-window LCS problems, and give an algorithm for these problems. This algorithm provides a refinement for the standard dot plot method, by allowing efficient window-window string comparison based on the LCS score, rather than the less sensitive Hamming score. In Section 8.2, we introduce the quasi-local LCS problem, which generalises the semi-local, window-substring and window-window LCS problems, and give an efficient algorithm for this problem. By application of this algorithm, in Section 8.3 we obtain an algorithm for sparse spliced alignment under an arbitrary rational edit distance metric, which improves on existing algorithms for this problem.

Some results presented in this work appeared incrementally in the author's publications [93, 94, 96, 95, 92]. The aim of this work is to consolidate these results, unifying the terminology and notation. However, a number of results have not been published before, and are original to this work.

Summarising the presented results, we conclude that semi-local string comparison turns out to be a useful algorithmic plug-in, which unifies, and often improves on, a number of previous approaches to various substring- and subsequence-related problems.

1.2 Terminology and notation

In addition to integers $\{\dots,-2,-1,0,1,2,\dots\}$, we will use *odd half-integers* $\left\{\dots,-\frac{5}{2},-\frac{3}{2},-\frac{1}{2},\frac{1}{2},\frac{3}{2},\frac{5}{2},\dots\right\}$. For ease of reading, odd half-integer variables will be indicated by hats (e.g. $\hat{\imath}$, $\hat{\jmath}$). Ordinary variable names (e.g. i, j, with possible subscripts or superscripts), will normally indicate integer variables, but can sometimes indicate a variable that may be either integer, or odd half-integer.

We denote integer and odd half-integer *intervals* by

$$[i:j] = \{i, i+1, \dots, j-1, j\}$$
$$\langle i:j\rangle = \left\{i+\tfrac{1}{2}, i+\tfrac{3}{2}, \dots, j-\tfrac{3}{2}, j-\tfrac{1}{2}\right\}$$

Note that in this notation, both an integer and an odd half-integer interval is defined by integer endpoints. To denote infinite intervals of integers and odd half-integers, we will use $-\infty$ for i and $+\infty$ for j where appropriate, so e.g. $[-\infty:+\infty]$ denotes the set of all integers, and $\langle-\infty:+\infty\rangle$ the set of all odd half-integers. For finite intervals $[i:j]$ and $\langle i:j\rangle$, we call the difference $j-i$ interval *length*.

When dealing with pairs of numbers, we will often use geometrical language and call such pairs *points*. When visualising points, we use the matrix indexing convention: the first coordinate in a pair increases downwards, and the second coordinate rightwards. We say that a point (i_0, j_0) *dominates*[1] point (i, j), if $i_0 < i$ and $j < j_0$. Visually, the dominated point is "below and to the left" of the dominating point. We will write $(i_0, j_0) \ll (i_1, j_1)$, if $i_0 < i_1$ and $j_0 < j_1$ (note that such two points do not dominate one another).

We use standard terminology for dominance and other partial orders. In particular, a set of elements forms a *chain*, if they are pairwise comparable, and an *antichain*, if they pairwise incomparable. An element in a partially ordered set is *minimal*, if it is not higher (in terms of the partial order) than any other element in the set. All minimal points in a partially ordered set form an antichain.

A function of an integer argument will be called *unit-monotone increasing* (respectively, *decreasing*), if the difference between every pair of successive values is either 0 or 1 (respectively, 0 or -1).

We will make extensive use of finite and infinite matrices, with integer (occasionally, rational or real) elements, and with integer or odd half-integer indices. Unless indicated otherwise, all definitions below apply to both finite and infinite matrices. Given finite or infinite index ranges I, J, a *vector over* I is indexed by $i \in I$, and a *matrix over* $I \times J$ is indexed $i \in I$, $j \in J$. A vector or matrix is *nonnegative*, if all its elements are nonnegative.

Sometimes we will consider matrices over non-consecutive index ranges. To reduce the amount of notation, we will occasionally perform operations on such matrices as if they were over consecutive intervals. This will have the following meaning: we remap the ranges to consecutive intervals preserving order, then we perform a matrix operation, and finally we remap the intervals back to the original ranges.

We will use parenthesis notation for indexing matrices, e.g. $A(i, j)$. We will use straightforward notation for selecting subvectors and submatrices; for example, given a matrix A over $[-\infty : +\infty]^2$, we denote by $A[i_0 : i_1, j_0 : j_1]$ the submatrix defined by the given intervals. A star $*$ will indicate that for a particular index, its whole range is selected implicitly, e.g. $A[*, j_0 : j_1] = A[-\infty : +\infty, j_0 : j_1]$. Given matrices A' over $I' \times J'$ and A'' over $I'' \times J''$, where $(I' \times I'') \cap (J' \times J'') = \emptyset$, and the ranges I', J', I'', J'' are not necessarily consecutive, we denote by $A = A' \bowtie A''$ the matrix over $(I' \cup I'') \times (J' \cup J'')$, obtained by merging the matrices A', A'': we have

$$A(i,j) = (A' \bowtie A'')(i,j) = \begin{cases} A'(i,j) & \text{if } i \in I',\ j \in J' \\ A''(i,j) & \text{if } i \in I'',\ j \in J'' \\ 0 & \text{otherwise} \end{cases}$$

[1]The standard definition of dominance requires $i < i_0$ instead of $i_0 < i$. Our definition is more convenient in the context of string applications.

We also extend this notation naturally to merging more than two matrices.

The matrices we consider (in particular, infinite matrices) can be *implicit*, i.e. represented by a compact data structure that allows access to every element in a specified (not necessarily constant) time.

Definition 1. *Let D be a matrix over $\langle i_0 : i_1\rangle \times \langle j_0 : j_1\rangle$. Its* distribution matrix D^Σ *over $[i_0 : i_1] \times [j_0 : j_1]$ is defined by*

$$D^\Sigma(i,j) = \sum\nolimits_{\hat{\imath}>i,\hat{\jmath}<j} D(\hat{\imath},\hat{\jmath})$$

for all $i \in [i_0 : i_1]$, $j \in [j_0 : j_1]$, $\hat{\imath} \in \langle i_0 : i_1\rangle$, $\hat{\jmath} \in \langle j_0 : j_1\rangle$.

Definition 2. *Let A be a matrix over $[i_0 : i_1] \times [j_0 : j_1]$. Its* density matrix $A^\square$ *over $\langle i_0 : i_1\rangle \times \langle j_0 : j_1\rangle$ is defined by*

$$A^\square(\hat{\imath},\hat{\jmath}) = A\big(\hat{\imath}+\tfrac{1}{2},\hat{\jmath}-\tfrac{1}{2}\big) - A\big(\hat{\imath}-\tfrac{1}{2},\hat{\jmath}-\tfrac{1}{2}\big) - A\big(\hat{\imath}+\tfrac{1}{2},\hat{\jmath}+\tfrac{1}{2}\big) + A\big(\hat{\imath}-\tfrac{1}{2},\hat{\jmath}+\tfrac{1}{2}\big)$$

for all $\hat{\imath} \in \langle i_0 : i_1\rangle$, $\hat{\jmath} \in \langle j_0 : j_1\rangle$.

The definitions of distribution and density matrices extend naturally to matrices over an infinite index range, as long as the sum in Definition 1 is always defined. This will be the case for all matrices considered in this work. Note that for any matrix D as above, and for all $\hat{\imath}$, $\hat{\jmath}$, we have

$$\big(D^\Sigma\big)^\square(\hat{\imath},\hat{\jmath}) = D(\hat{\imath},\hat{\jmath})$$

Also, for any matrix A as above, there exist vectors b over $[i_0 : i_1]$ and c over $[j_0 : j_1]$, such that for all i, j, we have

$$\big(A^\square\big)^\Sigma(i,j) + b(i) + c(j) = A(i,j)$$

If j_0, i_1 are finite, then we have $b(i) = A(i, j_0)$, $c(j) = A(i_1, j)$. An important special case is when b, c are both zero vectors.

Definition 3. *Matrix A will be called* simple, *if $\big(A^\square\big)^\Sigma = A$.*

The following classes of matrices play a fundamental role in optimisation theory (see [20] for an extensive survey).

Definition 4. *Matrix A is called* totally monotone, *if*

$$A(i,j) > A(i,j') : A(i',j) > A(i',j') \qquad \text{for all } i \le i',\ j \le j'$$

Definition 5. *Matrix A is called* a Monge matrix, *if*

$$A(i,j) + A(i',j') \le A(i,j') + A(i',j) \qquad \text{for all } i \le i',\ j \le j'$$

Equivalently, matrix A is a Monge matrix, if $A^\square$ is nonnegative. Matrix A is called an anti-Monge matrix, *if $-A$ is Monge.*

It is easy to see that Monge matrices are a subclass of totally monotone matrices. By Definition 5, a matrix is Monge, if and only if its density matrix is nonnegative. This condition is equivalent to the canonical structure theorem for Monge matrices, given by Burkard et al. [20].

1.3 Permutation and unit-Monge matrices

A *permutation matrix* is a (finite or infinite) square zero-one matrix, containing exactly one nonzero in every row and every column. Typically, permutation matrices will be over odd half-integer intervals. A zero-one matrix P over $I \times J$ is a permutation matrix, if and only if

$$\sum_{\hat{\jmath}} P(\hat{\imath},\hat{\jmath}) = 1 \qquad \sum_{\hat{\imath}} P(\hat{\imath},\hat{\jmath}) = 1$$

for all $\hat{\imath} \in I$, $\hat{\jmath} \in J$. An *identity matrix* is a (finite or infinite) permutation matrix Id, such that $Id(\hat{\imath},\hat{\jmath}) = 1$, iff $\hat{\imath} = \hat{\jmath}$. Further, given an $h \in [-\infty : +\infty]$, we define an infinite *offset identity matrix* as a permutation matrix Id_h, such that $Id_h(\hat{\imath},\hat{\jmath}) = 1$, iff $\hat{\jmath} - \hat{\imath} = h$. We have $Id_0 = Id$. Clearly, a finite or infinite identity or offset identity matrix, can be represented implicitly in constant space and with constant query time.

A permutation matrix P is *superdiagonal*, if $P(\hat{\imath},\hat{\jmath}) = 0$ for all $\hat{\imath} < \hat{\jmath}$. Clearly, a finite permutation matrix is superdiagonal, if and only if it is an identity matrix. However, the property of being superdiagonal is non-trivial for infinite permutation matrices,

An infinite permutation matrix P over $\langle -\infty : +\infty\rangle^2$ has *core* $\langle i_0 : i_1\rangle \times \langle j_0 : j_1\rangle$ and *offset* h, for given $i_0, i_1, j_0, j_1, h \in [-\infty : +\infty]$, if

$$\begin{aligned} &i_1 - i_0 = j_1 - j_0 \\ &j_0 - i_0 = j_1 - i_1 = h \\ &P(\hat{\imath},\hat{\jmath}) = Id(\hat{\imath} - h, \hat{\jmath}) = Id(\hat{\imath}, \hat{\jmath} + h) \end{aligned}$$

for all $\hat{\imath} \in \langle -\infty : i_0\rangle \cup \langle i_1 : +\infty\rangle$, $\hat{\jmath} \in \langle -\infty : j_0\rangle \cup \langle j_1 : +\infty\rangle$. In particular, an offset identity matrix Id_h has empty core and offset h. Clearly, a permutation matrix with a finite core can be represented implicitly in finite space and with constant query time.

From now on, instead of "index pairs corresponding to nonzeros", we will write simply "nonzeros", where this does not lead to confusion. We will normally assume that a permutation matrix is given by an efficient data structure that allows random access to the nonzeros both by rows and by columns.

Given a permutation matrix P over $I \times J$, and a set $I' \subseteq I$, we will denote by $P(I', \cdot)$ the permutation submatrix *row-induced by* I', i.e. the permutation submatrix obtained by deleting from P all columns in $I \setminus I'$, and then deleting from the remaining submatrix all zero rows. A column-induced permutation submatrix $P(\cdot, J')$ is defined analogously. Both these operations can be implemented in linear time by a sweep of the nonzeros of matrix P.

A *subpermutation matrix* is a (finite or infinite) zero-one matrix containing *at most* one nonzero in every row and every column.

The following subclass of Monge matrices plays a crucial role in this work.

Definition 6. *A square matrix A is called* a unit-Monge matrix*, if $A^{\square}$ is a permutation matrix. Matrix A is called* a unit-anti-Monge matrix*, if $-A$ is unit-Monge.*

By Definition 5, a unit-Monge (respectively, unit-anti-Monge) matrix over any index range is Monge (respectively, anti-Monge).

Matrices that are both unit-Monge and simple will be our main tool for the rest of this work. Note that such matrices are unit-monotone increasing in rows, and unit-monotone decreasing in columns. Furthermore, a square matrix A is simple unit-Monge, if and only if $A = P^{\Sigma}$, where P is a permutation matrix. The value $A(i_0, j_0) = P^{\Sigma}(i_0, j_0)$ is the number of (odd half-integer) nonzeros that the (integer) point (i_0, j_0) dominates in matrix P.

A permutation matrix P of size n can be regarded as an implicit representation of the simple unit-Monge matrix P^{Σ}. An individual element of P^{Σ} can be queried in time $O(n)$ by a single sweep of the nonzeros of P, counting those that are dominated. Thinking of the nonzeros of P as odd half-integer points in the plane, this procedure is known as geometric *dominance counting*.

Existing methods of computational geometry allow us to answer dominance counting queries much more efficiently than by a direct linear sweep, as long as a preprocessing of the point set is allowed.

Theorem 1. *Given a permutation matrix P of size n, there exists a data structure which*

- *has size $O\big(n \log n\big)$;*
- *can be built in time $O\big(n \log n\big)$;*
- *allows to query an individual element of the simple unit-Monge matrix P^{Σ} in time $O\big(\log^2 n\big)$;*

Proof. The required structure is a two-dimensional range tree [16] (see also [82]), built on the set of nonzeros in P. There are n nonzeros, hence the total number of nodes in the tree is $O\big(n \log n\big)$. A dominance counting query on the set of nonzeros can be answered by accessing $O\big(\log^2 n\big)$ of the tree nodes. □

Using recent results on dominance counting by JaJa et al. [53], the bounds given by Theorem 1 can be improved to size $O(n)$ and individual query time $O\big(\frac{\log n}{\log \log n}\big)$. However, the underlying data structure of Theorem 1 is simpler, requires a less powerful computation model, and is more

likely to be practical. Therefore, we will be using Theorem 1 as our main technique for implicit representation of simple unit-Monge matrices.

In addition to ordinary element queries described by Theorem 1, we will also deal with *incremental queries*, which are given an element of an implicit simple unit-Monge matrix, and return the value of an adjacent element. This kind of query can be answered directly from the permutation matrix, without any preprocessing.

Theorem 2. *Given a permutation matrix P of size n, and the value $P^\Sigma(i,j)$, $i,j \in [0:n]$, the values $P^\Sigma(i \pm 1, j)$, $P^\Sigma(i, j \pm 1)$, where they exist, can be queried in time $O(1)$.*

Proof. Consider a query of the type $P^\Sigma(i+1,j)$; other query types are obtained by symmetry. Let $\hat{\jmath} \in \langle 0:n \rangle$ be such that $P(i+\frac{1}{2}, \hat{\jmath}) = 1$; value $\hat{\jmath}$ can be obtained from the permutation representation of P in time $O(1)$. We have

$$P^\Sigma(i+1,j) = P^\Sigma(i,j) - \begin{cases} 1 & \text{if } \hat{\jmath} < j \\ 0 & \text{otherwise} \end{cases} \qquad \square$$

Incremental queries described by Theorem 2 can be used to answer *batch queries*, returning a set of elements in a row, column or diagonal of the implicit simple unit-Monge matrix. In particular, all elements in a given row, column or diagonal of matrix P^Σ can be obtained by a sequence of incremental queries in time $O(n)$, and a subset of r consecutive elements in time $O\big(r + \log^2 n\big)$.

1.4 Matrix distance multiplication and the seaweed monoid

We will make extensive use of the $(\min, +)$-algebra on integer or real numbers, where the operators min and + play the role of addition and multiplication, respectively. This algebra is often called *distance* (or *tropical*) algebra; for an extensive review of this and related topics, see e.g. Rote [85], Gondran and Minoux [43]. Our techniques are based on matrix-vector and matrix-matrix multiplication in the distance algebra.

Definition 7. *Let A be a matrix over $[i_0 : i_1] \times [j_0 : j_1]$. Let b, c be vectors over $[j_0 : j_1]$ and $[i_0 : i_1]$ respectively. The* distance product *$A \odot b = c$ is defined by*

$$c(i) = \min_j \big(A(i,j) + b(j)\big)$$

for all $i \in [i_0 : i_1]$, $j \in [j_0 : j_1]$.

Definition 8. *Let A, B, C be matrices over $[i_0 : i_1] \times [j_0 : j_1]$, $[j_0 : j_1] \times [k_0 : k_1]$, $[i_0 : i_1] \times [k_0 : k_1]$ respectively. The* distance product *$A \odot B = C$ is defined by*

$$C(i,k) = \min_j \big(A(i,j) + B(j,k)\big)$$

for all $i \in [i_0 : i_1]$, $j \in [j_0 : j_1]$, $k \in [k_0 : k_1]$.

It is straightforward to check that matrix distance multiplication is associative. The set of all square matrices with elements in $[0 : \infty]$ over a given index range forms a monoid with respect to distance multiplication. The identity element in this monoid is the matrix

$$E(i,j) = \begin{cases} 0 & \text{if } i = j \\ +\infty & \text{otherwise} \end{cases}$$

It is well-known that the set of all Monge matrices is closed under distance multiplication. What is slightly more surprising, but crucial for our method, is that the same is also true for the set of all simple unit-Monge matrices.

Lemma 1. *Let A, B, C be matrices, such that $A \odot B = C$. If A, B are Monge (respectively, simple unit-Monge), then C is also Monge (respectively, simple unit-Monge).*

Proof. First, let A, B be Monge matrices. Let $i \le i'$, $k \le k'$. By definition of matrix distance multiplication, we have

$$C(i,k') = \min_{j^*} \big(A(i,j^*) + B(j^*,k')\big)$$
$$C(i',k) = \min_{j^*} \big(A(i',j^*) + B(j^*,k)\big)$$

Let j, j' respectively be the values of j^* on which these minima are attained. Without loss of generality, suppose $j \le j'$. We have

$$\begin{aligned}
&C(i,k) + C(i',k') = && \text{(definition of } \odot\text{)} \\
&\min_{j^*} \big(A(i,j^*) + B(j^*,k)\big) + \min_{j^*} \big(A(i',j^*) + B(j^*,k')\big) \le \\
&\big(A(i,j) + B(j,k)\big) + \big(A(i',j') + B(j',k')\big) = && \text{(term rearrangement)} \\
&\big(A(i,j) + A(i',j')\big) + \big(B(j,k) + B(j',k')\big) \le && (A \text{ is Monge}) \\
&\big(A(i,j') + A(i',j)\big) + \big(B(j,k) + B(j',k')\big) = && \text{(term rearrangement)} \\
&\big(A(i,j') + B(j',k')\big) + \big(A(i',j) + B(j,k)\big) = && \text{(definition of } j,\, j'\text{)} \\
&C(i,k') + C(i',k)
\end{aligned}$$

The case $j \ge j'$ is treated symmetrically by the Monge property of B.

Now, let A, B be simple unit-Monge matrices over $[0 : n]$. We have $A = P_A^\Sigma$, $B = P_B^\Sigma$, where P_A, P_B are permutation matrices. Clearly, matrices

C and $C^{\square}$ are integer. It is also easy to check that matrix C is simple. Furthermore, matrix C is Monge, and therefore $C^{\square}$ is nonnegative. For any $i \in [0:n]$, we have

$$C(i,0) = \min_j\big(P_A^{\Sigma}(i,j) + P_B^{\Sigma}(j,0)\big) = \min_j\big(P_A^{\Sigma}(i,j) + 0\big) = 0$$
$$C(i,n) = \min_j\big(P_A^{\Sigma}(i,j) + P_B^{\Sigma}(j,n)\big) = \min_j\big(P_A^{\Sigma}(i,j) + n - j\big) = n - i$$

since the minimum is attained respectively at $j = 0$ and $j = n$. Therefore, for all $i \in \langle 0:n\rangle$, we have

$$\begin{aligned}
&\sum\nolimits_k C^{\square}(i,k) = && \text{(definition of } \square\text{)}\\
&\sum\nolimits_k \big(C(i+\tfrac{1}{2},k-\tfrac{1}{2}) - C(i-\tfrac{1}{2},k-\tfrac{1}{2}) -\\
&\qquad C(i+\tfrac{1}{2},k+\tfrac{1}{2}) + C(i-\tfrac{1}{2},k+\tfrac{1}{2})\big) = && \text{(term cancellation)}\\
&C(i+\tfrac{1}{2},0) - C(i-\tfrac{1}{2},0) - C(i+\tfrac{1}{2},n) + C(i-\tfrac{1}{2},n) =\\
&0 - 0 - (n-i-\tfrac{1}{2}) + (n-i+\tfrac{1}{2}) = 1
\end{aligned}$$

Symmetrically, for all $k \in \langle 0:n\rangle$, we have

$$\sum\nolimits_i C^{\square}(i,k) = 1$$

Taken together, the above properties imply that $C^{\square}$ is a permutation matrix, and therefore C is a simple unit-Monge matrix.

The proof is analogous (but more tedious) if A, B are simple unit-Monge matrices over an infinite index range. □

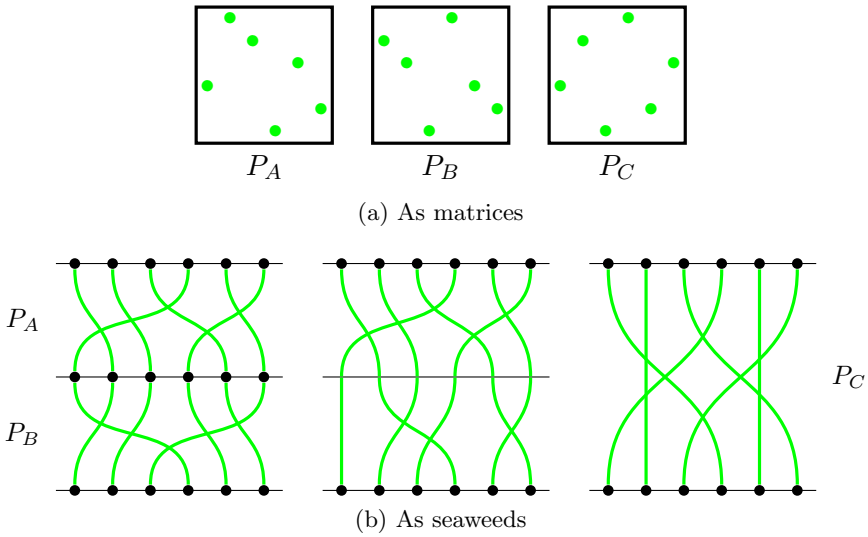
By Lemma 1, the sets of all square Monge matrices and of all simple unit-Monge matrices over a given index range are both submonoids of the distance multiplication monoid of general matrices. For Monge matrices, the identity element is the matrix E above, and for simple unit-Monge matrices, the identity element is the matrix

$$Id^{\Sigma}(i,j) = \begin{cases} j-i & \text{if } i \le j \\ 0 & \text{otherwise} \end{cases}$$

Lemma 1 gives us the basis for performing distance multiplication of simple unit-Monge matrices implicitly, by taking the density permutation matrices as input, and producing a density permutation matrix as output. This is illustrated by Figure 1.1. Subfigure 1.1a shows a triple of 6×6 permutation matrices P_A, P_B, P_C, with nonzeros indicated by green[2] bullets, such that $P_A^{\Sigma} \odot P_B^{\Sigma} = P_C^{\Sigma}$.

Further understanding of the distance multiplication monoid of implicit unit-Monge matrices can be gained by the following construction, which we

[2]For colour illustrations, the reader is referred to the online version of this work. If colour is not available, all references to colour can be ignored.



(a) As matrices

(b) As seaweeds

Figure 1.1: Matrix distance product $P_A^\Sigma = P_B^\Sigma \odot P_C^\Sigma$

call the *seaweed monoid*. Given a permutation matrix P over $I \times J$, represent the indices in sets I and J by nodes on two parallel lines, respecting the order of indices within each set. Represent every nonzero $P(\hat{\imath}, \hat{\jmath}) = 1$ by connecting node $\hat{\imath} \in I$ with node $\hat{\jmath} \in J$ by a continuous strictly monotone line called a *seaweed*. Unless P is the identity matrix Id, some of the seaweeds will have to cross. However, no "unnecessary" crossings are allowed; that is, a given pair of seaweeds may only cross at most once.

Consider the distance product $P_A^\Sigma \odot P_B^\Sigma = P_C^\Sigma$, where P_A, P_B, P_C are permutation matrices over $I \times J$, $J \times K$ and $I \times K$, respectively. We represent the indices by nodes on three parallel lines, and the nonzeros of the input matrices P_A, P_B by two sets of seaweeds connecting the corresponding points. The seaweed representation of the output matrix P_C can be obtained as follows. Let us remove the nodes representing the index set J, at each node $\hat{\jmath}$ joining together the two adjacent seaweeds, which represent nonzeros $P_A(\hat{\imath}, \hat{\jmath}) = 1$ and $P_B(\hat{\jmath}, \hat{k}) = 1$ for some $\hat{\imath}$, $\hat{k}$. We now have a configuration of seaweeds between nodes representing I and nodes representing K. However, some pairs of these seaweeds may cross twice. We now run through all the seaweed crossings, respecting the top-to-bottom order of crossings within each seaweed. For every crossing, we check whether the two seaweeds involved in it already have a previous crossing above the current one. If this is the case, then we undo the current crossing (that is, we cut the crossing out of the configuration, replacing it by two non-crossing seaweed pieces). After all the crossings have been processed, the resulting seaweed configuration represents the output matrix P_C. Subfigure 1.1b shows the sequence of seaweed configurations, which corresponds to the implicit distance product

in Subfigure 1.1a.

The seaweed monoid construction can be formalised as a language obtained from a free monoid over a set of generators, taken modulo a specific set of relations on the generators. The seaweed monoid of size n is generated by n elements id, g_1, g_2, $\ldots$, g_{n-1}. Generator id is the identity element. Intuitively, it corresponds to a configuration where all the seaweeds are parallel; in matrix notation, it corresponds to the simple unit-Monge matrix Id^{Σ}. Each of the remaining generators g_t corresponds to a configuration where all the seaweeds are parallel, except a pair of neighbouring seaweeds in positions $t - \frac{1}{2}$ and $t + \frac{1}{2}$, which do cross. In matrix notation, a generator g_t corresponds to a simple unit-Monge matrix P_t^{Σ}, where an *elementary transposition matrix* P_t is defined by the assignments

$$P_t \leftarrow Id$$
$$P_t\langle t-1 : t+1, t-1 : t+1\rangle \leftarrow \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$$

Concatenation of words in the generators corresponds to the composition of corresponding seaweed configurations. The relations defining the seaweed monoid consist of:

- *idempotence* relations $g_t^2 = g_t$ for all $t \in [1 : n-1]$;
- *commutativity* relations $g_t g_u = g_u g_t$ for all $t, u \in [1 : n-1]$, $u - t \geq 2$;
- *crossover* relations $g_t g_u g_t = g_u g_t g_u$ for all $t, u \in [1 : n-1]$, $u - t = 1$.

Intuitively, the idempotence relations describe the seaweeds' main double crossing property; the commutativity relations tell that a pair of independent seaweed crossings can be taken in an arbitrary order (note that pairs of crossing with $|t - u| \leq 1$ are not independent, so not all pairs of generators commute); and the crossover relations tell that for a given crossing of two seaweeds, a third seaweed passing next to the crossing on the left can be switched over to the right, and vice versa. We are now able to establish a formal connection between distance multiplication of simple unit-Monge matrices and the seaweed monoid.

Theorem 3. *The distance multiplication monoid of $n \times n$ simple unit-Monge matrices is isomorphic to the seaweed monoid of size n.*

Proof. It is straightforward to check that any simple unit-Monge matrix P^{Σ} can be decomposed into a distance product of matrices P_t^{Σ} for various values of t; this can be visualised as drawing a seaweed configuration for P, and decomposing it into individual seaweed crossings. Hence, matrices P_t^{Σ} serve as generators for the distance multiplication monoid of simple unit-Monge matrices. By using the defining relations of the seaweed monoid, it is also straightforward to check that multiplication in both monoids agrees on the

generators. By associativity of multiplication, this implies that multiplication in monoids agrees on all the elements, therefore the two monoids are isomorphic. □

While we will not be using the seaweed monoid directly in our algorithms, seaweeds will prove to be a useful exposition and visualisation tool for the rest of this work.

1.5 Matrix distance multiplication algorithms

In this section, we show that distance multiplication of Monge and simple unit-Monge matrices can be performed much more efficiently than a naive implementation of the definitions. One of the ingredients in our method is the classical algorithm by Aggarwal et al. [1] (see also [40]), which allows efficient searching in totally monotone matrices.

Lemma 2 ([1])**.** *Let A be an $n \times n$ implicit totally monotone matrix, where each element can be queried in time q. Then the problem of finding the minimum element in every row of A (the* row minima problem*) can be solved in time $O(qn)$.*

Our method is based on efficient matrix distance multiplication, exploiting the special properties of the matrices. We begin with matrix-vector multiplication. For generic, explicitly represented matrices, the fastest method for matrix-vector distance multiplication of size n is by direct application of Definition 7 in time $O(n^2)$. For implicit Monge matrices, the running time can be substantially reduced.

Theorem 4. *Let A be an $n \times n$ implicit Monge matrix, where each element can be queried in time q. Let b, c be n-vectors, such that $A \odot b = c$. Given vector b, vector c can be computed in time and memory $O(qn)$.*

Proof. Let $A' = A + e \cdot b^T$, so $A'(i,j) = A(i,j) + b(j)$. It easy to check that matrix A' is a Monge matrix. Clearly, each element of A' can be queried in time $q+O(1)$. The problem of computing the product $A \odot b = c$ is equivalent to the row minima problem in matrix A', which can be solved in time (and therefore also memory) $O(qn)$ by Lemma 2. □

Applying the above theorem to implicit unit-Monge matrices represented by Theorem 1 with $q = O(\log^2 n)$, we obtain an algorithm for matrix-vector distance multiplication, running in time $O(n \log^2 n)$. Using batch queries based on Theorem 2, this running time can be improved by a factor of $O(\log n)$ as follows.

Theorem 5. *Let P be an $n \times n$ permutation matrix. Let b, c be n-vectors, such that $P^\Sigma \odot b = c$. Given the nonzeros of P and the full vector b, vector c can be computed in time $O(n \log n)$ and memory $O(n)$.*

Proof. As in the proof of Theorem 4, we let $A' = A + e \cdot b^T$, so $A'(i,j) = A(i,j) + b(j)$. We then use the standard algorithm of [1] for finding row minima in a monotone (but not necessarily totally monotone) matrix. First, we obtain all elements in row $n/2$ of matrix A' by a row batch query based on Theorem 2, and compute the minimum element in this row. We are now faced with two subproblems of finding the row minima in the submatrix of A' with $i < n/2$ (respectively, $i > n/2$). By using the monotonicity property of matrix A', each of the subproblems can be reduced to an instance of the original problem of size $n/2$. Both the batch query and the problem reduction run in time and memory $O(n)$, therefore the total running time is $O(n+2\cdot n/2+2^2\cdot n/2^2+\ldots) = O(n \log n)$ and the total memory is $O(n)$. □

We now consider matrix-matrix multiplication. For generic matrices, the fastest known method for matrix distance multiplication of size n is a direct application of Definition 8 in time $O(n^3)$. For Monge matrices, the running time can be reduced as follows.

Theorem 6. *Let A, B, C be $n \times n$ matrices, such that A is Monge, and $A \odot B = C$. Given matrices A, B, matrix C can be computed in time and memory $O(n^2)$.*

Proof. The problem of computing the product $A \odot B = C$ is equivalent to n instances of the matrix-vector product $A \odot b = c$, where b (respectively, c) is a column of B (respectively, C). Every one of these instances can be solved in time $O(n)$ by Theorem 4, so the overall running time (and therefore also memory) is $n \cdot O(n) = O(n^2)$. □

For explicitly represented Monge matrices, the running time in Theorem 6 is clearly optimal. However, for implicit simple unit-Monge matrices, the distance multiplication time can be reduced even further. In [93, 96], we gave an algorithm running in time $O(n^{1.5})$. We now show that still further improvement is possible.

Theorem 7. *Let P_A, P_B, P_C be $n \times n$ permutation matrices, such that $P_A^\Sigma \odot P_B^\Sigma = P_C^\Sigma$. Given the nonzeros of P_A, P_B, the nonzeros of P_C can be computed in time $O(n \log n)$.*

Proof. Without loss of generality, let P_A, P_B, P_C be over $\langle 0 : n \rangle^2$. The algorithm is defined by recursion on n.

Recursion base. If $n = 1$, the computation is trivial.

Recursive step. Assume without loss of generality that $n > 1$ is even. Informally, the idea is to split the range of index j in the definition of matrix distance product (Definition 8) into two subranges of size $\frac{n}{2}$. For each of these subranges of j, we use the sparsity of the input permutation matrices P_A, P_B to reduce the range of each of the indices i, k into two disjoint (but

not necessarily contiguous) subsets of size $\frac{n}{2}$. We then call the algorithm recursively on the two resulting half-sized subproblems, and use the two returned half-sized permutation matrices to reconstruct the output permutation matrix P_C, relying on the distribution matrices' Monge properties.

We now describe the recursive step in more detail. Let

$$\begin{aligned} P_{A,lo} &= P_A\langle *, 0 : \tfrac{n}{2}\rangle & P_{A,hi} &= P_A\langle *, \tfrac{n}{2} : n\rangle \\ P_{B,lo} &= P_B\langle 0 : \tfrac{n}{2}, *\rangle & P_{B,hi} &= P_B\langle \tfrac{n}{2} : n, *\rangle \\ P^{\Sigma}_{A,lo} \odot P^{\Sigma}_{B,lo} &= P^{\Sigma}_{C,lo} & P^{\Sigma}_{A,hi} \odot P^{\Sigma}_{B,hi} &= P^{\Sigma}_{C,hi} \end{aligned}$$

Both $P_{C,lo}$, $P_{C,hi}$ are $n \times n$ subpermutation matrices. Matrix $P_{C,lo}$ (respectively, $P_{C,hi}$) can be obtained by deleting the zero rows and columns from $P_{A,lo}$, $P_{B,lo}$ (respectively, $P_{A,hi}$, $P_{B,hi}$), making a recursive call on the resulting half-sized problem, and then reinserting the zero rows and columns in the product matrix returned by the recursive call. Observe that $P_{C,lo} + P_{C,hi}$ is an $n \times n$ permutation matrix. We now have

$$P^{\Sigma}_C(i,k) = \min\big(P^{\Sigma}_{B,hi}(\tfrac{n}{2},k) + P^{\Sigma}_{C,lo}(i,k), P^{\Sigma}_{A,lo}(i,\tfrac{n}{2}) + P^{\Sigma}_{C,hi}(i,k)\big)$$

for all $i, k \in [0:n]$. In order to compute the nonzeros of matrix P_C efficiently, consider the difference of arguments of "min" in the above expression:

$$\begin{aligned} \delta(i,k) &= \big(P^{\Sigma}_{B,hi}(\tfrac{n}{2},k) + P^{\Sigma}_{C,lo}(i,k)\big) - \big(P^{\Sigma}_{A,lo}(i,\tfrac{n}{2}) + P^{\Sigma}_{C,hi}(i,k)\big) \\ &= \big(P^{\Sigma}_{B,hi}(\tfrac{n}{2},k) - P^{\Sigma}_{C,hi}(i,k)\big) - \big(P^{\Sigma}_{A,lo}(i,\tfrac{n}{2}) - P^{\Sigma}_{C,lo}(i,k)\big) \\ &= \sum\nolimits_{\hat{\imath}<i,\hat{k}<k} P_{C,hi}(\hat{\imath},\hat{k}) - \sum\nolimits_{\hat{\imath}>i,\hat{k}>k} P_{C,lo}(\hat{\imath},\hat{k}) \end{aligned}$$

From this, it is clear that function δ is unit-monotone increasing in each of its arguments.

The sign of function δ plays an important role in determining the positions of nonzeros in P_C. More precisely, we have $P_C(\hat{\imath},\hat{k}) = 1$, if and only if one of the following (mutually exclusive) conditions holds:

$$P_{C,lo}(\hat{\imath},\hat{k}) = 1 \text{ and } \delta(\hat{\imath}+\tfrac{1}{2},\hat{k}+\tfrac{1}{2}) \le 0 \tag{1.1}$$

$$P_{C,hi}(\hat{\imath},\hat{k}) = 1 \text{ and } \delta(\hat{\imath}-\tfrac{1}{2},\hat{k}-\tfrac{1}{2}) \ge 0 \tag{1.2}$$

$$\delta(\hat{\imath}-\tfrac{1}{2},\hat{k}-\tfrac{1}{2}) < 0 \text{ and } \delta(\hat{\imath}+\tfrac{1}{2},\hat{k}+\tfrac{1}{2}) > 0 \tag{1.3}$$

In order to perform the above checks efficiently, it is sufficient to find for each $d \in [-n+1 : n-1]$ a value $r(d) \in [1 : 2n-1]$, such that $r(d)+d$ is odd, and

$$\begin{aligned} &\delta(i,k) \le 0 \qquad \text{if } i+k < r(k-i) \\ &\delta(i,k) \ge 0 \qquad \text{if } i+k > r(k-i) \end{aligned}$$

for all $i, k \in [0:n]$ (note that the above list of two cases is exhaustive, since $r(k-i)-(i+k) = r(k-i)+(k-i)-2k$ must be odd, and therefore

$i+k \neq r(k-i)$). Such a value $r(d)$ is guaranteed to exist by the monotonicity of function δ. Furthermore, values $r(d)$ can be chosen so that $|r(\hat{d}+\frac{1}{2}) - r(\hat{d}-\frac{1}{2})| = 1$ for all $\hat{d} \in \langle -n+1 : n-1 \rangle$. Informally, array r defines a monotone rectilinear path, consisting of points $\big(\frac{r(d)-d}{2}, \frac{r(d)+d}{2}\big)$, from the bottom-left to the top-right corner of $\langle 0 : n \rangle^2$.

By definition of array r, for each d we have

$$w^-(d) = \delta\big(\tfrac{r(d)-d-1}{2}, \tfrac{r(d)+d-1}{2}\big) \in [-1, 0]$$
$$w^+(d) = \delta\big(\tfrac{r(d)-d+1}{2}, \tfrac{r(d)+d+1}{2}\big) \in [0, 1]$$

We call the values $w^-(d)$, $w^+(d)$ *witnesses* for $r(d)$.

Array r can be computed efficiently as follows. We loop from $d = -n+1$ to $d = n-1$. For each d, we obtain the value $r(d)$ along with its two witnesses.

Initially, we have $d = -n+1$, $r(-n+1) = n$; the witnesses $w^-(-n+1) = \delta(n-1, 0)$ and $w^+(-n+1) = \delta(n, 1)$ can be easily computed in time $O(1)$.

Now assume that for a current value of d, we have the value $r(d)$, and the witnesses $w^-(d)$, $w^+(d)$. Our next goal is to compute $r(d+1)$, along with its two witnesses. Let

$$w^* = \delta\big(\tfrac{r(d)-d-1}{2}, \tfrac{r(d)+d+1}{2}\big) \in [-1 : 1]$$

Value w^* can be obtained from either $w^-(d)$ or $w^+(d)$ by Theorem 2 in time $O(1)$. We now let

$$r(d+1) = r(d) + \begin{cases} 1 & \text{if } w^* \in [-1 : 0] \\ -1 & \text{if } w^* \in [0 : 1] \end{cases}$$

If $w^* = 0$, then the choice between 1 and -1 is made arbitrarily. Following this choice, we obtain the new witnesses as

$$w^-(d+1) = \begin{cases} \delta\big(\tfrac{r(d)-d-3}{2}, \tfrac{r(d)+d-1}{2}\big) & \text{if } w^* \in [-1 : 0] \\ w^* & \text{if } w^* \in [0 : 1] \end{cases}$$
$$w^+(d+1) = \begin{cases} w^* & \text{if } w^* \in [-1 : 0] \\ \delta\big(\tfrac{r(d)-d+1}{2}, \tfrac{r(d)+d+3}{2}\big) & \text{if } w^* \in [0 : 1] \end{cases}$$

In each case, the value for the new witness can be obtained from respectively $w^-(d)$, $w^+(d)$ by Theorem 2 in time $O(1)$. If $w^* = 0$, then the choices are made consistently with the arbitrary choice made in the definition of $r(d+1)$.

The described loop runs until $d = n-1$. At this point, we necessarily have $r(n-1) = n$, $w^-(n-1) = \delta(0, n-1)$ and $w^+(n-1) = \delta(1, n)$. The whole loop runs in time $O(n)$.

Given arrays r, w^-, w^+, conditions (1.1)–(1.3) can now be expressed as follows:

$$P_{C,lo}(\hat{\imath}, \hat{k}) = 1 \text{ and } \hat{\imath} + \hat{k} < r(\hat{k} - \hat{\imath}) \tag{1.4}$$

$$P_{C,hi}(\hat{\imath},\hat{k}) = 1 \text{ and } \hat{\imath}+\hat{k} > r(\hat{k}-\hat{\imath}) \tag{1.5}$$

$$\hat{\imath}+\hat{k} = r(\hat{k}-\hat{\imath}) \text{ and } w^-(\hat{k}-\hat{\imath}) = -1 \text{ and } w^+(\hat{k}-\hat{\imath}) = 1 \tag{1.6}$$

The nonzeros of P_C satisfying one of the conditions (1.4), (1.5) can be found in time $O(n)$ by a linear sweep of nonzeros of matrices $P_{C,lo}$ and $P_{C,hi}$. The nonzeros of P_C satisfying condition (1.6) can be found in time $O(n)$ by a linear sweep of the values $r(d)$ for all $d \in [-n+1 : n-1]$. For each d, we let $\hat{\imath} = \frac{r(d)+d}{2}$, $\hat{k} = \frac{r(d)-d}{2}$, and substitute these values into (1.6). We have now obtained all the nonzeros of matrix P_C.

End of recursive step.

Time analysis. The recursion tree is a balanced binary tree of height $\log n$. In the root node, the computation runs in time $O(n)$. In each subsequent level, the number of nodes doubles, and the running time per node decreases by a factor of 2. Therefore, the overall running time is $O(n \log n)$. □

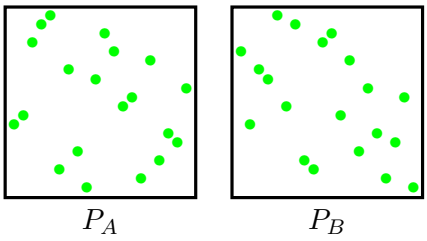
The proof of Theorem 7 is illustrated by Figure 1.2. Subfigure 1.2a shows a pair of input 20×20 permutation matrices P_A, P_B, with nonzeros indicated by green bullets. Subfigure 1.2b shows the partitioning of the implicit 20×20 matrix distance multiplication problem into two 10×10 subproblems. The nonzeros in the two subproblems are shown respectively by red stars and blue circles. Subfigure 1.2c shows a recursive step. The boundaries separating sets $\delta^{-1}([-10 : -1])$, $\delta^{-1}(\{0\})$, $\delta^{-1}([1 : 10])$ are indicated by the red and the blue line. Function r corresponds to an arbitrary monotone rectilinear path within $\delta^{-1}(\{0\})$, inclusive of the boundaries. In particular, either of the boundaries itself can be taken to define r. The nonzeros in the output matrix P_C satisfying (1.4), (1.5), (1.6) are indicated respectively by red stars, blue circles and green bullets; note that overall, there are 20 such nonzeros, and that they define a permutation matrix.

Theorem 7 gives an efficient algorithm for distance multiplication of finite simple unit-Monge matrices. We now extend this algorithm to infinite matrices. We consider two special cases:

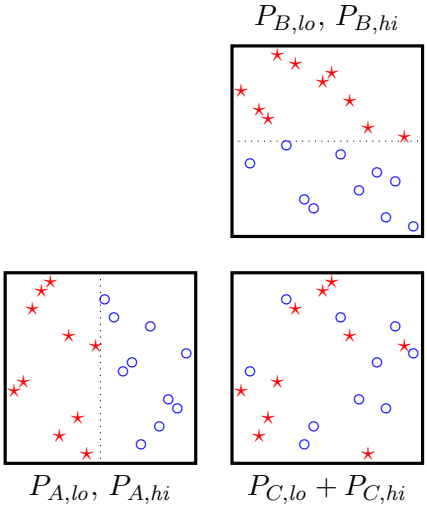
- both P_A, P_B have a semi-infinite core (Lemma 3);
- one of P_A, P_B has a finite core (Lemma 4).

Lemma 3. *Let $i_0, i_1 \in [-\infty : +\infty]$, $n = i_1 - i_0 \geq 0$. Let P_A, P_B, P_C be permutation matrices over $\langle -\infty : +\infty \rangle^2$, such that*

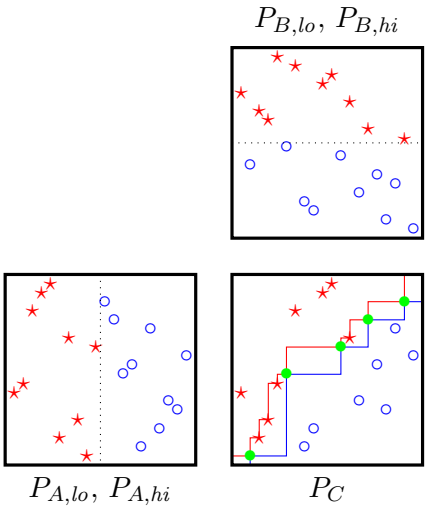
- *P_A has core $\langle i_0 : +\infty \rangle^2$ and offset 0*
- *P_B has core $\langle -\infty : i_1 \rangle^2$ and offset 0*
- *$P_A^\Sigma \odot P_B^\Sigma = P_C^\Sigma$*



(a) Input matrices P_A, P_B

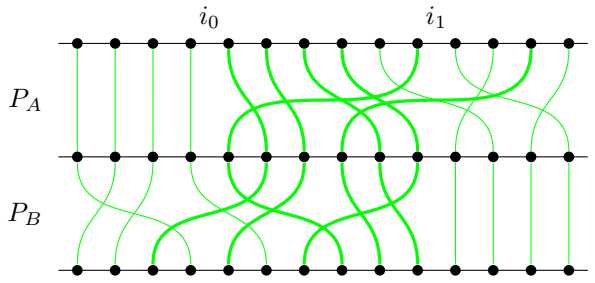


(b) Subproblems $P^{\Sigma}_{A,lo} \odot P^{\Sigma}_{B,lo} = P^{\Sigma}_{C,lo}$ and $P^{\Sigma}_{A,hi} \odot P^{\Sigma}_{B,hi} = P^{\Sigma}_{C,hi}$

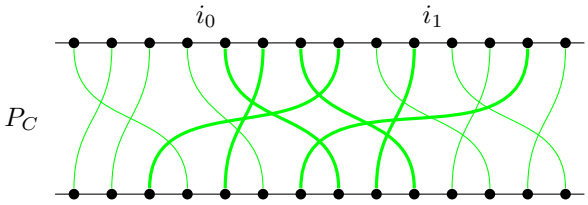


(c) Conversion of $P_{C,lo}$ and $P_{C,hi}$ into P_C

Figure 1.2: Proof of Theorem 7: $P^{\Sigma}_A = P^{\Sigma}_B \odot P^{\Sigma}_C$



(a) Input matrices P_A, P_B



(b) Output matrix P_C

Figure 1.3: Statement of Lemma 3: $P_A^\Sigma \odot P_B^\Sigma = P_C^\Sigma$

Given implicit representations of P_A, P_B with query time $O(1)$, an implicit representation of P_C with query time $O(1)$ can be computed in time $O(n \log n)$.

Proof. Without loss of generality, let $i_0 = 0$, $i_1 = n$. Let

$$\tilde{P}_A \leftarrow P_A\langle \cdot, 0 : n\rangle \qquad \tilde{P}_B \leftarrow P_B\langle 0 : n, \cdot\rangle \qquad \tilde{P}_A^\Sigma \odot \tilde{P}_B^\Sigma = \tilde{P}_C^\Sigma$$
$$P_C \leftarrow P_A\langle \cdot, n : +\infty\rangle \bowtie P_B\langle -\infty : 0, \cdot\rangle \bowtie \tilde{P}_C$$

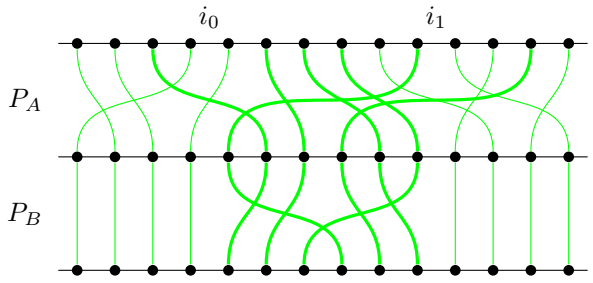
All index operations are performed in time $O(n)$. Implicit matrix distance multiplication is performed in time $O(n \log n)$ by Theorem 7. The overall running time is $O(n \log n)$. □

The statement of Lemma 3 is illustrated by Figure 1.3. Three horizontal lines represent respectively the index ranges of i, j, k. The nonzeros in P_A, P_B, P_C are shown by seaweeds; the thick seaweeds correspond to the nonzeros involved in the matrix distance multiplication, and the thin seaweeds to the remaining nonzeros.

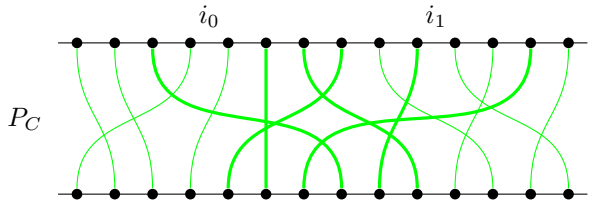
Lemma 4. *Let $i_0, i_1 \in [-\infty : +\infty]$, $n = i_1 - i_0 \geq 0$. Let P_A, P_B, P_C be permutation matrices over $\langle -\infty : +\infty\rangle^2$, such that*

- *P_B has core $\langle i_0 : i_1\rangle^2$ and offset 0*
- *$P_A^\Sigma \odot P_B^\Sigma = P_C^\Sigma$*

Given implicit representations of P_A, P_B with query time $O(1)$, an implicit representation of P_C with query time $O(1)$ can be computed in time $O(n \log n)$.



(a) Input matrices P_A, P_B



(b) Output matrix P_C

Figure 1.4: Statement of Lemma 4: $P_A^\Sigma \odot P_B^\Sigma = P_C^\Sigma$

Proof. Without loss of generality, let $i_0 = 0$, $i_1 = n$. Let

$$\tilde{P}_A \leftarrow P_A\langle \cdot, 0 : n\rangle \qquad \tilde{P}_B \leftarrow P_B\langle 0 : n, 0 : n\rangle \qquad \tilde{P}_A^\Sigma \odot \tilde{P}_B^\Sigma = \tilde{P}_C^\Sigma$$
$$P_C \leftarrow P_A\langle \cdot, -\infty : 0\rangle \bowtie P_A\langle \cdot, n : +\infty\rangle \bowtie \tilde{P}_C$$

All index operations are performed in time $O(n)$. Implicit matrix distance multiplication is performed in time $O(n \log n)$ by Theorem 7. The overall running time is $O(n \log n)$. □

The statement of Lemma 4 is illustrated by Figure 1.4, using the same conventions as Figure 1.3.

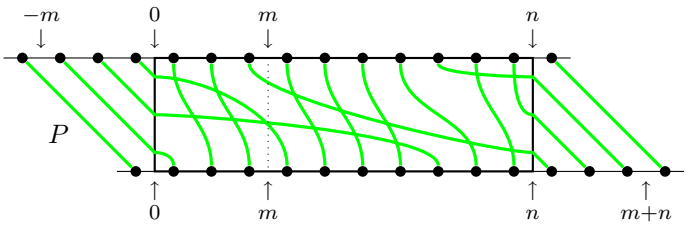
Lemma 5. *Let P be a superdiagonal permutation matrix over $\langle -\infty : +\infty\rangle^2$, with core size $m + n$ and offset m. There exist superdiagonal permutation matrices $P_0, \ldots, P_{\lfloor n/m \rfloor}$, each with core size $2m$ and offset m, such that $P_0^\Sigma \odot \cdots \odot P_{\lceil n/m \rceil}^\Sigma = P^\Sigma$. Given the core nonzeros of P, the core nonzeros of all of $P_0, \ldots, P_{\lceil n/m \rceil}$ can be computed in time $O(n)$.*

Proof. Without loss of generality, let P have core $\langle -m : n\rangle \times \langle 0 : m + n\rangle$. We define the decomposition recursively as follows.

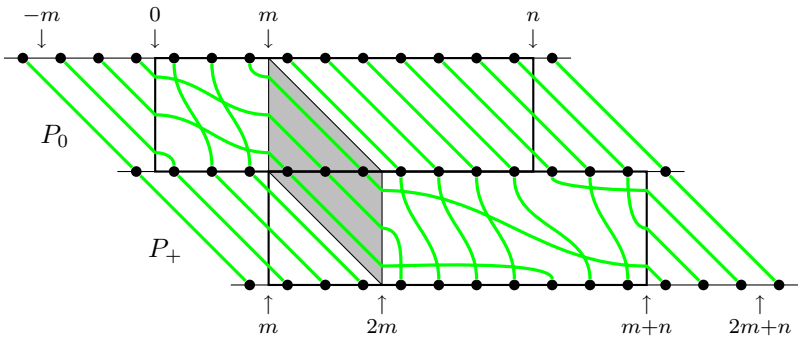
Recursion base. If $n \le m$, the decomposition is trivial: $P = P_0$.

Recursive step. We partition matrix P as

$$P = P\langle -\infty : m, -\infty : m\rangle \bowtie P\langle -\infty : m, m : +\infty\rangle \bowtie$$



(a) Input matrix P



(b) Decomposition matrices P_0^Σ, P_+^Σ

Figure 1.5: Proof of Lemma 5: $P^\Sigma = P_0^\Sigma \odot P_+^\Sigma$

$$P\langle m : +\infty, m : +\infty\rangle$$

Since matrix P is superdiagonal, the submatix $P\langle m : +\infty, -\infty : m\rangle$ does not contain any nonzeros, and therefore it is not included in the above decomposition.

We construct permutation matrices P_0, P_+ as shown in Figure 1.5. Intuitively, each core nonzero $P(\hat{\imath}, \hat{\jmath})$ within the submatrix $P\langle -\infty : m, -\infty : m\rangle$ is preserved as $P_0(\hat{\imath}, \hat{\jmath})$; each core nonzero $P(\hat{\imath}, \hat{\jmath})$ within the submatrix $P\langle m : +\infty, m : +\infty\rangle$ is preserved as $P_+(\hat{\imath} + m, \hat{\jmath} + m)$. The remaining core nonzeros are within the submatrix $P\langle -\infty : m, m : +\infty\rangle$; each of these nonzeros $P(\hat{\imath}, \hat{\jmath})$ is preserved as a pair of nonzeros $P_0(\hat{\imath}, \hat{t})$, $P_+(\hat{t}, \hat{\jmath} + m)$; the intermediate index $\hat{t} \in \langle m : 2m\rangle$ is chosen so that the resulting nonzeros do not dominate one another in P_0, and the dominance relations of P are preserved in P_+.

By construction, we have $P^\Sigma = P_0^\Sigma \odot P_+^\Sigma$. The decomposition is then applied recursively to matrix P_+.

End of recursive step.

Time analysis. Each recursive step can be implemented in time and memory $O(m)$, therefore the full decomposition can be obtained in time $O(m{\cdot}n/m) = O(n)$. □

In Figure 1.5, the $m \times n$ rectangle corresponding to the core of P is split

into an $m \times m$ square corresponding to the core of P_0, and an $m \times (n-m)$ rectangle corresponding to the core of P_+. The resulting rectangles are arranged vertically with a shift by m. The seaweeds that do not cross the partition between the rectangles are preserved by the construction. The seaweeds that do cross the partition line are also preserved, by passing them through a parallelogram-shaped "buffer zone". Note the latter class of seaweeds are all uncrossed in P_0, and keep their original crossings from P in P_+.

Chapter 2

Semi-local string comparison

2.1 Semi-local LCS

We will consider strings of characters taken from an alphabet. No a priori assumptions are made on the size of the alphabet and on the model of computation; we will make specific assumptions in different contexts (e.g. a fixed finite alphabet with only equality comparisons, or an alphabet of integers up to a given n with standard arithmetic operations, etc.) Two alphabet characters α, β *match*, if $\alpha = \beta$, and *mismatch* otherwise. We extend the alphabet by a special *wildcard character* '?', which by definition matches all the other characters in the alphabet. We denote by $\backsim$ (respectively, $\sim$) a string of wildcard characters extending infinitely to the left (respectively, right).

It will be convenient to index strings by odd half-integer, rather than integer indices, e.g. string $a = \alpha_{\frac{1}{2}}\alpha_{\frac{3}{2}}\dots\alpha_{m-\frac{1}{2}}$. We will index strings similarly to matrices, writing e.g. $a(\hat{i}) = \alpha_{\hat{i}}$, $a\langle i : j\rangle = \alpha_{i+\frac{1}{2}}\dots\alpha_{j-\frac{1}{2}}$. String concatenation will be denoted by juxtaposition.

Given a string, we distinguish between its contiguous *substrings*, and not necessarily contiguous *subsequences*. Special cases of a substring are *a prefix* and *a suffix* of a string. Given a string a of length m, we use the *take/drop notation* of [98] for prefixes and suffixes of a:

$$\begin{aligned} a \upharpoonright k &= a\langle 0 : k\rangle & a \downharpoonright k &= a\langle k : m\rangle \\ a \restriction k &= a\langle m-k : m\rangle & a \lfloor k &= a\langle 0 : m-k\rangle \end{aligned}$$

Unless indicated otherwise, our algorithms will take as input a string a of length m, and a string b of length n.

Definition 9. *Given strings a, b, the* longest common subsequence (LCS) problem *asks for the length of the longest string that is a subsequence of both a and b. We will call this length the* LCS score *of strings a, b.*

A special case of the LCS problem is the *subsequence recognition problem*, which, assuming $m \geq n$, asks whether a contains b itself as a subsequence. This problem has been considered e.g. by Aho et al. [2] as the "subsequence matching problem"; they gave an algorithm running in time $O(m)$. Algorithms for the general LCS problem are more computationally intensive; we will consider them in Sections 3.1, 4.1.

Definition 10. *Given strings a, b, the* semi-local LCS problem *asks for the LCS scores as follows:*

- *a against every substring of b (the* string-substring LCS scores*);*
- *every prefix of a against every suffix of b (the* prefix-suffix LCS scores*);*
- *symmetrically, the* substring-string LCS scores *and the* suffix-prefix LCS scores*, defined as above but with the roles of a and b exchanged.*

A traditional distinction, especially in computational biology, is between global (full string against full string) and local (all substrings against all substrings) comparison. Our problem lies in between, hence the term "semi-local". It turns out that this is a very natural and useful generalisation of the LCS problem. Many string comparison algorithms output either a single optimal comparison score across all local comparisons, or a number of local comparison scores that are "sufficiently close" to the globally optimal. In contrast with this approach, Definition 10 requires to output all the locally optimal comparison scores.

The LCS problem is clearly a special case of the semi-local LCS problem. Another special case is the *local subsequence recognition problem*, which asks for the substrings in a containing b as a subsequence. We will consider algorithms for the local subsequence recognition problem in Section 4.4, and for the general semi-local LCS problem in Sections 3.1, 4.1.

In certain contexts, e.g. when m is much higher than n, we may not be able to solve all four components of the semi-local LCS problem efficiently. In such cases, we may wish to settle for its following asymmetric restriction.

Definition 11. *Given strings a, b, the* three-way semi-local LCS problem *asks for the string-substring, prefix-suffix and suffix-prefix LCS scores as in Definition 10, but excludes the substring-string LCS scores.*

When considering the three-way version of the semi-local LCS problem, we will occasionally use the term *full semi-local LCS* for the standard four-way version.

2.2 Alignment dags and highest-score matrices

It is well-known that an instance of the LCS problem can be represented by a dag (directed acyclic graph) on a rectangular grid of nodes, where character matches correspond to edges scoring 1, and mismatches to edges scoring 0.

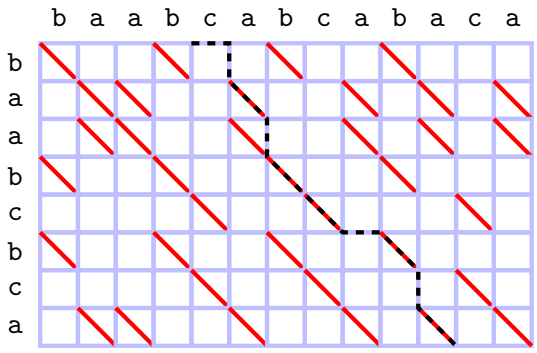


Figure 2.1: Alignment dag $G_{a,b}$ and a highest-scoring path

Definition 12. *An* alignment dag *is a weighted dag, defined on the set of nodes* $v_{l,i}$, $l \in [l_0 : l_1]$, $i \in [i_0, i_1]$. *The edge and path weights are called* scores. *For all* $l \in [l_0 : l_1]$, $\hat{l} \in \langle l_0 : l_1 \rangle$, $i \in [i_0, i_1]$, $\hat{\imath} \in \langle i_0 : i_1 \rangle$, *the alignment dag contains:*

- *the horizontal edge* $v_{l,\hat{\imath}-\frac{1}{2}} \rightarrow v_{l,\hat{\imath}+\frac{1}{2}}$ *and the vertical edge* $v_{\hat{l}-\frac{1}{2},i} \rightarrow v_{\hat{l}+\frac{1}{2},i}$, *both with score* 0*;*
- *the diagonal edge* $v_{\hat{l}-\frac{1}{2},\hat{\imath}-\frac{1}{2}} \rightarrow v_{\hat{l}+\frac{1}{2},\hat{\imath}+\frac{1}{2}}$ *with score either* 0 *or* 1.

An alignment dag can be viewed as an $(l_1 - l_0) \times (i_1 - i_0)$ grid of *cells*. An instance of the semi-local LCS problem on strings a, b corresponds to an $m \times n$ alignment dag $G_{a,b}$; a cell indexed by $\hat{l} \in \langle 0 : m \rangle$, $\hat{\imath} \in \langle 0 : n \rangle$ is called a *match cell*, if $a(\hat{l}) = b(\hat{\imath})$, and a *mismatch cell* otherwise. The diagonal edges in match cells have score 1, and in mismatch cells score 0. Clearly, the diagonal edges with score 0 do not affect maximum node-to-node scores, and can therefore be ignored. Figure 2.1 shows the alignment dag corresponding to strings $a =$ "`baabcbca`", $b =$ "`baabcabcabaca`" (an example borrowed from [7]).

Particular examples of an alignment dag are the *full-mismatch dag* and the *full-match dag*, which consist entirely of mismatch or match cells, respectively. The dag $G_{a,b}$ is the full-mismatch dag when the strings a, b have no characters in common, and is the full-match dag where both strings consist of a single repeated character, or when one of the strings consists entirely of wildcard characters.

Given an instance of the LCS problem on strings a, b, common string-substring, suffix-prefix, prefix-suffix, and substring-string subsequences correspond, respectively, to paths of the following form in the alignment dag $G_{a,b}$:

$$v_{0,i} \rightsquigarrow v_{m,i'} \quad v_{l,0} \rightsquigarrow v_{m,i'} \quad v_{0,i} \rightsquigarrow v_{l',n} \quad v_{l,0} \rightsquigarrow v_{l',n} \tag{2.1}$$

where $l, l' \in [0:m]$, $i, i' \in [0:n]$. The length of each subsequence is equal to the total score of its corresponding path.

The solution to the semi-local LCS problem is equivalent to finding the highest path scores for each of the four path types (2.1). This is also equivalent to finding the corresponding shortest distances in an undirected graph, obtained from the alignment dag by assigning length 1 to vertical and horizontal edges, assigning lengths 0 and 2 to diagonal edges in match and mismatch cells respectively, and ignoring edge directions. Thus, the problem is equivalent to the problem of finding distances between boundary nodes and all nodes on a special case of a weighted undirected planar graph. This problem has been previously studied by Schmidt [88] on real-weighted grid dags, and by Klein [59] and Cabello and Chambers [21] on general real-weighted undirected planar graphs. In contrast with these approaches, we exploit both the special structure of the alignment dag, and the discreteness of the weights.

The analysis of the four path types (2.1) can be reduced to a single type, by extending one of the input strings with wildcards to infinity in both directions. Accordingly, we need to consider an infinite alignment dag with $i_0 = -\infty$, $i_1 = +\infty$.

Definition 13. *Consider an $m \times \infty$ alignment dag $G_{a,\smile b\sim}$. The corresponding* highest-score matrix[1] *is a matrix over $[-\infty : +\infty]^2$, defined by*

$$H_{a,\smile b\sim}(i,j) = \max score(v_{0,i} \rightsquigarrow v_{m,j})$$

where $i, j \in [-\infty : +\infty]$, and the maximum is taken across all paths between the given endpoints. If $i = j$, we have $H_{a,\smile b\sim}(i,j) = 0$. By convention, if $j < i$, then we let $H_{a,\smile b\sim}(i,j) = j - i < 0$.

In Figure 2.1, the highlighted path has score 5, and corresponds to the value $H_{a,\smile b\sim}(4,11) = 5$, which is equal to the LCS score of string a against substring $b\langle 4:11\rangle =$ "`cabcaba`". Figure 2.2 shows a finite fragment of the highest-score matrix $H_{a,\smile b\sim}$, giving just the string-substring LCS scores; the value $H_{a,\smile b\sim}(4,11) = 5$ is circled.

The solution for each of the four components (2.1) of the LCS problem can now be obtained from the highest-score matrix $H_{a,\smile b\sim}$ as follows:

$$\begin{aligned}
\max score(v_{0,j} \rightsquigarrow v_{m,j'}) &= H_{a,\smile b\sim}(j, j') \\
\max score(v_{i,0} \rightsquigarrow v_{m,j'}) &= H_{a,\smile b\sim}(-i, j') - i \\
\max score(v_{0,j} \rightsquigarrow v_{i',n}) &= H_{a,\smile b\sim}(j, m+n-i') - m + i' \\
\max score(v_{i,0} \rightsquigarrow v_{i',n}) &= H_{a,\smile b\sim}(-i, m+n-i') - m - i + i'
\end{aligned}$$

[1] These matrices are called "DIST matrices" e.g. in [88, 27], and "score matrices" in [94].We have chosen a different terminology to reflect better the score-maximising nature of the matrix elements, and to avoid confusion with pairwise substitution score matrices used in comparative genomics (see e.g. [54]).

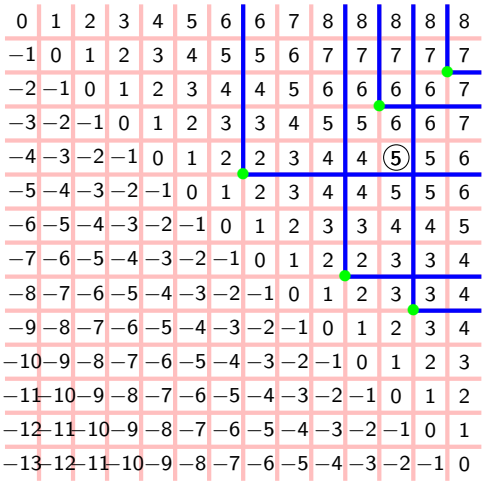


Figure 2.2: A fragment of matrices $H_{a,\smile b\sim}$ and $P_{a,\smile b\sim}$

where $i, i' \in [0 : m]$, $j, j' \in [0 : n]$, and the maximum is taken across all paths between the given endpoints.

Special properties of highest-score matrices have been extensively used in algorithm design. These properties are captured by the following theorem.

Theorem 8. *Consider an $m \times \infty$ alignment dag $G_{a,\smile b\sim}$ Its corresponding highest-score matrix $H_{a,\smile b\sim}$ is unit-anti-Monge. In particular, we have*

$$H_{a,\smile b\sim}(i,j) = j - i - P^{\Sigma}_{a,\smile b\sim}(i,j)$$

where $P_{a,\smile b\sim}$ is a superdiagonal permutation matrix over $\langle -\infty : +\infty\rangle^2$.

Proof. Let $i, j \in \langle -\infty : +\infty\rangle$. Any crossing pair of paths $v_{0,i+\frac{1}{2}} \rightsquigarrow v_{m,j-\frac{1}{2}}$ and $v_{0,i-\frac{1}{2}} \rightsquigarrow v_{m,j+\frac{1}{2}}$ can be rearranged into a non-crossing pair of paths $v_{0,i-\frac{1}{2}} \rightsquigarrow v_{m,j-\frac{1}{2}}$ and $v_{0,i+\frac{1}{2}} \rightsquigarrow v_{m,j+\frac{1}{2}}$ of the same total score. Therefore, we have $H^{\square}_{a,\smile b\sim}(i,j) \le 0$, hence matrix $H_{a,\smile b\sim}$ is anti-Monge, and matrix $P^{\Sigma}_{a,\smile b\sim}$ is Monge. Furthermore, we have

$$\begin{aligned}&P^{\Sigma}_{a,\smile b\sim}(i-\tfrac{1}{2}, m+n) - P^{\Sigma}_{a,\smile b\sim}(i+\tfrac{1}{2}, m+n) = \\ &1 - H_{a,\smile b\sim}(i-\tfrac{1}{2}, m+n) + H_{a,\smile b\sim}(i+\tfrac{1}{2}, m+n) = 1 - m + m = 1\end{aligned}$$

and

$$\begin{aligned}&P^{\Sigma}_{a,\smile b\sim}(-m, j+\tfrac{1}{2}) - P^{\Sigma}_{a,\smile b\sim}(-m, j-\tfrac{1}{2}) = \\ &\qquad 1 - H_{a,\smile b\sim}(-m, j+\tfrac{1}{2}) + H_{a,\smile b\sim}(-m, j-\tfrac{1}{2}) = 1 - m + m = 1\end{aligned}$$

Together, the above properties imply that $P^{\Sigma}_{a,\smile b\sim}$ is a simple unit-Monge matrix, so $P_{a,\smile b\sim}$ is a permutation matrix. □

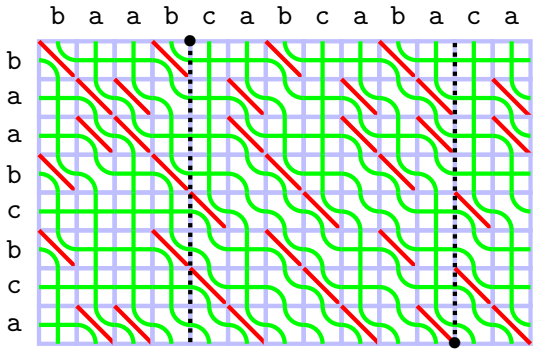


Figure 2.3: Alignment dag $G_{a,b}$ and nonzeros of $P_{a,\smile b\sim}$ as seaweeds

The key idea of our approach is to regard the highest-score matrix $H_{a,\smile b\sim}$ as implicitly represented by the permutation matrix $P_{a,\smile b\sim}$.

In Figure 2.2, the definition of implicit highest score matrix is illustrated by an odd half-integer grid of edges. Red (respectively, blue) edge colouring indicates that the two elements of matrix $H_{a,\smile b\sim}$ separated by the edge differ by 1 (respectively, that they are equal). The nonzeros of the permutation matrix P_A within the given finite section of the matrix are shown by green bullets.

Figure 2.3 shows an alternative graphical representation of the implicit highest-score matrix, given directly on the alignment dag. Nonzeros of $P_{a,\smile b\sim}$ are represented by seaweeds, laid out as paths in the dual graph. In particular, every nonzero $P_{a,\smile b\sim}(i,j) = 1$, where $i, j \in \langle 0 : n\rangle$, is represented by a seaweed originating between the nodes $v_{0,i-\frac{1}{2}}$ and $v_{0,i+\frac{1}{2}}$, and terminating between the nodes $v_{m,j-\frac{1}{2}}$ and $v_{m,j+\frac{1}{2}}$. The remaining seaweeds, originating or terminating at the sides of the dag, correspond to nonzeros $P_{a,\smile b\sim}(i,j) = 1$, where either $i \in \langle -m : 0\rangle$ or $j \in \langle n : n+m\rangle$ (or both). In particular, every nonzero $P_{a,\smile b\sim}(i,j) = 1$, where $i \in \langle -m : 0\rangle$ (respectively, $j \in \langle n : m+n\rangle$) is represented by a seaweed originating between the nodes $v_{-i-\frac{1}{2},0}$ and $v_{-i+\frac{1}{2},0}$ (respectively, terminating between the nodes $v_{m+n-j-\frac{1}{2},n}$ and $v_{m+n-j+\frac{1}{2},n}$). For the purposes of this section, the specific layout of the seaweeds between their endpoints is not important. However, this layout will become meaningful in the context of the algorithms described in the next chapter.

In Figure 2.2, the nonzeros of $P_{a,\smile b\sim}$ that are dominated by the entry $P^{\Sigma}_{a,\smile b\sim}(4,11) = 2$ correspond to the dots lying below and to the left of the circled entry. In Figure 2.3, these dominated nonzeros correspond to seaweeds fitting completely between the two vertical lines $i = 4$ and $j = 11$. Note that in both cases, there are exactly two dominated nonzeros, and that $H_{a,\smile b\sim}(4,11) = 11 - 4 - 2 = 5$.

Recall that outside the range of string b, the alignment graph contains

only match cells. This property carries over to the corresponding permutation matrix: it has core $\langle -m, n\rangle \times \langle 0, m+n\rangle$ and offset m, and contains $m+n$ core nonzeros. In Figure 2.3, these core nonzeros are represented by the full set of $m+n = 8+13 = 21$ seaweeds.

With minimal modification, the described method can also be applied to the three-way, rather than full, semi-local LCS problem.

Definition 14. *A* three-way slice *of matrix $H_{a,\smile b\sim}$ is a pair of submatrices*

$$H^{\llcorner}_{a,\smile b\sim} = \big(H_{a,\smile b\sim}[0 : +\infty, *], H_{a,\smile b\sim}[*, -\infty : n]\big)$$

Similarly, a three-way slice *of matrix $P_{a,\smile b\sim}$ is a pair of submatrices*

$$P^{\llcorner}_{a,\smile b\sim} = \big(P_{a,\smile b\sim}\langle 0 : +\infty, *\rangle, P_{a,\smile b\sim}\langle *, -\infty : n\rangle\big)$$

The three-way slice $H^{\llcorner}_{a,\smile b\sim}$ is sufficient for obtaining the first three components in (2.1), corresponding to the three-way semi-local LCS problem. In its turn, $H^{\llcorner}_{a,\smile b\sim}$ can be represented implicitly by the three-way slice $P^{\llcorner}_{a,\smile b\sim}$. The number of core nonzeros within $P^{\llcorner}_{a,\smile b\sim}$ is at least n and at most $\min(m+n, 2n)$; note that for $m \geq n$, this number is independent of m.

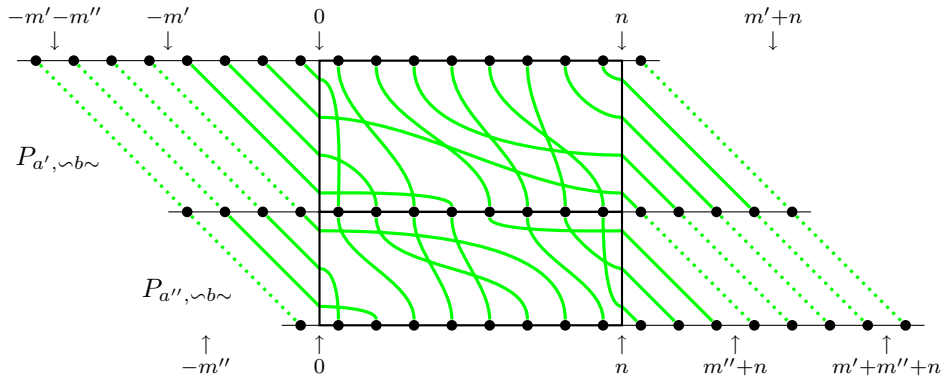
Both the full implicit highest-score matrices and their three-way slices can be processed into an efficient data structure of Theorem 1 for answering individual element queries.

2.3 Highest-score matrix composition

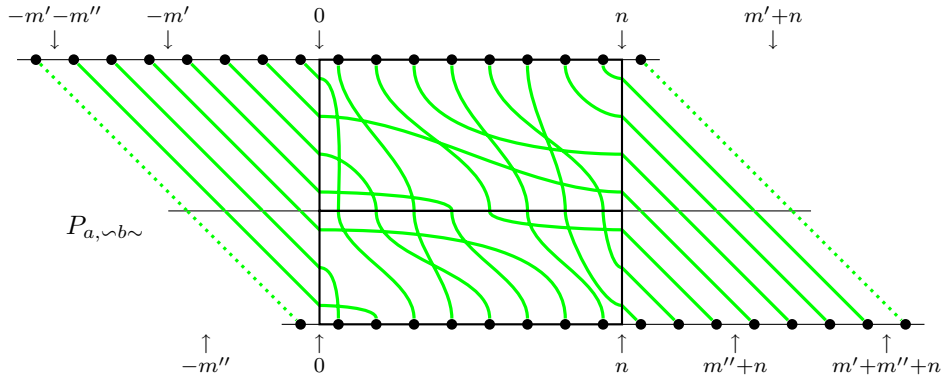
We now describe how the techniques of previous sections can be applied within the divide-and-conquer framework. Consider the semi-local LCS problem for string $a = a'a''$ against b, where strings a', a'', b are of length m', m'', n respectively. Without loss of generality, we assume $m' \geq m''$. The alignment dag $G_{a,\smile b\sim}$ consists of alignment subdags $G_{a',\smile b\sim}$, $G_{a'',\smile b\sim}$, sharing a horizontal row of n nodes and $n-1$ edges, which are simultaneously at the bottom of $G_{a',\smile b\sim}$ and at the top of $G_{a'',\smile b\sim}$. We will say that dag $G_{a,\smile b\sim}$ is the *composite* of dags $G_{a',\smile b\sim}$ and $G_{a'',\smile b\sim}$.

Our goal is, given the respective highest-score matrices $H_{a',\smile b\sim}$, $H_{a'',\smile b\sim}$, to compute matrix $H_{a,\smile b\sim}$ efficiently. We call this procedure *highest-score matrix composition*. Using the method of Section 2.2, matrices $H_{a',\smile b\sim}$, $H_{a'',\smile b\sim}$, $H_{a,\smile b\sim}$ can be represented implicitly by permutation matrices $P_{a',\smile b\sim}$, $P_{a'',\smile b\sim}$, $P_{a,\smile b\sim}$ over $\langle -\infty : +\infty\rangle$, with respective core sizes $m'+n$, $m''+n$, $m'+m''+n$ and offsets m', m'', $m'+m''$, such that $P^{\Sigma}_{a',\smile b\sim} \odot P^{\Sigma}_{a'',\smile b\sim} = P^{\Sigma}_{a,\smile b\sim}$.

Figure 2.4 shows an example of highest-score matrix composition represented by implicit matrices. The nonzeros in the matrices are shown by seaweeds; since in this case there is no explicit underlying alignment dag, the



(a) Input matrices $P_{a',\smile b\sim}$, $P_{a'',\smile b\sim}$



(b) Output matrix $P_{a,\smile b\sim}$

Figure 2.4: Highest-score matrix composition: $P^{\Sigma}_{a',\smile b\sim} \odot P^{\Sigma}_{a'',\smile b\sim} = P^{\Sigma}_{a,\smile b\sim}$

layout of every seaweed should be regarded as completely arbitrary (except for disallowing double crossings).

Observe that if only a single row of the highest-score composition is required, this can be easily computed by matrix-vector distance multiplication. An equivalent procedure is given (using different terminology and notation) in [66, 27, 57], based on techniques from [55, 14].

Theorem 9. *Given the core elements of row i in matrix $H_{a',\smile b\sim}$, and the core nonzeros of matrix $P_{a'',\smile b\sim}$, it is possible to compute the core elements of row i in matrix $H_{a,\smile b\sim}$ in time $O(n \log n)$ and memory $O(n)$.*

Proof. By Theorem 5. □

We now give an efficient algorithm for full highest-score matrix composition.

Theorem 10. *Given the core nonzeros of matrices $P_{a',\smile b\sim}$, $P_{a'',\smile b\sim}$, it is possible to compute the core nonzeros of matrix $P_{a,\smile b\sim}$ in time $O\big(m' + n \log \min(m'', n)\big)$.*

Proof. By Lemma 5, we obtain a decomposition

$$P^{\Sigma}_{a'',\smile b\sim} = P^{\Sigma}_{0} \odot \cdots \odot P^{\Sigma}_{\lfloor n/m'' \rfloor}$$

where each of P_0, ..., $P_{\lfloor n/m \rfloor}$ has core size $2m''$ and offset m''. Then, we compute

$$P^{\Sigma}_{a,\smile b\sim} = P^{\Sigma}_{a',\smile b\sim} \odot P^{\Sigma}_{a'',\smile b\sim} = P^{\Sigma}_{a',\smile b\sim} \odot (P^{\Sigma}_{0} \odot \cdots \odot P^{\Sigma}_{\lfloor n/m'' \rfloor}) =$$
$$\big((P^{\Sigma}_{a',\smile b\sim} \odot P^{\Sigma}_{0}) \odot \cdots\big) \odot P^{\Sigma}_{\lfloor n/m'' \rfloor}$$

By Lemma 4, each of the above distance multiplications can be performed in time $O(m'' \log m'')$, resulting in an implicit representation for matrix $P_{a,\smile b\sim}$ with query time $O(1)$. All the nonzeros of $P_{a,\smile b\sim}$ can be queried from this representation in time $O(m' + n)$. The overall running time is $O\big((n/m'') \cdot m'' \log m'' + (m' + n)\big) = O(m' + n \log m'')$. □

Similarly to the composition of full highest-score matrices, we can define the composition of their three-way slices. In this case, the input and output size is independent of values m', m'', and the computation can be performed efficiently even when m', m'' are large (but even more efficiently, if m'' happens to be small).

Corollary 1. *Given the core nonzeros of the three-way slices*

$$P^{\llcorner}_{a',\smile b\sim} = \big(P_{a',\smile b\sim}\langle 0 : +\infty, * \rangle, P_{a',\smile b\sim}\langle *, -\infty : n \rangle\big)$$
$$P^{\llcorner}_{a'',\smile b\sim} = \big(P_{a'',\smile b\sim}\langle 0 : +\infty, * \rangle, P_{a'',\smile b\sim}\langle *, -\infty : n \rangle\big)$$

it is possible to compute the core nonzeros of the three-way slice

$$P^{\llcorner}_{a,\smile b\sim} = \big(P_{a,\smile b\sim}\langle 0 : +\infty, * \rangle, P_{a,\smile b\sim}\langle *, -\infty : n \rangle\big)$$

and all the nonzeros of the submatrix

$$P^{\urcorner}_{a,\smile b\sim} = P_{a,\smile b\sim}\langle -m' : +\infty, -\infty : m'' + n \rangle$$

in time $O\big(n \log \min(m'', n)\big)$.

Proof. Observe that the number of core nonzeros within each of the three-way slices is at most n. The computation runs as in Theorem 10 (although the current corollary will be typically used when $n < m''$, in which case the decomposition by Lemma 5 becomes trivial). In the final stage of the algorithm, at most $3n$ core nonzeros of $P_{a,\smile b\sim}$ have to be queried, therefore the overall running time is $O\big(n \log \min(m'', n)\big)$. □

The submatrix $P^{\urcorner}_{a,\smile b\sim}$, obtained alongside the three-way slice $P^{\llcorner}_{a,\smile b\sim}$ in Corollary 1, contains at most n nonzeros. This submatrix will be called the *cross-way slice* of $P_{a,\smile b\sim}$. Notice that, while the definition of a three-way slice $P^{\llcorner}_{a,\smile b\sim}$ depends only on n, the definition of a cross-way slice $P^{\urcorner}_{a,\smile b\sim}$ also depends on m', m'', and therefore on a particular decomposition $a = a'a''$.

2.4 Weighted scores and edit distances

The concept of LCS score is generalised by that of *weighted alignment score* (see e.g. [52]). An *alignment* of strings a, b is obtained by putting a subsequence of a into one-to-one correspondence with a (not necessarily identical) subsequence of b, character by character and respecting the index order. The corresponding pair of characters, one from a and the other from b, are said to be *aligned*. A character not aligned with a character of another string is said to be aligned with a *gap* in that string. Hence, four types of character alignment arise, each of which is given a real *weight*:

- a pair of matching characters, with weight $w_=$;
- a pair of mismatching characters, with weight $w_\#$;
- a gap against a character, with weight $w_\dashv$;
- a character against a gap, with weight $w_\vdash$.

Some of these weights may be negative. Aligning a matching pair of characters is considered to be better than aligning a mismatching pair of characters, which in its turn is not worse than aligning each of the two characters against a gap. Therefore, we assume $w_= > w_\# \geq w_\dashv + w_\vdash$. In particular, the LCS score corresponds to taking $w_= = 1$, $w_\# = w_\dashv = w_\vdash = 0$.

Definition 15. *The* alignment score *for strings a, b is the maximum total weight of character alignments in an alignment of a and b.*

Clearly, the alignment score corresponds to a shortest path in a generalised alignment dag, where diagonal match, diagonal mismatch, horizontal and vertical edges have weight $w_=$, $w_\#$, $w_\dashv$, $w_\vdash$, respectively.

We show that without loss of generality, we can restrict ourselves to alignment scores with $w_= = 1$, $w_\dashv = w_\vdash = 0$. Indeed, given general weights, we solve the alignment score problem with *normalised weights*

$$w^*_= = 1 \qquad w^*_\# = \frac{w_\# - w_\dashv - w_\vdash}{w_= - w_\dashv - w_\vdash} \qquad w^*_\dashv = w^*_\vdash = 0$$

Then the score w of any alignment with the original weights can be found from the score w^* of the corresponding alignment with normalised weights as

$$w = w^* \cdot (w_= - w_\dashv - w_\vdash) + m \cdot w_\vdash + n \cdot w_\dashv$$

In this work, we will mostly restrict ourselves to alignment scores that satisfy the following rationality condition.

Definition 16. *A set of alignment score weights will be called* rational*, if the corresponding normalised weights (in particular, $w^*_\#$) are rational numbers.*

Given a rational set of normalised weights, the semi-local alignment score problem on strings a, b can be reduced to the semi-local LCS problem as follows. Let $w_{\#} = \frac{\mu}{2\nu} < 1$, where μ, ν are positive natural numbers. We consider the *subdivided alignment dag*, defined on the set of nodes $v_{l,i}$, $l \in \left\{0, \frac{1}{2\nu}, \frac{2}{2\nu}, \ldots, m\right\}$, $i \in \left\{0, \frac{1}{2\nu}, \frac{2}{2\nu}, \ldots, n\right\}$; the horizontal, vertical and diagonal edges are defined analogously to the ordinary alignment dag. The subdivided alignment dag can be viewed as an $2m\nu \times 2n\nu$ grid of cells, indexed by $\hat{l}_0 + \frac{\hat{l}_1}{2\nu}$, $\hat{\imath}_0 + \frac{\hat{\imath}_1}{2\nu}$, where $\hat{l}_0 \in \langle 0 : m\rangle$, $\hat{\imath}_0 \in \langle 0 : n\rangle$, $\hat{l}_1, \hat{\imath}_1 \in \langle -\nu : \nu\rangle$. A cell contains a diagonal edge; this edge has score $\frac{1}{\nu}$, if either $\hat{l}_1 = \hat{\imath}_1 < \mu - \nu$, or both $a(\hat{l}_0) = b(\hat{\imath}_0)$ and $\hat{l}_1 = \hat{\imath}_1$; the diagonal edge has score 0 otherwise. It is easy to see that the alignment score between strings a and b corresponds to the highest-scoring path in the subdivided alignment dag.

All the techniques of the previous sections clearly apply to the subdivided alignment dag, assuming that ν is a constant. In particular, we can extend naturally Definitions 10 and 11 to define the *semi-local* and the *three-way semi-local alignment score problems*. The output of the semi-local alignment score problem corresponds to a conceptually infinite *semi-local alignment score matrix*, which is an anti-Monge matrix that can be represented implicitly by a permutation matrix with core size $(m+n)\cdot\nu$. Given an implicit semi-local alignment score matrix, individual semi-local alignment scores can be queried in polylogarithmic time by Theorem 1.

Finally, we can adapt the same approach to comparing strings by means of an *edit distance metric*. Here, we think of string a being transformed into string b by a sequence of weighted *character edits* of one of three types:

- character insertion, with weight w_{in};
- character deletion, with weight w_{del};
- character substitution, with weight w_{sub}.

Definition 17. *The* edit distance *between strings a, b is the minimum total weight of a sequence of character edits transforming a into b.*

In particular, taking $w_{in} = w_{del} = 1$, $w_{sub} = 2$ corresponds to the *LCS distance* (also called the *indel distance*) [79, 10]; taking $w_{in} = w_{del} = w_{sub} = 1$ corresponds to the *Levenshtein distance* (also called the *indelsub distance*) [67]; taking $w_{in} = 0$, $w_{del} \geq w_{sub} > 0$ corresponds to the *episode distance* [30].

The relationship between string alignment and string editing is straightforward: given a set of weights, the edit distance problem corresponds to the alignment score problem with weights

$$w_{=} = 0 \qquad w_{\#} = -w_{sub} \qquad w_{\dashv} = -w_{in} \qquad w_{\vdash} = -w_{del}$$

The resulting set of weights is rational, if $\frac{w_{del}+w_{in}}{w_{sub}}$ is a rational number. In this case, all the techniques of the previous sections apply also to semi-local edit distances.

Chapter 3

The seaweed method

3.1 The seaweed algorithm

A classical solution to the global LCS problem is given by the dynamic programming algorithm, discovered independently by Needleman and Wunsch (without an explicit analysis) [79], and by Wagner and Fischer [97]. This algorithm assumes a character comparison model that only allows comparison outcomes "equal" and "unequal", and the unit-cost RAM computation model. The dynamic programming algorithm runs in time $O(mn)$. In the course of the computation, the LCS problem is solved for all prefixes of input string a against all prefixes of input string b.

A naive algorithm for the semi-local LCS problem runs in time $O\big((m+n)^4\big)$. Based on the ideas of Schmidt [88], Alves et al. [7] gave an algorithm for the string-substring LCS problem that runs in time $O(mn)$, which therefore extends the functionality of the standard dynamic programming algorithm, while matching its asymptotic running time. In the course of the computation, the string-substring LCS problem is solved for all prefixes of a against all prefixes of b.

We now give a simple algorithm for the semi-local LCS problem, which further improves on the functionality of the above algorithms, while still matching their model assumptions and asymptotic running time. We call it the *seaweed algorithm*, since it has a simple interpretation in terms of seaweeds introduced in Chapter 1.

Algorithm 1. *Semi-local LCS: the seaweed algorithm.*

Input: strings a, b of length m, n, respectively.

Output: implicit highest-score matrix $P_{a,\smile b\sim}$, represented by core nonzeros.

Description. The output permutation matrix $P_{a,\smile b\sim}$ has core $\langle -m : n\rangle \times \langle 0 : m+n\rangle$ and offset m. We will maintain a variable matrix P with the same core and offset. Let initially $P \leftarrow Id_m$. We sweep the cells of the alignment dag in an arbitrary order compatible with the top-to-bottom and

left-to-right partial order of the cells. For each cell, we perform an update on matrix P. At the end of the sweep, we will have $P = P_{a,\smile b\sim}$.

Consider a cell indexed by $\hat{l} \in \langle 0 : m\rangle$, $\hat{\imath} \in \langle 0 : n\rangle$. We define the cell's *parameters* to be characters $a(\hat{l})$, $b(\hat{\imath})$. Let $i^* = \hat{\imath} + m - \hat{l}$. The update is performed on a 2×2 induced permutation submatrix of P as follows:

$$P\langle \cdot, i^* - 1 : i^* + 1\rangle \leftarrow \begin{cases} \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right) & \text{if } a(\hat{l}) \neq b(\hat{\imath}) \text{ and } P\langle \cdot, i^* - 1 : i^* + 1\rangle = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) \\ \text{unchanged otherwise} \end{cases}$$

The current cell can be regarded as an automaton, performing the update on the submatrix from an *input state* into the *output state*.

The sequence of updates on matrix P can be interpreted as the following sequence of updates on the alignment dag. We start with a trivial full-match dag, which consists entirely of match cells. We then sweep the cells in the order described above. In each step, we transform a match cell into a mismatch cell, if the corresponding characters mismatch in the input strings. By Theorem 8, the algorithm maintains the invariant "current state of matrix P is the implicit highest-score matrix for the current state of the alignment dag". Therefore, at the end of the sweep, we have $P = P_{a,\smile b\sim}$.

Cost analysis. For every cell, the 2×2 column-induced submatrix $P\langle \cdot, i^* - 1 : i^* + 1\rangle$ can be obtained from matrix P in time $O(1)$. The cell update also runs in time $O(1)$. Therefore, the overall running time is $O(mn)$.

The memory cost is dominated by storing the input and the linear representation of the current matrix P. Therefore, the overall memory cost is $O(m + n)$. □

In the course of the computation by Algorithm 1, the semi-local LCS problem is solved implicitly for all prefixes of a against all prefixes of b. The algorithm can be interpreted in terms of seaweeds as follows. Each seaweed is traced across the alignment dag in the top-to-bottom or left-to-right direction. A seaweed runs in a straight line by default; however, its direction may be affected by match cells, and by other seaweeds. Every cell has two seaweeds passing through it, one entering across the top edge and another across the left-hand edge. In a match cell, both seaweeds "bend away" from each other, so the seaweed entering at the top exits on the right, and the seaweed entering on the left exits at the bottom. In a mismatch cell, the two seaweeds keep straight and cross each other, if and only if this pair of seaweeds have not previously crossed; otherwise, they bend away as in a match cell. Therefore, any given pair of seaweeds are only allowed to cross at most once in the course of the computation. Notice that the same property of crossing at most once also holds for any pair of highest-scoring paths in the dag.

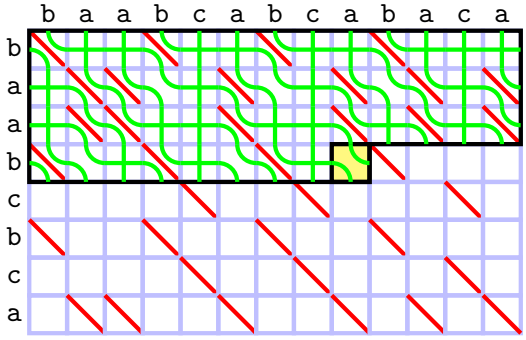


Figure 3.1: A snapshot of Algorithm 1 (the seaweed algorithm)

Figure 3.1 shows a snapshot of Algorithm 1. The dag area that has already been processed is shown by the dark border; the cell currently being processed is shaded. Since the two seaweeds crossing in the current cell have previously crossed, the current step will leave the implicit highest-score matrix unchanged, so that the second crossing is not allowed. The final layout of the seaweeds is the one given in Figure 2.3, which describes the full sequence of states of the implicit highest-score matrix in Algorithm 1.

Recall that the dag cells in Algorithm 1 can be processed in any order consistent with the left-to-right and top-to-bottom dependency partial order. In particular, the cell processing order can be fixed so that the algorithm will compute incrementally the implicit highest-score matrix for all prefixes of string a against string b. By keeping the algorithm's intermediate data, we obtain a data structure that allows efficient LCS queries for every prefix of a against every substring of b. As in the classical dynamic programming approach, this data structure can be used to *trace back* (i.e. to obtain character by character) the actual LCS corresponding to a prefix-substring LCS query, in time proportional to the size of the output (i.e. the length of the output subsequence). Alternatively, a technique similar to memory-efficient dynamic programming by Hirschberg [47] can be applied to achieve prefix-substring LCS traceback in the same asymptotic time, but in a linear amount of memory.

Under the "equal/unequal" character comparison model, Algorithm 1 matches the lower bound on the (global) LCS problem by Aho et al. [3] (see also a survey by Bergroth et al. [17] and references therein). Therefore, in this model the algorithm is asymptotically optimal.

3.2 Incremental LCS and semi-local LCS

The *incremental LCS problem* was introduced by Landau et al. [64], and by Kim and Park [58]. Given a fixed text string, the problem asks its LCS score against a variable pattern string, which can be modified on-line by either

appending or prepending a character. An extension, called *fully-incremental LCS problem*, was introduced by Ishida et al. [51]. Here, both input strings can be modified on-line in a similar fashion. In both versions of the problem, the goal is to maintain a data structure that will store the LCS score for the input strings, and will allow efficient on-line updates of this score.

Let a, b denote the current state of each input string, and m, n their respective current size. Works [64, 58] give incremental LCS algorithms with worst-case update time $O(m)$, where input string a is kept fixed. Work [51] extends this result to a fully-incremental LCS algorithm with worst-case update time $O(m)$ (respectively, $O(n)$) when input string a (respectively, b) is kept fixed.

We now give an algorithm for the fully-incremental LCS problem, matching the above algorithms in running time. Our algorithm is a straightforward generalisation of Algorithm 1. Intuitively, the dynamic data structure consists of the endpoints of all the seaweeds in the current state of the core alignment dag. Prepending or appending a character to string a (respectively, b) corresponds to adding a new row of cells along the top or bottom (respectively, left or right) boundary of the core dag.

The same technique also extends to the case where the dynamic data structure is required to support, in addition to the global LCS score, also semi-local LCS queries. By Theorem 1, a data structure allowing efficient semi-local LCS score queries can be maintained at an extra time $O\big((m+n)\log(m+n)\big)$ per character update.

We now give another generalisation of incremental string comparison. Consider a fixed text string of length n and a variable pattern string, which can be modified on-line by either appending or prepending a block of characters from a pre-specified set of *admissible blocks*. The set of admissible blocks is known in advance, and off-line preprocessing of this set is allowed. The *block-incremental LCS problem* asks, as before, to maintain a data structure that will store the LCS score for the text against the pattern, and will allow efficient on-line updates of this score.

Consider an individual block update, and let l be the corresponding block length. Such an update can be done naively as l single-character updates, giving the block update time $O(nl)$.

We now give an algorithm for the block-incremental LCS problem, that improves on the naive algorithm in running time. The set of admissible blocks is preprocessed off-line by computing the implicit highest-score matrix for the text string against every admissible block. The preprocessing runs in time $O\big(n \cdot L\big)$, where L is the total length of the admissible blocks. Given the implicit highest-score matrices, an individual block update can be performed by Theorem 10 in time $O(n \log l)$.

3.3 Common-substring LCS and semi-local LCS

The *common-substring LCS problem* was introduced by Landau et al. [66, 27]. Given a text string of length n and an unspecified number of pattern strings, the problem asks for the LCS score of the text against each of the patterns. The pattern strings may share a common substring of length l; we assume $l \leq n$. A pattern string may contain several copies of the common substring; the locations of all the copies are known in advance. The goal is, given the text, to preprocess the common substring so as to minimise the LCS computation time for each occurrence of the common substring in the patterns.

The problem can be solved naively by computing the LCS score for the text against each of the patterns, ignoring the common-substring structure. The resulting algorithm does no preprocessing, and runs in time $O(nl)$ for each occurrence of the common substring.

An improved algorithm is given in [66, 27]. This algorithm, following some preprocessing in time $O(nl)$, runs in time $O(n)$ for each occurrence of the common substring.

We now give an algorithm for the common-substring LCS problem, that matches the above algorithm both in preprocessing and running time. We preprocess the common substring in time $O(nl)$, obtaining the implicit highest-score matrix for the text against the common substring. For every pattern string, row 0 of the implicit highest-score matrix can now be computed incrementally by repeated application of Theorem 9. Each incremental update takes time $O(n)$ per occurrence of the common substring in the pattern, and the same time $O(n)$ per pattern character outside any such occurrence.

We now consider the more general *semi-local common-substring LCS problem*. As in the ordinary semi-local LCS problem, string-substring, substring-string, prefix-suffix and suffix-prefix LCS score queries are now allowed between the text and each of the patterns.

Similarly to the global common-substring LCS problem, its semi-local version can be solved naively by computing the implicit highest-score matrix for the text against each of the patterns, ignoring the common-substring structure. The resulting algorithm does no preprocessing, and runs in time $O(nl)$ for each occurrence of the common substring.

We now give an algorithm for the semi-local common-substring LCS problem, improving on the naive algorithm in running time. As before, we preprocess the common substring in time $O(nl)$, obtaining the implicit highest-score matrix for the text against the common substring. For every pattern string, the implicit highest-score matrix can now be computed incrementally, starting from an arbitrary occurrence of the common substring. The resulting algorithm can be regarded as a special case of the block-incremental LCS algorithm from Section 3.2. Each incremental up-

date takes time $O(n \log l)$ per occurrence of the common substring in the pattern, and $O(n)$ per pattern character outside any such occurrence. Overall, the algorithm takes time $O(n)$ for the first occurrence of the common substring in a pattern, and time $O(n \log l)$ for each subsequent occurrence in the same pattern. In particular, if the common substring only occurs in every pattern string once, our algorithm improves on the algorithm of [66, 27] in functionality, without any increase in the asymptotic running time.

Chapter 4

The micro-block seaweed method

4.1 The micro-block seaweed algorithm

In the previous chapter, we assumed the character comparison model that only allows comparison outcomes "equal" and "unequal". As mentioned in Section 3.1, the LCS problem in this model has a lower bound of $\Omega(mn)$, which is matched by both the standard dynamic programming algorithm, and by the seaweed algorithm. Both these algorithms sweep the alignment dag cell by cell, and perform in every cell a constant amount of work, assuming the unit-cost RAM computation model.

We now switch to a more powerful character comparison model, assuming that the alphabet is a totally ordered set, and comparison outcomes are "less than", "equal" and "greater than". In this model, we no longer need to process every dag cell individually, so algorithms with running time $o(mn)$ become possible. This is true even if the computation model assumption is weakened, so that character comparisons and arithmetic operations are charged using the log-cost RAM model.

We assume without loss of generality that $m \leq n$, and that m and n are reasonably close, so $m = \Omega\big(\frac{\log n}{\log \log n}\big)$. In such a setting, LCS computation can be accelerated by the method originated by Arlazarov et al. [11], often called the "four Russians method". In this work, we call it the *micro-block method*, adapting the terminology of Bille and Gørtz [18]. Using the micro-block method, Masek and Paterson [73] gave an algorithm for the (global) LCS problem running in time $O\big(\frac{mn}{\log n}\big)$ for a constant-size alphabet[1], and in time $O\big(\frac{mn(\log \log n)^2}{\log n}\big)$ for an unbounded-size alphabet (the latter was observed in [81]).

[1] In the unit-cost RAM model, the algorithm of [73] can be accelerated by another factor of $O(\log n)$ (see e.g. [100]) for a constant-size alphabet. This technique does not seem to apply in the case of an unbounded-size alphabet.

We now give an algorithm for semi-local LCS running in subquadratic time, which achieves a slight improvement on Algorithm 1 in running time. Our algorithm also matches the algorithm of [73] in running time for an unbounded-size alphabet, while improving on it in functionality. In the case of a constant-sized alphabet, the running time of our algorithm remains unchanged, while the algorithm by Masek and Paterson is accelerated by a factor of $O\big((\log\log n)^2\big)$.

Algorithm 2. *Semi-local LCS: the micro-block seaweed algorithm.*

Input, output: as in Algorithm 1; we let $t = \frac{\log n}{4\cdot\log\log n}$, where the logarithms are base 2, and assume that $t \le m \le n$.

Description. Without loss of generality, we may assume that $m = n$; otherwise, we can partition string b into $\lceil m/n \rceil$ blocks of size at most m, and process each block separately by the current algorithm. Also, without loss of generality, we may assume that the alphabet size is at most $2n$, and that the characters are encoded by values in the range $\langle -n : n\rangle$. We call two strings of equal length *isomorphic*, if one can obtained from the other by a permutation of the alphabet.

As in Algorithm 1, we will maintain a variable matrix P with the same core and offset as the output matrix $P_{a,\smile b\sim}$. We let initially $P \leftarrow Id_m$. The main idea of the algorithm is to sweep the alignment dag in *micro-blocks* of size t; this size is chosen so that running time can be saved by precomputing all possible updates in advance, rather than performing every update as it appears in the alignment dag. At the end of the sweep, we will have $P = P_{a,\smile b\sim}$.

The described idea by itself is sufficient to obtain a subquadratic algorithm in the unit-cost RAM model. In this case, we can sweep the micro-blocks of the alignment dag in an arbitrary order compatible with the top-to-bottom and left-to-right partial order of the micro-blocks. However, in order to perform the computation efficiently in the log-cost RAM model, we must fix the order of the micro-blocks to be a specific recursive quadtree order. The root of the recursion tree is the whole dag of size n, the children of a block of size h are four subblocks of size $h/2$, and the leaves are the micro-blocks of size t. For each micro-block, we perform an update on matrix P.

Consider any block of cells of size h, indexed by $\langle l, l+h\rangle \times \langle i, i+h\rangle$, where $l \in [0 : m-h]$, $i \in [0 : n-h]$. We define the block's *parameter sequence* as the sequence of characters in the substrings $a\langle l : l+h\rangle$, $b\langle i : i+h\rangle$. Let $i^* = i + m - l$. The current block can be regarded as an automaton, performing the update on the $2h \times 2h$ column-induced permutation submatrix $P\langle \cdot, i^* - h, i^* + h\rangle$ from an *input state* into the *output state*.

The elements of the parameter sequence are characters, encoded by values in the range $\langle -n : n\rangle$. The input and output states are described by the row and column indices of the nonzeros; the natural range of such values

is also $\langle -n : n \rangle$. However, in order to perform the computation efficiently in the log-cost RAM model, these ranges have to be remapped to smaller ranges in every level of the recursion. For a block of size h, the parameter sequence and the input and output states consist each of $2h$ values, ranging over $\langle -h : h \rangle$. For each of the four block's children of size $\frac{h}{2}$, the parameter sequence and the input and output states consist each of h values; therefore, these values can be remapped bijectively to the range $\langle -\frac{h}{2} : \frac{h}{2} \rangle$, preserving their linear order. Such a remapping can be easily performed in $O(h)$ operations.

We process a block of size h in the recursion tree as follows. First, we form the parameter sequence and the input state for its top-left child block, and remap their elements from range $\langle -h : h \rangle$ to range $\langle -\frac{h}{2} : \frac{h}{2} \rangle$. Then, we call the algorithm recursively, obtaining the output state of the top-left child block, and remap its elements from range $\langle -\frac{h}{2} : \frac{h}{2} \rangle$ back to range $\langle -h : h \rangle$. We repeat the same procedure (forming parameter sequences and input states, remapping their elements to a reduced range, performing the recursive call, remapping the output state back to the original range) on the top-right and bottom-left child blocks, and then on the bottom-right child block.

The base of the recursion is a micro-block of size t. In this case, the update is performed on a $2t \times 2t$ column-induced permutation submatrix of P as follows:

$$P\langle \cdot, i^* - t : i^* + t \rangle \leftarrow \\ \mathit{update}\big(a\langle l : l + t \rangle, b\langle i : i + t \rangle, P\langle \cdot, i^* - t : i^* + t \rangle\big)$$

The parameter sequence and the input state consist each of $2t$ values, ranging over $\langle -t : t \rangle$. For each of the at most $(2t)^{2t+2t} = (2t)^{4t}$ possible combinations of the parameter and input values, the output values given by the function *update* are precomputed in advance, using Algorithm 1.

Similarly to Algorithm 1, the sequence of updates on matrix P corresponds to the following sequence of updates on the alignment dag. We start with a trivial full-match dag. We then sweep the dag in micro-blocks of size t, in the quadtree order described by the above recursion. In each step, we transform a full-match micro-block into a micro-block defined by the input strings. The algorithm maintains the invariant "current state of matrix P is the implicit highest-score matrix for the current state of the alignment dag". Therefore, at the end of the sweep, we have $P = P_{a,\curvearrowright b\sim}$.

Cost analysis. In the precomputation stage, there are at most $(2t)^{4t}$ problem instances, each of which runs in time $O(t^2 \log t)$ in the log-cost RAM model. Therefore, the running time of the precomputation is $O\big((2t)^{4t} \cdot t^2 \log t\big) = O\big(2^{4t \cdot \log(2t)} \cdot t^2 \log t\big) = o\big(2^{\frac{\log n}{\log \log n} \cdot \log \log n} \cdot (\log n)^{O(1)}\big) = o(2^{\log n} \cdot (\log n)^{O(1)}) = o(n \cdot (\log n)^{O(1)})$, which is clearly dominated by the main computation stage.

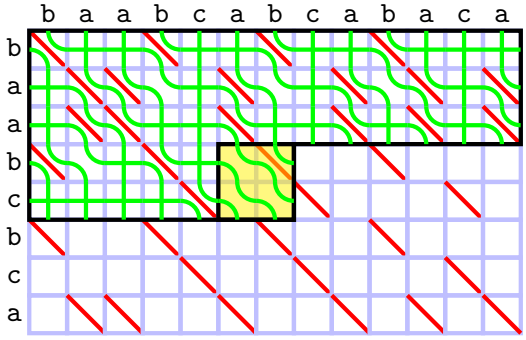


Figure 4.1: A snapshot of Algorithm 2 (the micro-block seaweed algorithm)

In the main computation stage, the running time of the recursion is dominated by its base. There are $\frac{mn}{t^2}$ micro-block update steps, each of which runs in time $O(t \log t)$ in the log-cost RAM model. Therefore, the total running time of the algorithm is $\frac{mn}{t^2} \cdot O(t \log t) = O\big(\frac{mn \log t}{t}\big) = O\big(\frac{mn(\log\log n)^2}{\log n}\big)$. □

Figure 4.1 shows a snapshot of Algorithm 2, using the same conventions as Figure 3.1. For simplicity, this illustration ignores the recursive quadtree micro-block ordering, and instead assumes an ordering similar to that of Figure 3.1, yielding a subquadratic algorithm in the unit-cost RAM model only. As in Algorithm 1, the final layout of the seaweeds is the one given in Figure 2.3.

4.2 Cyclic LCS

Given strings a, b of length m, n respectively, the *cyclic LCS problem* asks for the highest LCS score between a and all cyclic shifts of b (or, equivalently, all cyclic shifts of a and all cyclic shifts of b).

Cyclic string comparison has been considered by Maes [70], Bunke and Bühler [19], Landau et al. [64], Schmidt [88], Marzal and Barrachina [72]. Works [64, 88] give algorithms that solve the cyclic LCS problem in worst-case time $O(mn)$.

We now give a new algorithm for the cyclic LCS problem, improving on the existing algorithms in running time. First, we call Algorithm 2 on strings a and bb (a concatenation of string b with itself). Then, we perform n string-substring LCS queries for a against every substring of bb of length n, and take the maximum score among these queries. The overall running time is dominated by the call to Algorithm 2, which runs in time $O\big(\frac{mn(\log\log n)^2}{\log n}\big)$.

4.3 Longest repeating subsequence

Given a string a of length n, the *longest repeating subsequence problem* asks for the length of the longest subsequence of a that is a *square*, i.e. a concatenation of two identical strings.

This problem has been considered under the name "longest tandem scattered subsequence problem" by Kosowski [60], who gave an algorithm running in time $O(n^2)$.

We now give a new algorithm for the longest repeating subsequence problem, improving on the existing algorithm in running time. First, we call Algorithm 2 on string a against itself. Then, we perform $n-1$ prefix-suffix LCS queries for every possible non-trivial prefix-suffix decomposition of a, and take the maximum score among these queries. The overall running time is dominated by the call to Algorithm 2, which runs in time $O\big(\frac{n^2(\log\log n)^2}{\log n}\big)$.

4.4 Approximate pattern matching

Approximate pattern matching is a classical generalisation of both the alignment score (or, equivalently, edit distance) problem, and of ordinary pattern matching. Given a text string t of length m and a pattern string p of length n, the *approximate pattern matching problem* asks to find the substrings of the text that are locally closest to the pattern, i.e. that have the locally highest alignment score (or, equivalently, lowest edit distance) against the pattern. The precise definition of "locally" may vary in different versions of the problem. Some well-known types of approximate pattern matching are:

- the *complete approximate matching problem,* which assumes an alignment score with arbitrary weights, and asks for the highest-scoring prefix in every suffix of the text (that is, the row maxima of the highest-score matrix $H_{p,\backsim t\sim}$);
- the *threshold approximate matching problem,* which assumes an alignment score with arbitrary weights, and, given a threshold score h, asks for all substrings of the text that have alignments score at least h against the pattern;
- the *minimal-window subsequence recognition problem,* which asks for all inclusion-minimal substrings in the text containing the pattern as a substring (that is, the dominance-minimal global maxima of the highest-score matrix $H_{p,\backsim t\sim}$, as long as the global maximum of m is attained, and assuming the LCS alignment score).
- the *fixed-window subsequence recognition problem,* which, given a window length w, asks for all substrings of length w of the textAS containing the pattern as a substring (that is, the global maxima of the

highest-score matrix $H_{p,\smile t\sim}$ on the diagonal $j - i = w$, as long as the global maximum of m is attained, and assuming the LCS alignment score).

A classical algorithm by Sellers [89], which is a modification of the standard dynamic programming algorithm, solves the complete approximate pattern matching problem in time $O(mn)$. Assuming a rational set of weights, and keeping the model assumptions of Section 4.1, the micro-block method gives an algorithm running in time $O\big(\frac{mn}{\log n}\big)$ for a constant-size alphabet, and in time $O\big(\frac{mn(\log\log n)^2}{\log n}\big)$ for an unbounded-size alphabet. Various extensions of the problem have been considered by Landau and Vishkin [65], Cormode and Muthukrishnan [26] and many others (see e.g. a survey by Navarro [78] and references therein).

The minimal-window and fixed-window subsequence recognition problems are considered by Das et al. [30] as "episode matching problems". For both problems, they give an algorithm with running in time $O\big(\frac{mn}{\log n}\big)$ for a constant-size alphabet, which again can be modified to an algorithm running in time $O\big(\frac{mn(\log\log n)^2}{\log n}\big)$ for an unbounded-size alphabet. A multi-pattern version of the problems has been considered by Cégielski et al. [23].

We now give a new unified algorithm for the described three versions of approximate pattern matching. Our algorithm matches the algorithms based on [73] and on [30] in running time for an unbounded-size alphabet.

The new algorithm is as follows. First, we call Algorithm 2 on strings p, t (in case of rational weights, via the subdivided alignment dag of Section 2.4), obtaining the implicit highest-score matrix $P_{p,\smile t\sim}$. By Theorem 1, we then build a data structure that allows to query any element of the highest-score matrix $H_{p,\smile t\sim}$ in polylogarithmic time. Since matrix $H_{p,\smile t\sim}$ is anti-Monge, all the row maxima can now be found efficiently by the algorithm of Lemma 2. The overall running time is dominated by the call to Algorithm 2, which runs in time $O\big(\frac{mn(\log\log n)^2}{\log n}\big)$.

Chapter 5

Periodic string comparison

5.1 The periodic seaweed algorithm

In many string comparison applications, one or both of the input strings may have periodic structure. In this chapter, we show how to exploit such structure efficiently, using a variant of the seaweed method.

Consider the problem of comparing a finite string a of length m against a string b, which is infinite in both directions and *periodic*: $b = u^{\pm\infty} = \ldots uuuu \ldots$ The *period string* u is finite of length p.

Definition 18. *Given strings a, u, the* periodic string-substring LCS problem *asks for the LCS score of a against every finite substring of $b = u^{\pm\infty}$.*

Without loss of generality, we assume that every character of a occurs in u at least once. Clearly, the length of the substring of b in Definition 18 can be restricted to be at most mp.

The definition of the alignment dag (Definition 12) extends naturally to the periodic string-substring LCS problem. The alignment dag is itself *periodic*: the edges $v_{l,\hat{\imath}-\frac{1}{2}+kp} \rightarrow v_{l,\hat{\imath}+\frac{1}{2}+kp}$ (respectively, $v_{\hat{l}-\frac{1}{2},i+kp} \rightarrow v_{\hat{l}+\frac{1}{2},i+kp}$, $v_{\hat{l}-\frac{1}{2},\hat{\imath}-\frac{1}{2}+kp} \rightarrow v_{\hat{l}+\frac{1}{2},\hat{\imath}+\frac{1}{2}+kp}$) have equal scores for all $l \in [l_0 : l_1]$, $\hat{l} \in \langle l_0 : l_1 \rangle$, $i \in [i_0, i_1]$, $\hat{\imath} \in \langle i_0 : i_1 \rangle$, $k \in [-\infty : +\infty]$. Such an alignment dag can also be regarded as a horizontal composition of an infinite sequence of *period subdags*, each of which is isomorphic to the $m \times p$ alignment dag $G_{a,u}$.

Consider the highest-score matrix $H_{a,b}$ and its implicit representation $P_{a,b}$; note that, since string b is already infinite, it does not require any extension by wildcards. Matrices $H_{a,b}$, $P_{a,b}$ are again *periodic*: we have $H_{a,b}(i,j) = H_{a,b}(i+p, j+p)$ for all $i, j \in [-\infty : \infty]$, and $P_{a,b}(\hat{\imath}, \hat{\jmath}) = H_{a,b}(\hat{\imath}+p, \hat{\jmath}+p)$ for all $\hat{\imath}, \hat{\jmath} \in \langle -\infty : \infty \rangle$. To represent such matrices, it is sufficient to store the p nonzeros of the *horizontal period submatrix* $P_{a,b}\langle 0 : p, * \rangle$, or, symmetrically, of the *vertical period submatrix* $P_{a,b}\langle *, 0 : p \rangle$. The nonzero sets of the two period submatrices can be obtained from one

another in time $O(p)$; we will be using both of them simultaneously where necessary.

The periodic string-substring LCS problem can be solved by a simple extension of the seaweed algorithm (Algorithm 1). Following the periodic structure of the highest-score matrix, the seaweed pattern is also periodic. Hence, the seaweeds only need to be traced within a single period subdag, with appropriate wraparound.

Algorithm 3. *Periodic string-substring LCS: the periodic seaweed algorithm.*

Input: strings a, u of length m, p, respectively.

Output: implicit highest-score matrix $P_{a,b}$, represented by nonzeros of (say) vertical period submatrix $P_{a,b}\langle *, 0 : p\rangle$, where $b = u^{\pm\infty}$.

Description. The output matrix is periodic with period p. We will maintain a variable matrix P with the same period. We let initially $P \leftarrow Id_m$ (which is a periodic matrix). Then, we sweep the cells of the period subdag as follows. In the outer loop, we run through the rows of cells top-to-bottom. For the current row $\hat{l} \in \langle 0 : m\rangle$, we start the inner loop at an arbitrary match cell $\hat{\imath}_0 \in \langle 0 : p\rangle$, so we have $a(\hat{l}) = b(\hat{\imath})$. Such a match cell is guaranteed to exist by the assumption that every character of a occurs in u at least once. Then, we sweep the cells from $\hat{\imath} = \hat{\imath}_0$ left-to-right, wrapping around from $\hat{\imath} = p - \frac{1}{2}$ to $\hat{\imath} = \frac{1}{2}$, and continuing the sweep left-to-right up to $\hat{\imath} = \hat{\imath}_0 - 1$. For each cell, we perform an update on matrix P. At the end of the sweep, we will have $P = P_{a,b}$.

Consider a cell indexed by $\hat{l} \in \langle 0 : m\rangle$, $\hat{\imath} \in \langle 0 : p\rangle$. We define the cell's *parameters* to be characters $a(\hat{l})$, $b(\hat{\imath})$. Let $i^* = \hat{\imath} + m - l$. As in Algorithm 1, the update is performed on a 2×2 column-induced permutation submatrix of P as follows:

$$P\langle \cdot, i^* - 1 : i^* + 1\rangle \leftarrow \begin{cases} \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right) & \text{if } a(\hat{l}) \neq b(\hat{\imath}) \text{ and } P\langle \cdot, i^* - 1 : i^* + 1\rangle = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) \\ \text{unchanged otherwise} \end{cases}$$

Note that the first update in an inner loop is always trivial: we have $a(\hat{l}) = b(\hat{\imath}_0)$, therefore P remains unchanged.

The sequence of updates on matrix P can be interpreted as a sequence of updates on the alignment dag, as described in Algorithm 1, but now including the wraparound. Therefore, at the end of the sweep, we have $P = P_{a,b}$.

Cost analysis. For every cell, the 2×2 column-induced submatrix $P\langle \cdot, i^* - 1 : i^* + 1\rangle$ can be obtained from the vertical period submatrix of P in time $O(1)$. The cell update also runs in time $O(1)$. Therefore, the overall running time is $O(mp)$.

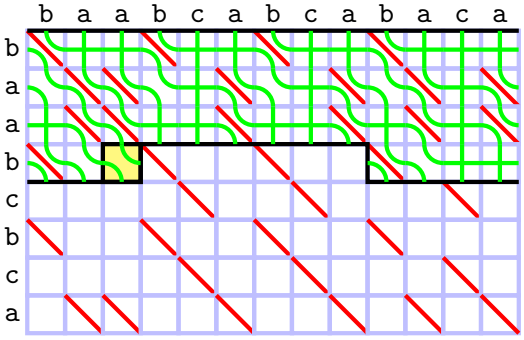


Figure 5.1: A snapshot of Algorithm 3 (the periodic seaweed algorithm)

The memory cost is dominated by storing the input and the period submatrix of the current matrix P. Therefore, the overall memory cost is $O(m+p)$. □

Figure 5.1 shows a snapshot of Algorithm 3, using the same conventions as Figure 3.1.

Note that the cell updating order in Algorithm 3 is significantly more restricted than in Algorithm 1, due to the extra data dependencies caused by the wraparound. This seems to rule out the possibility of a micro-block version of the algorithm.

5.2 Tandem alignment

The periodic LCS problem has many variations that can be solved by an application of the periodic seaweed algorithm.

The first such variation is the *tandem LCS problem*. The problem asks for the LCS score of a string a of length m against a tandem k-repeat string $b = u^k$ of length $n = kp$. As before, we assume that every character of a occurs in u at least once. We may assume that $k \leq m$ (since for $k \geq m$, every character of a can be matched to a different copy of u in b, and therefore the LCS score between a and b is equal to m).

The tandem LCS problem can be solved naively by considering the LCS problem directly on strings a and b, ignoring the periodic structure of string b. The standard dynamic programming algorithm [79, 97] solves the problem in time $O(mn) = O(mkp)$. This running time can be slightly improved by the micro-block precomputation method [73].

The tandem LCS problem can also be regarded as a special case of the common-substring LCS problem [66, 27] (see also Section 3.3). Using this technique, the problem can be solved in time $O\big(m(k+p)\big)$. The techniques of Landau et al. [27, 63] give an algorithm for the tandem LCS problem, parameterised by the LCS score of the input strings; however, the worst-case

running time of this algorithm is still $O\big(m(k+p)\big)$. Landau [62] asked if the running time for the tandem LCS problem can be improved to $O\big(m(\log k + p)\big)$.

We now give an algorithm that improves on the current algorithms in time and functionality, and even exceeds Landau's expectation. First, we call Algorithm 3 on strings a and u. Then, we count the number of nonzeros dominated by point $(0, n)$, i.e. nonzeros in the submatrix $P_{a,b}\langle 0 : +\infty, -\infty : n\rangle$. Given the (say) horizontal period submatrix $P_{a,b}\langle 0 : p, *\rangle$, this can be done by a sweep of its p nonzeros, counting every nonzero with appropriate multiplicity. More precisely, every nonzero $P_{a,b}(i, j) = 1$, $i \in \langle 0 : p\rangle$, $j \in \langle -\infty : \infty\rangle$, is counted with multiplicity $k - \lfloor j/p \rfloor$, if $j \in \langle 0 : n\rangle$, and is skipped (counted with multiplicity 0) otherwise. The solution to the tandem LCS problem is then obtained by Theorem 8. The overall running time is dominated by the call to Algorithm 3, which runs in time $O(mp)$.

Another set of variations on the periodic LCS problem was introduced by Benson [15] as the *tandem alignment problem*. Instead of asking for all string-substring LCS scores of a against $b = u^{\pm\infty}$, the tandem alignment problem asks for a substring of b that is closest to a in terms of alignment score (or edit distance), under different restrictions on the substring. In particular:

- the *pattern global, text global (PGTG) tandem alignment problem* restricts the substring of b to consist of a whole number of copies of u, i.e. to be of the form $u^k = uu \dots u$ for an arbitrary integer k;
- the *tandem cyclic alignment problem* restricts the substring of b to be of length kp for an arbitrary integer k (but it may not consist of a whole number of copies of u);
- the *pattern local, text global (PLTG) tandem alignment problem* leaves the substring of b unrestricted.

All three versions of the tandem alignment problem can be regarded as special cases of the approximate pattern matching problem (see Section 4.4) on strings a of length m and $b' = u^m$ of length $n = kp$ (but with the roles of the text and the pattern reversed). Therefore, the tandem LCS problem can be solved naively by considering the approximate pattern matching problem directly on strings a and b', ignoring the periodic structure of string b'. Given an arbitrary (real) set of alignment weights, the classical algorithm by Sellers [89] solves the problem in time $O(mn) = O(mkp)$. For a rational set of weights, the running time can again be slightly improved by the micro-block precomputation method (see Section 4.4).

The PGTG and PLTG tandem alignment problems can be solved more efficiently by the technique of *wraparound dynamic programming* [76, 37] (see also [15]) in time $O(mp)$. For the tandem cyclic alignment problem,

Benson [15] modified this technique to give an algorithm running in time $O(mp \log p)$ and memory $O(mp)$.

We now give a new algorithm for the tandem cyclic alignment problem, which improves on the existing algorithm in running time, assuming a rational set of alignment weights. The running time of the new algorithm matches the current algorithms for the PGTG and PLTG tandem alignment problems.

Given input strings a, u, we first solve the periodic string-substring problem by calling Algorithm 3. This gives us a period submatrix of matrix $P_{a,b}$, where $b = u^{\pm\infty}$. Then, for each k, $0 < k < m$, we perform independently the following procedure. We solve the tandem LCS problem for strings a and u^k by the method described earlier in this section, counting every nonzero in the period submatrix $P_{a,b}$ with an appropriate multiplicity. This gives us the LCS score for a against u^k for every k. We then update this score incrementally, obtaining the LCS score for string a against a window of length p in b, sliding through p successive positions. This is equivalent to querying p successive elements in a diagonal of matrix $P_{a,b}$, which can be achieved by $2p$ incremental dominance counting queries. By Theorem 2, every one of these queries can be performed in time $O(1)$.

The call to Algorithm 3 runs in time $O(mp)$; its output is shared by the tandem LCS computation for all k. For each k, the running time of the remaining computation is $O(p)$. Therefore, the combined running time for all values of k is $m \cdot O(p) = O(mp)$. Overall, the algorithm runs in time $O(mp)$.

Chapter 6

Permutation string comparison

6.1 Semi-local LCS between permutations

An important special case of string comparison is where each of the input strings a, b is a *permutation string*, i.e. a string that consists of all distinct characters. Without loss of generality, we may assume that $m = n$, and that both strings are permutations of a given totally ordered set of size n. The semi-local LCS problem on permutations is equivalent to finding the length of the longest increasing subsequence (LIS) in every substring of a given permutation string. In the rest of this section, we give an efficient algorithm for this problem.

For consistency with the notation in previous chapters, we will assume that a permutation string of length n is indexed by odd half-integers $\langle 0 : n \rangle$, and is over the alphabet $\langle 0 : n \rangle$, unless indicated otherwise. The *identity permutation* string of length n is the string $id = \left(\frac{1}{2}, \frac{3}{2}, \ldots, n - \frac{1}{2}\right)$. Given a string a, we denote by $\Sigma(a)$ the set of characters appearing in a at least once. For a set of characters S, we denote by $a|_S$ the *filtered subsequence* of a, which consists only of those characters that belong to S.

Algorithm 4. *Semi-local LCS between permutations.*

Input: permutation strings a, b of length n over an alphabet of size n.

Output: implicit highest-score matrix $P_{a,\smile b\sim}$, represented by core nonzeros.

Description. Recursion on n.

Recursion base. If $n = 1$, the computation is trivial.

Recursive step. Assume without loss of generality that $n > 1$ is even. We partition the input string a into a concatenation $a = a'a''$ of two strings of length $\frac{n}{2}$. Each of the strings a', a'' is a permutation string over $\frac{n}{2}$ characters.

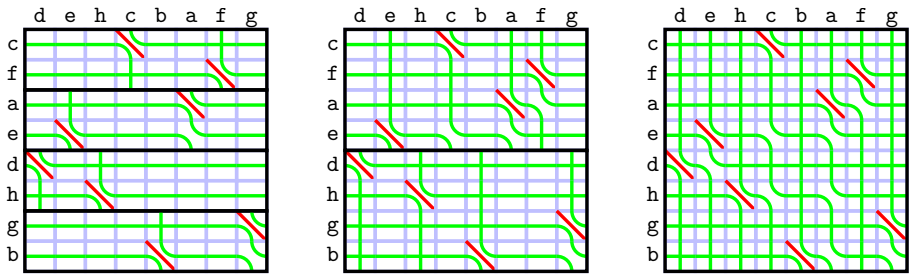


Figure 6.1: An execution of Algorithm 4

The implicit highest-score matrices $P_{a',\smile b\sim}$, $P_{a'',\smile b\sim}$ contain each $\frac{3n}{2}$ core nonzeros. Note that for all $\hat{\imath} \in \langle 0 : n\rangle$, we have $P_{a',\smile b\sim}(\hat{\imath},\hat{\imath}) = 1$, whenever $b(\hat{\imath}) \notin \Sigma(a')$. There are exactly $\frac{n}{2}$ such *trivial* core nonzeros in $P_{a',\smile b\sim}$. The remaining n core nonzeros in $P_{a',\smile b\sim}$ can be obtained by solving recursively the semi-local LCS problem on strings a' and $b' = b|_{\Sigma(a')}$, both of which are permutations strings over the character set $\Sigma(a_1) = \Sigma(b')$ of size $\frac{n}{2}$. Similarly, there are exactly $\frac{n}{2}$ trivial core nonzeros in $P_{a'',\smile b\sim}$, and the remaining n core nonzeros can be obtained by solving recursively the semi-local LCS problem on strings a'' and $b'' = b|_{\Sigma(a'')}$. Strings b', b'' can be computed easily from strings a', a'', b, at the cost of sorting their character sets.

Finally, given matrices $P_{a',\smile b\sim}$, $P_{a'',\smile b\sim}$, matrix $P_{a,\smile b\sim}$ is computed by a call to the algorithm of Theorem 10, which calls the algorithm of Theorem 7 as a subroutine. Note that we now have two nested recursions: the current recursion, and the recursion of Theorem 7.

End of recursive step.

Cost analysis. The recursion tree is a balanced binary tree of height $\log n$. In the root node, the running time is dominated by the call to the algorithm of Theorem 10, and is therefore $O(n \log n)$. In each subsequent level of the recursion tree, the number of nodes doubles, and the running time per node is reduced by at least a factor of 2. Therefore, the running time per level is $O(n \log n)$. The overall running time is $\log n \cdot O(n \log n) = O(n \log^2 n)$. □

Figure 6.1 shows an execution of Algorithm 4.

By keeping the algorithm's intermediate data, we obtain a data structure that allows efficient traceback of any semi-local LCS query on a pair of permutations, in time proportional to the size of the output (i.e. the length of the output subsequence). A related problem of tracing back LIS in *every* substring of a *fixed size* in a permutation has been studied by Albert et al. [6] and by Chen et al. [24]. In particular, work [24] gives an algorithm that runs in time proportional to the size of the output (i.e. the combined lengths of all the output subsequences). In the same work, the algorithm is also generalised for tracing back the LIS in an arbitrary subset of n substrings, possibly of different sizes. In both versions of the problem, the size of the

output, and therefore the algorithm's running time, can be as high as $\Theta(n^2)$. In contrast, Algorithm 4 allows efficient LIS traceback for any individual substring.

6.2 Cyclic LCS between permutations

The cyclic LCS problem has been defined in Section 4.2. Given permutation strings a, b of length n, the cyclic LCS problem on a, b is equivalent to the LIS problem on a circular string.

This problem has been considered by Albert et al. [5], who gave a Monte Carlo randomised algorithm, running in time $O(n^{1.5} \log n)$ with small error probability.

We now give a new algorithm for cyclic LCS between permutations, that improves on the above algorithm both in running time, and by being deterministic. First, we call Algorithm 4, obtaining the implicit highest-score matrix $P_{a,\backsim b\sim}$. Then, we run the algorithm of Theorem 10 on matrix $P_{a,\backsim b\sim}$ against itself, obtaining the implicit highest-score matrix $P_{aa,\backsim b\sim}$. Finally, we perform n substring-string LCS queries for every substring of aa of length n against string b. The overall running time is dominated by the call to Algorithm 4, which runs in time $O(n \log^2 n)$.

A version of the cyclic LCS problem between permutations, parameterised by the output LCS length l, has also been considered by Albert et al. [5], who gave an algorithm running in time $O(nl \log n)$. This was improved upon by Deorowicz [33], who gave an algorithm running in time $O\big(\min(nl, n \log n + l^3 \log n)\big)$. Our algorithm described above improves on the algorithm of [33], unless $l = o\big((n \log n)^{1/3}\big)$.

6.3 Longest pattern-avoiding subsequences

Two given permutation strings a, b of equal length (but generally over different alphabets) are called *isomorphic*, if they have the same relative order of characters, i.e. $a(\hat{\imath}) < a(\hat{\jmath})$ iff $b(\hat{\imath}) < b(\hat{\jmath})$ for all $\hat{\imath}$, $\hat{\jmath}$. Given a target permutation string t of length n and a pattern permutation string p of fixed length, the *longest p-isomorphic subsequence problem*, or simply the *longest p-subsequence problem*, asks for the longest subsequence of t that is isomorphic to p. More generally, given a set of pattern permutation strings X, the *longest X-subsequence problem* asks for the longest subsequence of t that is isomorphic to any pattern string in p. For example, the LIS problem can be interpreted as the longest X-subsequence problem, where X is a set of identity permutation strings, one of each length $m \in [1 : n]$.

Given a set of *antipattern* permutation strings Y, the *longest Y-avoiding subsequence problem* asks for the longest subsequence of t that *does not* contain a subsequence isomorphic to any string in Y. For example, the LIS

problem on a permutation string can be interpreted as the longest {"21"}-avoiding subsequence problem. For a detailed introduction into these problems and their connections, see the work by Albert et al. [4] and references therein.

The LIS problem is the only nontrivial example of the longest Y-avoiding subsequence problem with antipatterns of length 2. Albert et al. [4] gave the full classification of the longest Y-avoiding subsequence problem for all sets of antipatterns of length 3. There are 10 non-trivial sets of such antipatterns. For each of these sets, the algorithms given in [4] run in polynomial time, ranging from $O(n \log n)$ to $O(n^5)$. Two particular antipattern sets considered in [4] are (in that work's original notation):

$$C_3 = \{\texttt{"132"}, \texttt{"213"}, \texttt{"321"}\}$$
$$C_4 = \{\texttt{"132"}, \texttt{"213"}, \texttt{"312"}\}$$

For both these antipattern sets, algorithms given in [4] run in time $O(n^2 \log n)$.

We now give new algorithms for the longest C_3- and C_4-avoiding subsequence problems, improving on the above algorithms in running time.

Permutations avoiding the antipattern set C_3 are all cyclic rotations of an increasing permutation string. The longest C_3-avoiding subsequence in the target string can be found by the algorithm described in Section 6.2, running in time $O(n \log^2 n)$.

Permutations avoiding the antipattern set C_4 are all obtained from an increasing permutation by reversing some suffix. The longest C_4-avoiding subsequence in the target string t can be found as follows. First, we call the standard LIS algorithm on t, obtaining explicitly prefix-prefix LCS scores

$$lcs\big(t \restriction (\hat{\imath} + \tfrac{1}{2}), id \restriction (t(\hat{\imath}) + \tfrac{1}{2})\big) = lcs\big(t \restriction (\hat{\imath} - \tfrac{1}{2}), id \restriction (t(\hat{\imath}) - \tfrac{1}{2})\big) + 1$$

for all $\hat{\imath} \in \langle 0 : n \rangle$. Independently, we call Algorithm 4 on t against the reverse identity permutation id^R, and use Theorem 1 to process its output into a data structure that allows efficient queries of all suffix-prefix LCS scores $lcs\big(t \downarrow k, id^R \downarrow l\big)$ for all $k, l \in [0 : n]$. Finally, we obtain the solution to the longest C_4-avoiding subsequence problem as

$$\max_{\hat{\imath}} \Big(lcs\big(t \restriction (\hat{\imath} + \tfrac{1}{2}), id \restriction (t(\hat{\imath}) + \tfrac{1}{2})\big) + lcs\big(t \downarrow (\hat{\imath} + \tfrac{1}{2}), id^R \downarrow (t(\hat{\imath}) + \tfrac{1}{2})\big) \Big)$$

for all $\hat{\imath} \in \langle 0 : n \rangle$. The overall running time is dominated by the call to Algorithm 4, which runs in time $O(n \log^2 n)$.

6.4 Longest piecewise monotone subsequences

The classical LIS problem asks for the longest increasing (or, equivalently, decreasing) subsequence in a permutation string. A natural generalisation

is to ask for the longest subsequence that consists of a constant number of monotone pieces. In particular, given a permutation string a of length n, the *longest k-piece increasing subsequence* (respectively, *longest k-modal subsequence*) problem asks for the longest subsequence in a that is a concatenation of at most k sequences, all of which are increasing (respectively, alternate between increasing and decreasing). In the case of the longest k-modal subsequence problem, we assume without loss of generality that k is even. Both problems can be solved as an instance of the LCS problem, comparing the input permutation string a against string id^k, i.e. the concatenation of k copies of the identity permutation id (respectively, against string $(id\, id^R)^{k/2}$, i.e. the concatenation of k alternating copies of id and its reverse id^R). The resulting alignment dag is of size $n \times kn$, and contains kn match cells. Using standard sparse LCS algorithms [50, 10], such an instance of the LCS problem can be solved in time $O(nk \log n)$. Demange et al. [32] gave a similar algorithm for the longest k-modal subsequence problem, also running in time $O(nk \log n)$.

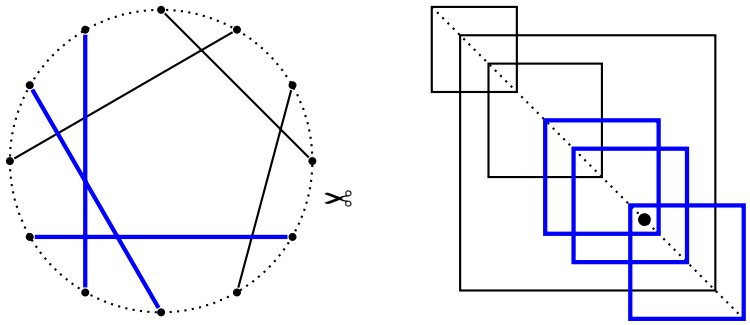
We now give a new algorithm for the longest k-piece increasing subsequence and the longest k-modal subsequence problems, improving on the above algorithms in running time, unless k is very small.

Our algorithm is as follows. In the case of the longest k-piece increasing subsequence problem, we run Algorithm 4, obtaining the implicit highest-score matrix $P_{id,a}$. Then, we extract the three-way slice $P^{\llcorner}_{id,a}$, and run on it the Corollary 1 algorithm $\log k$ times, obtaining the three-way slice $P^{\llcorner}_{id^k,a}$. In the case of the longest k-modal subsequence problem, we assume without loss of generality that k is even. We run Algorithm 4 twice, obtaining the implicit highest-score matrices $P_{id,a}$ and $P_{id^R,a}$, from which we obtain matrix $P_{id\, id^R,a}$ by Theorem 10. Then, we extract the three-way slice $P^{\llcorner}_{id\, id^R,a}$, and run on it the Corollary 1 algorithm $\log k - 1$ times, obtaining the three-way slice $P^{\llcorner}_{(id\, id^R)^{k/2},a}$. Finally, for both problems we use the resulting three-way slice to query the (global) LCS score. The described algorithm runs in time $O(n \log^2 n) + \log k \cdot O(n \log n) = O(n \log^2 n)$. This is an improvement on both the sparse LCS approach and the algorithm of [32], as long as $k \geq \log n$.

6.5 Maximum clique in a circle graph

A *circle graph* [35, 42] is defined as the intersection graph of a set of chords in a circle, i.e. the graph where each node represents a chord, and two nodes are adjacent, whenever the corresponding chords intersect. We consider the maximum clique problem on a circle graph. The problem is illustrated by Figure 6.2, where Subfigure 6.2a shows in blue a set of chords defining a circle graph, with one of the maximum cliques shown in bold.

The *interval model* of a circle graph is obtained by cutting the circle at an arbitrary point and laying it out on a line, so that the chords become



(a) The chord model (b) An interval model

Figure 6.2: A circle graph and its maximum clique

(closed) intervals. The original circle graph is isomorphic to the overlap graph of its interval model, i.e. the graph where each node represents an interval, and two nodes are adjacent, whenever the corresponding intervals intersect but do not contain one another. In Subfigure 6.2a, the cut point is shown by scissors. Subfigure 6.2b shows the corresponding interval model; the dotted diagonal line contains the intervals, each defined by the diagonal of blue a square. The squares corresponding to the maximum clique are shown in bold.

It has long been known that the maximum clique problem in a circle graph on n nodes is solvable in polynomial time [38]. A number of algorithms have been proposed for this problem [86, 48, 74, 9]; the problem has also been studied in the context of line arrangements in the hyperbolic plane [56, 34]. Given an interval model of a circle graph, the running time of the above algorithms is $O(n^2)$ in the worst case, i.e. when the input graph is dense. In [94, 96], we gave an algorithm running in time $O(n^{1.5})$.

We now give a new algorithm for the maximum clique problem in a circle graph, improving on existing algorithms in running time. The algorithm is based on the fast matrix distance multiplication procedure of Theorem 7.

Our algorithm takes as input the interval model of a circle graph G on n nodes. Without loss of generality, we may assume that the set of interval endpoints is $\langle 0 : 2n\rangle$. The interval model is represented by a permutation string a of size $2n$, where for each left (respectively, right) interval endpoint $\hat{\imath} \in \langle 0 : 2n\rangle$, $a(\hat{\imath})$ is the corresponding right (respectively, left) endpoint. Note that for all $\hat{\imath} < \hat{\jmath}$, an interval with left endpoint $\hat{\imath}$ does not contain an interval with left endpoint $\hat{\jmath}$, if and only if $a(\hat{\imath}) < a(\hat{\jmath})$. Various alternative representations of interval models (e.g. the ones used in [86, 9]) can be converted to this representation in linear time.

In the interval model, a clique corresponds to a set of pairwise intersecting intervals, none of which contains another interval from the set. Recall that intervals in the line satisfy the *Helly property*: if all intervals in a set

intersect pairwise, then they all intersect at a common point. In our context, we only need to consider integer indices as intersection points.

Consider a clique in G. Let $k \in [1 : 2n-1]$ be a common intersection point of the intervals representing the clique, which is guaranteed to exist by the Helly property. Since the intervals representing the clique cannot contain one another, the sequence of their right endpoints is an increasing subsequence of a. Let id be the identity permutation string of length $2n$. From the observations above, it follows that the clique corresponds to a common subsequence of a prefix $a \restriction k$ and a suffix $id \downharpoonright k$. Therefore, the maximum clique can be solved as an instance of the semi-local LCS problem.

Algorithm 5. *Maximum clique in a circle graph.*

Input: interval model of circle graph G, represented by permutation string a of size $2n$.

Output: maximum-size clique of G, represented by the set of (say) left endpoints of the corresponding intervals.

Description.

First phase. We run Algorithm 4 on the input permutation string a against the identity permutation string id, obtaining an implicit highest-score matrix with $4n$ core nonzeros. We then build the data structure of Theorem 1 for querying semi-local LCS scores of a against id.

Second phase. For each $k \in [1 : 2n-1]$, we query the LCS score of prefix $a \restriction k$ against suffix $id \downharpoonright k$. The maximum of the $2n$ returned values gives the size of the maximum clique in G, and the corresponding value k gives a common intersection point of the clique intervals.

Third phase. The intervals defining the maximum clique can now be obtained by running a standard LIS algorithm on string $(a \restriction k)|_{\Sigma(id \downharpoonright k)}$.

Cost analysis.

First phase. The running time of Algorithm 4 is $O(n \log^2 n)$.

Second phase. By Theorem 1, the combined running time of all the prefix-suffix queries is $O(n \log^2 n)$, if the queries are performed independently. This time can be reduced to $O(n)$ by observing that the queries can be performed as a single diagonal batch query.

Third phase. The LIS algorithm runs in time $O(n \log n)$.

Total. The overall running time is $O(n \log^2 n)$. □

Like many algorithmic problems, the problem of finding a maximum clique in a circle graph admits various parameterised versions. Some relevant parameters are:

- the size l of the maximum clique;

- the *thickness* d of the interval model, i.e. the maximum number of intervals containing a point, taken across all points in the line;
- the number e of graph edges.

For any interval model of a non-trivial circle graph, we have $l \leq d \leq n \leq e \leq n^2$. Notice that, given a permutation representing an interval model, its thickness can be found in time $O(n \log^2 n)$ by building a range tree on the corresponding set of planar points, and then performing $O(n)$ dominance counting queries.

Apostolico et al. [9] give algorithms for the parameterised version of the maximum clique problem in a circle graph, running in time $O(n \log n + e)$ and $O(n \log n + nl \log(n/l))$. They also describe an algorithm for the maximum independent set problem, parameterised by the interval model's thickness.

We now give a new algorithm for the maximum clique problem in a circle graph, parameterised by the thickness of the input interval model. Our algorithm improves on the parameterised algorithms of [9] for most values of the parameters. The algorithm is an extended version of Algorithm 5.

Algorithm 6. *Maximum clique in a circle graph, parameterised by thickness.*

Input: interval model of circle graph G, represented by string a of size $2n$.

Output: maximum-size clique of G, represented by the set of (say) left endpoints of the corresponding intervals.

Parameter: thickness d, $d \leq n$, of the input interval model.

Description.

First phase. We run Algorithm 4 on string $a \restriction (r+1)$ against string $id \downharpoonright rd$, independently for all $r \in [0 : 2n/d - 1]$. As will be shown in the algorithm's analysis, in each run we obtain an implicit highest-score matrix with at most $4d$ non-trivial core nonzeros. For every r, we then build the data structure of Theorem 1 for querying semi-local LCS scores of $a \restriction (r+1)$ against $id \downharpoonright rd$.

Second phase. For each $k \in [1 : 2n - 1]$, we query the LCS score of prefix $a \restriction k = \big(a \restriction (r+1)d\big) \restriction k$ against suffix $id \downharpoonright k = (id \downharpoonright rd) \downharpoonright (k - rd)$, where $r = \lfloor k/d \rfloor$. The maximum of the $2n$ returned values gives the size of the maximum clique in G, and the corresponding value k gives a common intersection point of the clique intervals.

Third phase. The intervals defining the maximum clique can now be obtained by running a standard LIS algorithm on string $(a \restriction k)|_{\Sigma(id \downharpoonright k)}$.

Cost analysis.

First phase. We have $a \restriction (r+1)d = (a \restriction rd)\big((a \downharpoonright rd) \restriction d\big)$. The alignment dag of $a \restriction rd$ against $id \downharpoonright rd$ contains at most d match cells, since every match corresponds to an interval containing point rd, and there can be at most d

such intervals by the definition of thickness. The alignment dag of $(a \lfloor rd) \rceil d$ against $id \lfloor rd$ also contains at most d match cells, since the length of the string $(a \lfloor rd) \rceil d$ is d. The alignment dag of $a \rceil (r+1)d$ against $id \lfloor rd$ is the composition of the above two alignment dags, and therefore contains at most $d + d = 2d$ matches. Therefore, the time for each run of Algorithm 4 is $O(d \log^2 d)$, and the overall running time of this phase is $O(n/d \cdot d \log^2 d) = O(n \log^2 d)$.

Second phase. By Theorem 1, the combined running time of all the prefix-suffix queries is $O(n \log^2 d)$, if the queries are performed independently. This time can be reduced to $O(n/d \cdot d) = O(n)$ by observing that the queries can be performed as a single diagonal batch query.

Third phase. The alignment dag of $a \rceil k$ against $id \lfloor k$ contains at most d matches, since every such match corresponds to an interval containing point k. Therefore, string $(a \rceil k)|_{\Sigma(id \lfloor k)}$ has length at most d. The LIS algorithm runs in time $O(d \log d)$.

Total. The resulting overall running time is $O(n \log^2 d)$. □

Algorithm 6 improves on the $O(n \log n + e)$ algorithm of [9], unless $e = o(n \log^2 d) = O(n \log^2 n)$. It also improves on the $O(n \log n + nl \log(n/l))$ algorithm of [9], unless $l = o\big(\frac{\log^2 d}{\log n}\big) = O(\log n)$.

6.6 Maximum common pattern between linear graphs

The concept of a *linear graph*, introduced by Davydov and Batzoglou [31], is similar to an interval model of a circle graph defined in Section 6.5. Fertin et al. [36] considered the problem of finding the maximum common pattern in a set of n linear graphs, each defined by at most m intervals. Common patterns are defined as ordered subsets of intervals that are isomorphic with respect to interval disjointness, containment and overlapping. These three interval properties are denoted respectively by symbols $<$, $\sqsubset$ and $\between$. The structure of the common pattern may be restricted by only considering patterns where the intervals must pairwise satisfy a prescribed subset of these properties. The resulting *maximum common S-structured pattern (S-MCSP)* problem is parameterised by the nonempty set $S \subseteq \{<, \sqsubset, \between\}$ of prescribed properties. For example, the $\{\between\}$-MCSP problem asks for the maximum commonly-structured subset of pairwise overlapping intervals; for $n = 1$ this is equivalent to finding the maximum clique of a circle graph, and for general n is equivalent to finding the minimum-sized clique among maximum cliques of the n input circle graphs. The $\{<, \sqsubset\}$-MCSP problem asks for the maximum commonly-structured subset of intervals, no two of which are overlapping; for $n = 1$ this is equivalent to finding the maximum independent set of a circle graph; however, for general n the maximum commonly-structured independent set of the n input circle graphs may be

significantly different from (and smaller than) each of the n individual maximum independent sets. The $\{<, \sqsubset, \between\}$-MCSP problem asks for the maximum commonly-structured subset of intervals without any a priori restriction on its structure.

Extending and generalising a number of previous results, paper [36] considers the S-MCSP problem for each of seven nonempty subsets of $\{<, \sqsubset, \between\}$. For some of these seven variants, the algorithms use as a subroutine the algorithm of [94, 96] for the maximum clique problem in a circle graph. By plugging in the more efficient Algorithm 5, we can obtain improved algorithms for those variants of the S-MCSP problem, where finding the maximum clique in a circle graph is a bottleneck.

In particular, the $\{\between\}$-MCSP problem is solved in [36] by finding the maximum clique independently for n circle graphs, each corresponding to one of the input linear graphs, in overall time $O(nm^{1.5})$. By plugging in Algorithm 5, the running time is improved to $O(nm \log^2 m)$.

The $\{<, \between\}$-MCSP problem is shown in [36] to be NP-hard, and to admit a polynomial-time $h(k)$-approximation, where $h(k) = \sum_{1 \le i \le k} 1/i$; for the rest of this section, k denotes the size of the solution. The approximation is obtained by finding the maximum clique for $nm \log m$ different circle graphs, in overall time $O(nm^{2.5} \log^2 m)$. By plugging in Algorithm 5, the running time of the approximation algorithm is improved to $O(nm^2 \log^4 m)$.

The $\{\sqsubset, \between\}$-MCSP problem is also shown in [36] to be NP-hard, and to admit a polynomial-time $k^{1/2}$-approximation. The approximation is obtained by combining exact solutions for the $\{\sqsubset\}$-MCSP and $\{\between\}$-MCSP problems on the same input sets. The exact solution for the $\{\between\}$-MCSP is the bottleneck; by plugging in the improved algorithm for this problem described above, the running time of the approximation algorithm for the $\{\sqsubset, \between\}$-MCSP problem is improved from $O(nm^{1.5})$ to $O(nm \log^2 m)$.

Finally, paper [36] argues that the $\{<, \sqsubset, \between\}$-MCSP problem is NP-hard, and gives several polynomial-time approximation algorithms. In particular, it gives an $O(k^{2/3})$-approximation algorithm running in time $O(nm^{1.5})$, and an $O\big((k \log k)^{1/2}\big)$-approximation algorithm running in time $O(nm^{2.5} \log m)$. Again, the exact solution for the $\{\between\}$-MCSP is the bottleneck; by plugging in the improved algorithm, the running times of the approximation algorithms improve respectively to $O(nm \log^2 m)$ and $O(nm^2 \log^4 m)$.

Chapter 7

Compressed string comparison

7.1 Grammar-compressed strings

Algorithms on compressed strings is an area of steadily increasing importance in algorithm theory. Early examples of such algorithms were given e.g. by Amir et al. [8] and by Rytter [87].

Let t be a string of length m (typically large). We call t a *grammar-compressed string* (*GC-string*), when it is represented implicitly by a special type of context-free grammar, called a *straight-line program (SLP)*. An SLP of length $\bar{m}$, $\bar{m} \leq m$, is a sequence of $\bar{m}$ *statements*. A statement numbered k, $1 \leq k \leq \bar{m}$, has one of the following forms:

$$t_k = \alpha \quad \text{where } \alpha \text{ is an alphabet character}$$
$$t_k = t_i t_j \quad \text{where } 1 \leq i, j < k$$

We identify every symbol t_r with the string it represents; in particular, we have $t = t_{\bar{m}}$. Note that, in general, the uncompressed text length m can be exponential in the GC-text length $\bar{m}$.

Grammar compression includes as a special case the well-known LZ78 and LZW compression schemes by Ziv, Lempel and Welch [102, 99]. Both these schemes can be expressed by an SLP that consists of three sections:

- in the first section, all statements are of the form $t_k = \alpha$;
- in the second section, all statements are of the form $t_k = t_i t_j$, where statement j is from the first section;
- in the third section, all statements are of the form $t_k = t_{k-1} t_j$, where statement j is from the second section.

It should also be noted that certain other compression methods, such as e.g. LZ77 [101] and run-length compression, do not fit directly into the grammar compression model.

Our goal is to design efficient algorithms on GC-strings. While we do not allow text decompression (since, in the worst case, this could be extremely inefficient), we will assume that standard arithmetic operations on integers up to m can be performed in constant time. This assumption is necessary, since most natural counting problems on GC-strings produce a numerical output that may be as high as $O(m)$. The same assumption on the computation model is made implicitly in previous works, e.g. by Cégielski et al. [22].

7.2 Three-way semi-local LCS on GC-strings

Recall that the LCS problem on a pair plain strings can be solved in time $O(\frac{mn}{\log(m+n)})$, assuming m and n are reasonably close [73, 28]. The LCS problem on a pair GC-strings has been considered by Lifshits and Lohrey [69], and proven to be NP-hard.

Let us consider first the LCS problem on a pair of strings, one of which is a GC-string and the other a plain string. Let string t (the *text string*) of length m be represented by an SLP of length $\bar{m}$, and let string p (the *pattern string*) of length n be represented explicitly. We aim at algorithms with running time and memory that are low-degree polynomial in $\bar{m}$, n, but are independent of m (which could be exponential in $\bar{m}$). This rules out any attempt at solving the semi-local LCS problem, since the resulting implicit highest-score matrix requires memory $O(m+n)$. However, we are still able to consider the three-way semi-local LCS problem, excluding the computation of LCS on substrings of t.

The described version of the LCS problem can be regarded as a special case of the edit distance problem between a context-free language given by a grammar of size $\bar{m}$, and a string of size n. For this more general problem, Myers [77] gave an algorithm running in time $O(\bar{m}n^3 + \bar{m}\log\bar{m}\cdot n^2)$. In [92], we gave an algorithm for the three-way semi-local LCS problem, running in time $O(\bar{m}n^{1.5})$. Lifshits [68] asked whether the LCS problem can be solved in time $O(\bar{m}n)$.

A new algorithm for the three-way semi-local LCS problem can be obtained by plugging into our previous algorithm [92] the fast matrix distance multiplication procedure of Theorem 7. The resulting algorithm improves on existing algorithms in running time, and approaches an answer to Lifshits' question within a logarithmic factor.

Algorithm 7. *Three-way semi-local LCS.*

Input: string t of length m, represented by an SLP of length $\bar{m}$; string p of length n, represented explicitly.

Output: three-way slice $P^{\llcorner}_{t,\smile p\sim}$.

Description. Recursion on the SLP representing t.

Recursion base. If $\bar{m} = m = 1$, then $P^{\llcorner}_{t,\smile p\sim} = P_{t,\smile p\sim}$ can be computed by a linear sweep of string p.

Recursive step. Let $t = t't''$ be the SLP statement defining string t. We call the algorithm recursively to obtain three-way slices $P^{\llcorner}_{t',\smile p\sim}$, $P^{\llcorner}_{t'',\smile p\sim}$, and then compute their composition $P^{\llcorner}_{t,\smile p\sim}$ by Corollary 1.

End of recursive step.

Cost analysis. By Corollary 1, each three-way slice composition runs in time $O(n \log n)$. There are $\bar{m}$ recursive steps in total, therefore the whole recursion runs in time $O(\bar{m}n \log n)$. □

Algorithm 7 provides, as a special case, an algorithm for the LCS problem between a GC-string and a plain string, running in time $O(\bar{m}n \log n)$; the LCS score can easily be queried from the algorithm's output by Theorem 8. This running time should be contrasted with standard uncompressed LCS algorithms, running in time $O\big(\frac{mn}{\log(m+n)}\big)$ [73, 28], and with the NP-hardness of the LCS problem on two GC-strings [69].

Hermelin et al. [46] gave a more detailed analysis of this problem's complexity, by considering the weighted alignment problem on a pair of GC-strings a, b of total compressed length $\bar{r} = \bar{m} + \bar{n}$, parameterised by the strings' total plain length $r = m + n$. They gave an algorithm running in time $O(\bar{r}^{1.34} r^{1.34})$ for general weights, and in time $O(\bar{r}^{1.4} r^{1.2})$ for rational weights.

In the case of rational weights, the parameterised running time of weighted GC-string alignment can be improved by the following straightforward algorithm. First, we uncompress one of the input strings — say, string b. Then, we run Algorithm 7 on the GC-string a against the plain version of string b. The resulting running time is $O(\bar{m}n \log n) = O(\bar{r}r \log r)$.

7.3 Subsequence recognition on GC-strings

The (global) subsequence recognition problem has been defined in Section 2.1; it is a simple special case of the (global) LCS problem. In Section 4.4, we considered local (minimal-window, fixed-window) subsequence recognition problems; they are special cases of both the semi-local LCS problem, and the approximate matching problem. In this section, we consider these problems in the context of a GC-compressed text.

Consider a text string t and a pattern string p. For brevity, a substring of t containing p as a subsequence will be called *p-matching*. A p-matching substring will be called *minimally p-matching*, if no its proper substring is p-matching.

Given a text string t and a pattern string p, the global subsequence recognition problem asks whether the whole text t is p-matching. Global subsequence recognition on a GC-text can be performed by the following simple folklore algorithm. For convenience, we generalise the problem's output: instead of a Boolean value, the algorithm will return an integer.

Algorithm 8. *Global subsequence recognition.*

Input: string t of length m, represented by an SLP of length $\bar{m}$; string p of length n, represented explicitly.

Output: an integer k, giving the length of the longest prefix of p that is a subsequence of t. String t contains p as a subsequence, iff $k = n$.

Description. Recursion on the SLP representing t.

Recursion base. If $\bar{m} = m = 1$, then the value $k \in \{0, 1\}$ is determined by a single character comparison.

Recursive step. Let $t = t't''$ be the SLP statement defining string t. Let k' be the length of the longest prefix of p that is a subsequence of t'. Let k'' be the length of the longest prefix of $P \lfloor k'$ that is a subsequence of t''. We call the algorithm recursively to obtain k' and k'', and then return $k = k' + k''$.

End of recursive step.

Cost analysis. The running time of the algorithm is $O(\bar{m}k)$. The proof is by induction. The running time of the recursive calls is respectively $O(\bar{m}k')$ and $O(\bar{m}k'')$. The overall running time of the algorithm is $O(\bar{m}k') + O(\bar{m}k'') + O(1) = O(\bar{m}k)$. In the worst case, this is $O(\bar{m}n)$. □

We now consider local subsequence recognition. The minimum-window subsequence recognition problem asks for the locations of all substrings of t that are minimally p-matching. Clearly, the output size for this *reporting version* of the problem may be exponential in $\bar{m}$; therefore, we will parameterise the running time by the output size. We will also consider the *counting version* of the problem, that only asks the overall number of minimally p-matching substrings.

Alternative approaches to local subsequence recognition are given by the fixed-window subsequence recognition problem, which asks for all the p-matching substrings of a fixed length w, and the bounded minimal-window subsequence recognition problem, which asks for all the minimally p-matching substrings below a fixed length w.

The minimal-window, fixed-window and bounded minimal-window subsequence recognition problems on a GC-text against an uncompressed pattern have been considered by Cégielski et al. [22]. They gave algorithms that run in time $O(\bar{m}n^2 \log n + output)$ for the reporting version, and $O(\bar{m}n^2 \log n)$ for the counting versions of the problem.

We now show how the three-way semi-local LCS algorithm of Section 7.2 can be used to provide more efficient local subsequence recognition. Although the definition of local subsequence recognition (Section 4.4) involves the highest-score matrix $H_{p,\smile t\sim}$, it will now be more convenient to switch to the "dual" matrix $H_{t,\smile p\sim}$ (more precisely, the three-way slice $H^{\llcorner}_{t,\smile p\sim}$, represented implicitly by the three-way slice $P^{\llcorner}_{t,\smile p\sim}$).

Algorithm 9. *Local subsequence recognition.*

Input: string t of length m, represented by an SLP of length $\bar{m}$; string p of length n, represented explicitly.

Output: positions, or count, of minimally p-matching substrings in t.

Description.

First phase. We build on Algorithm 7, extending every recursive step by the reporting of minimally p-matching substrings that span the boundary between symbols in the currently considered SLP statement.

Recursion base. If $\bar{m} = m = 1$, then the three-way slice $P^{\llcorner}_{t,\smile p\sim} = P_{t,\smile p\sim}$ can be computed by a linear sweep of string p. No substring of t can be p-matching (unless $n = 1$, in which case the whole problem is trivial).

Recursive step. Let $t = t't''$ be the SLP statement defining string t. We call the algorithm recursively to obtain three-way slices $P^{\llcorner}_{t',\smile p\sim}$, $P^{\llcorner}_{t'',\smile p\sim}$, and then compute both the three-way slice composition $P^{\llcorner}_{t,\smile p\sim}$ and the cross-way slice $P^{\urcorner}_{t,\smile p\sim}$ by Corollary 1.

A substring $t\langle i : k\rangle$ is p-matching, iff point $(-i, m+n-k)$ does not dominate any nonzeros in $P_{t,\smile p\sim}$. Let us call the substring $t\langle i : k\rangle$ *spanning*, if $i \in [0 : m'-1]$, $k \in [m'+1 : m]$, i.e. the substring consists of a non-empty suffix of t' and a non-empty prefix of t''. For a spanning substring, any nonzeros dominated by point $(-i, m+n-k)$ must belong to the cross-way slice

$$P^{\urcorner}_{t,\smile p\sim} = P_{t,\smile p\sim}\langle -m' : +\infty, -\infty : m'' + n\rangle$$

Recall that this slice has at most n nonzeros. Consider the antichain of all dominance-minimal nonzeros in $P^{\urcorner}_{t,\smile p\sim}$, and denote them by

$$(\hat{\imath}_0, \hat{k}_0) \ll (\hat{\imath}_1, \hat{k}_1) \ll \cdots \ll (\hat{\imath}_{s-1}, \hat{k}_{s-1})$$

where $s \leq n$. A spanning substring $t\langle i : k\rangle$ is minimally p-matching, iff $(-i, m+n-k)$ is one of the $s-1$ points in the antichain

$$(\hat{\imath}_0 + \tfrac{1}{2}, \hat{k}_1 - \tfrac{1}{2}) \ll (\hat{\imath}_1 + \tfrac{1}{2}, \hat{k}_2 - \tfrac{1}{2}) \ll \cdots \ll (\hat{\imath}_{s-2} + \tfrac{1}{2}, \hat{k}_{s-1} - \tfrac{1}{2})$$

Since not all these points may correspond to spanning substrings of t, the number of minimally p-matching spanning substrings is at most $s-1 \leq n-1$.

End of recursive step.

Second phase. For every SLP symbol, we now have the positions of its minimally p-matching spanning substrings, which are at most $n-1$. By another recursion on the structure of the SLP, it is now straightforward to obtain either the positions or the count of all minimally p-matching substrings in string t.

Cost analysis.

First phase. As in Algorithm 7, each three-way slice composition runs in time $O(n \log n)$. The antichain of dominance-minimal nonzeros in $P^{\urcorner}_{t,\backsim p\sim}$ can be found in time $O(n)$. Hence, the running time of a recursive step is $O(n \log n)$. There are $\bar{m}$ recursive steps in total, therefore the whole recursion runs in time $O(\bar{m}n \log n)$.

Second phase. Given the output of the first phase, the positions of all p-matching substrings in t can now be found in time $O(\bar{m}n + \mathit{output})$; the count of such substrings can be obtained in time $O(\bar{m}n)$.

Total. The overall running time is $O(\bar{m}n \log n + \mathit{output})$ for the reporting version, and $O(\bar{m}n \log n)$ for the counting version. □

An algorithm for the fixed-window subsequence recognition problem can be obtained from Algorithm 9 as follows. Substrings $t\langle i : k\rangle$ of length w correspond to points on the diagonal $(-i, m+n-k)$, $k-i = w$, of the highest-score matrix $H_{t,\backsim p\sim}$. Therefore, given the antichain of all $s \leq n$ dominance-minimal nonzeros in $P^{\urcorner}_{t,\backsim p\sim}$ computed by Algorithm 9, a spanning substring $t\langle i : k\rangle$, $k-i = w$, is p-matching, iff $-i$ belongs to the union of $s-1$ (possibly empty) intervals

$$\left[\hat{\imath}_0 + \tfrac{1}{2} : \hat{k}_1 - \tfrac{1}{2} - w\right] \cup \left[\hat{\imath}_1 + \tfrac{1}{2} : \hat{k}_2 - \tfrac{1}{2} - w\right] \cup \cdots \cup \left[\hat{\imath}_{s-2} + \tfrac{1}{2} : \hat{k}_{s-1} - \tfrac{1}{2} - w\right]$$

An interval $[i' : k']$ in the above expression is considered empty, if $i' > k'$. In every recursive step, the above union of intervals can be computed in time $O(n)$, and each element corresponding to a spanning substring of t can be reported in constant time.

An algorithm for the bounded minimal-window subsequence recognition problem can be obtained from Algorithm 9 by discarding in every recursive step the minimally p-matching substrings of length exceeding w.

The overall running time of both the above modifications of Algorithm 9 is still $O(\bar{m}n \log n + \mathit{output})$ for the reporting version, and $O(\bar{m}n \log n)$ for the counting version.

Chapter 8

Beyond semi-locality

8.1 Window-local LCS and alignment plots

So far, we have considered mostly global and semi-local string comparison. Our aim now is to approach local string comparison — the type of string comparison that is the most important for biological applications, but also the most difficult. In this chapter, we consider a version of local string comparison that is restricted to a fixed subset of *prescribed* substrings in one of the input strings, comparing them to all substrings in the other string.

An important special case is where all the prescribed substrings have equal length. Given a fixed parameter w, we call a substring of length w a *window* in the corresponding string.

String comparison in windows has a long history. One of its early instances is *dot plots* (also known as *diagonal plots* or *dot matrices*), introduced by Gibbs and McIntyre [41] and by Maizel and Lenk [71]. In addition to numerical scores, dot plots provide a convenient visualisation of string comparison. In the context of dot plots, processing a pair of windows is usually referred to as *filtering*. The standard filtering method compares every window of string a against every window of string b in terms of their *Hamming score*, i.e. the count of matching characters along the main diagonal of the windows' Cartesian product. A Hamming-filtered dot plot can be computed in time $O(mn)$ by the algorithm of [71, 75]. This algorithm has been implemented in several software packages (see e.g. [91, 84, 25]). A faster suffix-tree based algorithm has been proposed and implemented by Krumsiek et al. [61]. Enhancement of the dot plot approach have been proposed by Huang and Zhang [49] and by Putonti et al. [83].

Numerous other methods of local string comparison have been proposed. The *Smith–Waterman–Gotoh algorithm* [90, 44] allows one to obtain the highest-scoring pair across all substring pairs in the input strings. It can also be generalised to report all substring pairs scoring above a certain threshold. A significant drawback of the Smith–Waterman–Gotoh algorithm is that it

generally favours long, less precise substring alignments over short, more precise ones (as noted e.g. by Arslan et al. [13]). The quality of the alignment is also dependent on the scoring scheme: for example, for the LCS score, the algorithm only provides the trivial global comparison, so the method is generally only useful for weighted alignment scores with sufficiently high penalties (negative score weights) for gaps.

In contrast with the Smith–Waterman–Gotoh algorithm, the dot plot method gives the user more flexibility to select the biologically significant substring alignments, by providing all the local scores between fixed-size windows of the input strings. However, the Hamming scoring scheme used by this method within each window pair is less sensitive than even the LCS score, and especially than the weighted alignment score used by Smith–Waterman–Gotoh. This tradeoff motivates us to combine the best features of the two approaches in the following definition.

Definition 19. *Given strings a, b, the* window-window *(respectively,* window-substring*)* LCS problem *asks for the LCS score of for every window in a against every window (respectively, substring) in b.*

The window-window LCS problem can be seen as a refinement of the dot plot method and a complement to the Smith–Waterman–Gotoh method. As in the dot plot method, we compute all window-window comparison scores between the input strings. However, instead of the Hamming score, our method is based on the LCS score, and is therefore potentially more sensitive. The method can be further extended to use weighted alignment scores. By analogy with Hamming-filtered dot plots, we call the resulting matrix of window-window alignment scores an *alignment-filtered dot plot*, or simply an *alignment plot*. A similar method has been proposed recently for detection of alignment-conserved regions in DNA [80].

Note that the solution of the window-substring LCS problem can be represented in space $O(mn \log n)$ by giving the implicit three-way highest-score matrix for each window of a against b. An individual window-substring LCS score query can be performed on this data structure by Theorem 1 in time $O(\log^2 n)$. The same data structure can be used to obtain the explicit solution of the window-window LCS problem in time $O(mn)$ by performing a diagonal batch query on each of the implicit highest-score matrices. Thus, we can treat both the window-substring and the window-window LCS problems simultaneously.

A naive algorithm for the window-window LCS problem runs in time $O(mnw^2)$, and for the window-substring LCS problem runs in time $O(mn^3w)$. This can be improved upon by running the seaweed algorithm (Algorithm 1) independently for each window of string a against whole b. The resulting algorithm runs in time $O(mnw)$ for both problems. If window length w is sufficiently large, the running time can be improved slightly by using the micro-block seaweed algorithm (Algorithm 2).

We now give an algorithm for the window-window and window-substring LCS problems that provides a further substantial improvement on the above approach, and matches the asymptotic running time of both the Hamming-scored dot plot and the Smith–Waterman–Gotoh methods.

Algorithm 10. *Window-window and window-substring LCS.*

Input: strings a, b of length m, n, respectively; window length w.

Output: implicit highest-score matrix for every window of a against full b.

Description. For simplicity, we assume that m is a power of 2. We call a substring of the form $a\langle r \cdot 2^s : (r+1) \cdot 2^s \rangle$, $r, s \in [-\infty : +\infty]$, a *canonical substring*. In particular, both the whole string a, and every one of its individual characters, are canonical substrings. Every substring of a can be decomposed into a concatenation of $O(\log m)$ canonical substrings.

In the following, by processing a substring a' of a, we mean computing the implicit highest-score matrix $P_{a',\backsim b\sim}$.

First phase. We process all canonical substrings of a by recursion on m, with one-character substrings at the base of the recursion.

Recursion base. For $m = 1$, matrix $P_{a,\backsim b\sim}$ is computed by a linear sweep of string b.

Recursive step. For $m > 1$, we have $a = a'a''$, where substrings a', a'' are canonical. We call the first phase recursively on each of a', a'' against b, obtaining highest-score matrices $P_{a',\backsim b\sim}$, $P_{a'',\backsim b\sim}$. Then, we obtain the highest-score matrix $P_{a,\backsim b\sim}$ by Theorem 10.

End of recursive step.

Second phase. We represent each prescribed substring $a\langle i, j\rangle$ by a *prescribed point* $(i+\frac{1}{2}, j-\frac{1}{2}) \in \langle 0 : m\rangle^2$. We then partition the range $[0 : m]^2$ recursively into regular half-sized square blocks, as long as these blocks contain any prescribed points. Given indices $i_0, j_0 \in [0 : m]$ and block size h, a block is defined by the range $\langle i_0 - h : i_0\rangle \times \langle j_0 : j_0 + h\rangle$. The blocks with no prescribed points, as well as 1×1 blocks containing a prescribed point, are at the base of the recursion.

Throughout the recursion, we maintain the following invariant: either $j_0 - i_0 \leq 0$, or the substring $a\langle i_0 : j_0\rangle$ has been processed, and we have the implicit highest-score matrix $P_{a\langle i_0:j_0\rangle,\backsim b\sim}$.

At the beginning of a recursive call, we establish whether the current block contains any prescribed points. This check is easy to perform in constant time: the current block contains a positive number of prescribed points, iff $j_0 - i_0 < w < j_0 - i_0 + 2h$.

Recursion base. If the number of prescribed points in the current block is zero, we do nothing and terminate the current recursive call.

The current block now contains at least one prescribed point. If $h = 1$, then it contains exactly one prescribed point $(i_0 - \frac{1}{2}, j_0 + \frac{1}{2})$, which corresponds to substring $a\langle i_0 - 1 : j_0 + 1\rangle$. By the invariant, we already have the implicit highest-score matrix $P_{a\langle i_0:j_0\rangle,\backsim b\sim}$, Since the one-character substrings $a(i_0 - \frac{1}{2})$, $a(j_0 + \frac{1}{2})$ are canonical, we also already have the matrices $P_{a(i_0-\frac{1}{2}),\backsim b\sim}$, $P_{a(j_0+\frac{1}{2}),\backsim b\sim}$. We can now obtain the matrix

$$P_{a\langle i_0-1:j_0+1\rangle,\backsim b\sim} = P_{a(i_0-\frac{1}{2})\, a\langle i_0:j_0\rangle\, a(j_0+\frac{1}{2}),\backsim b\sim}$$

by two applications of Theorem 10, each having $m' = j_0 - i_0$, $m'' = 1$.

Recursive step. We partition the current block into four $\frac{h}{2} \times \frac{h}{2}$ regular subblocks. By the invariant, we already have the implicit highest-score matrix $P_{a\langle i_0:j_0\rangle,\backsim b\sim}$. Since the one-character substrings $a\langle i_0 - \frac{h}{2} : i_0\rangle$, $a\langle j_0 : j_0 + \frac{h}{2}\rangle$ are canonical, we also already have the matrices $P_{a\langle i_0-\frac{h}{2}:i_0\rangle,\backsim b\sim}$, $P_{a\langle j_0:j_0+\frac{h}{2}\rangle,\backsim b\sim}$. We can now obtain the matrices

$$\begin{aligned}
P_{a\langle i_0-\frac{h}{2}:j_0\rangle,\backsim b\sim} &= P_{a\langle i_0-\frac{h}{2}:i_0\rangle\, a\langle i_0:j_0\rangle,\backsim b\sim} \\
P_{a\langle i_0:j_0+\frac{h}{2}\rangle,\backsim b\sim} &= P_{a\langle i_0:j_0\rangle\, a\langle j_0:j_0+\frac{h}{2}\rangle,\backsim b\sim} \\
P_{a\langle i_0-\frac{h}{2}:j_0+\frac{h}{2}\rangle,\backsim b\sim} &= P_{a\langle i_0-\frac{h}{2}:j_0\rangle\, a\langle j_0:j_0+\frac{h}{2}\rangle,\backsim b\sim} = P_{a\langle i_0-\frac{h}{2}:i_0\rangle\, a\langle i_0:j_0+\frac{h}{2}\rangle,\backsim b\sim}
\end{aligned}$$

by three applications of Theorem 10, each having $m' = j_0 - i_0$, $m'' = h$.

We have now established the invariant for each of the four subblocks, and make a recursive call on each of them.

End of recursive step.

Cost analysis.

First phase. The running time is dominated by the bottom level of the recursion tree, and is therefore $m/2 \cdot O(n) = O(nm)$.

Second phase. The recursion tree is an unbalanced tree of degree 4 and of height $\log m$. Consider a level corresponding to block size h. Since all the prescribed points lie on a single diagonal, there can be at most $2m/h$ nodes at the current level, each corresponding to a block containing a positive number of prescribed points. The amount of work in every such node is $O(n \log h)$, hence the amount of work per level is $O(2m/h \cdot n \log h) = O(nm/h \cdot \log h)$. The running time for the whole recursion tree is dominated by the bottom level ($h = 1$), and is therefore $O(nm)$.

Total. The running time for both the first and the second phase, and therefore the overall running time, is $O(mn)$.

Memory. Storing the implicit highest-score matrices for all $O(m)$ canonical substrings requires memory $O(mn)$. However, only the matrices for canonical substrings of length at most w are actually required, and even these

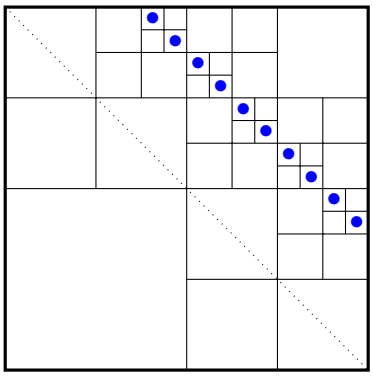


Figure 8.1: An execution of Algorithm 10

matrices need not be all stored simultaneously. By processing the canonical substrings incrementally within a sliding window of length w, and discarding the data after the window has passed, the memory cost can be reduced to $O(wn)$. □

Note that the asymptotic running time of the algorithm $O(mn)$ is independent of the window length w.

Figure 8.1 shows an execution of the second stage of Algorithm 10 on a string of length 16 with window size 7. The prescribed points are shown by blue bullets, and the resulting block partitioning by black lines.

8.2 Quasi-local LCS

We now consider an arbitrary set of prescribed substrings in string a, and denote their number by k, $m \leq k \leq m^2$.

Definition 20. *Given strings a, b, the* quasi-local LCS problem *asks for the LCS score of every prescribed substring in a against every substring in b.*

The quasi-local LCS problem includes as special cases semi-local, window-window, window-substring and fully-local LCS problems, as well as length-constrained local alignment considered by Arslan and Eğecioğlu [12]. Note that the solution of the quasi-local LCS problem can be represented in space $O(kn)$ by giving the implicit highest-score matrix for each prescribed substring of a against b. An individual quasi-local LCS score query can be performed on this data structure in time $O(\log^2 n)$.

A naive algorithm for the quasi-local LCS problem runs in time $O(mn^3k)$. This can be improved upon by running the seaweed algorithm (Algorithm 1) independently for each prescribed substring a against whole b. The resulting algorithm runs in time $O(mnk)$. If all the prescribed substrings are sufficiently long, the running time can be improved slightly by using the micro-block seaweed algorithm (Algorithm 2).

We now give an algorithm for the quasi-local LCS problem that provides a further improvement on the above approach.

Algorithm 11. *Quasi-local LCS.*

Input: strings a, b of length m, n, respectively; a set of k endpoint index pairs for the prescribed substrings in a.

Output: implicit highest-score matrix for every prescribed substring of a against full b.

Description. The algorithm is based on principles similar to the ones of Algorithm 10.

First phase. As in Algorithm 10.

Second phase. Similarly to Algorithm 10, we represent each prescribed substring by a prescribed point. In order to establish efficiently the number of prescribed points located in a given block, we build a range tree [16] on the set of prescribed points, allowing efficient orthogonal range counting queries.

We then proceed by recursion as in Algorithm 10. At the beginning of a recursive call, we query from the range tree the total number of prescribed points in the current block. Otherwise, the second phase is the same as in Algorithm 10.

Cost analysis.

First phase. As in Algorithm 10.

Second phase. The recursion tree is an unbalanced tree of degree 4 and of height $\log m$. Let us call a leaf of the recursion tree *useful*, if it corresponds to a 1×1 block containing a prescribed point, and *useless* if it corresponds to an empty block. Overall, the tree has k useful leaves. Every internal (i.e. non-leaf) node in the tree must have a useful leaf as a descendant, therefore there are at most k internal nodes per level, hence $O(k \log m)$ nodes overall. The amount of work per node in $O(n \log m)$, therefore the running time of the whole recursion tree is $O(k \log m \cdot n \log m) = O(nk \log^2 m)$.

For values of k close to the fully-local case $k = \binom{m}{2} = O(m^2)$, a sharper analysis is possible. In this case, the running time of the whole recursion tree is $O(nm^2)$.

Total. The overall running time is dominated by the second phase, and is therefore $O(nk \log^2 m)$. For values of k close to $\binom{m}{2}$, the running time is $O(nm^2)$. □

Note that in the fully-local case, the same asymptotic time can be obtained by running m independent instances of the seaweed algorithm (Algorithm 1), each instance computing the implicit highest-score matrices incrementally for $O(n)$ different substrings of a.

Figure 8.1 shows an execution of the second stage of Algorithm 11, using the same conventions as Figure 8.1.

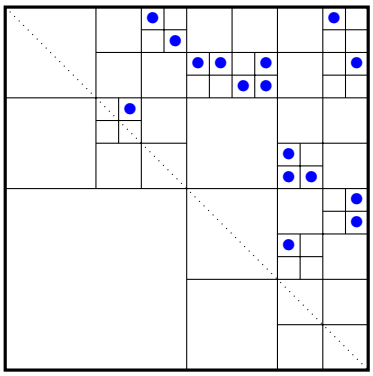


Figure 8.2: An execution of Algorithm 11

8.3 Sparse spliced alignment

Assembling a gene from candidate exons is an important problem in computational biology. Several alternative approaches to this problem have been developed over time. One of the most successful approaches is *spliced alignment* by Gelfand et al. [39] (see also [45]), which scores different candidate exon chains within a DNA sequence by comparing them to a known related gene sequence. In this method, the two sequences are modelled respectively by strings a, b of lengths m, n; we assume that $m = \Theta(n)$. A subset of substrings in string a are marked as candidate exons. The comparison between sequences is made by string alignment. The algorithm for spliced alignment given in [39] runs in time $O(n^3)$.

In general, the number of candidate exons k may be as high as $O(n^2)$. The method of *sparse spliced alignment* makes a realistic assumption that, prior to the assembly, the set of candidate exons undergoes some filtering, after which only a small fraction of candidate exons remains. Kent et al. [57] give an algorithm for sparse spliced alignment that, in the special case $k = O(n)$, runs in time $O(n^{2.5})$. For higher values of k, the algorithm provides a smooth transition in running time to the dense case $k = O(n^2)$, where its running time $O(n^3)$ is asymptotically equal to the algorithm of [39].

We now consider the problem of sparse spliced alignment. We keep the notation and terminology of the previous sections; in particular, candidate exons are represented by prescribed substrings of string a. We say that substring $a\langle i' : j' \rangle$ *precedes* substring $a\langle i'' : j'' \rangle$, if $j' < i''$. A *chain* of substrings is a chain in the partial order of substring precedence. We identify every chain with the string obtained by concatenating all its component substrings in the order of precedence.

Our sparse spliced alignment algorithm is based on the efficient method of quasi-local string comparison developed in Section 8.2. This improves the

running time of the bottleneck procedure from [57]. The algorithm also uses a generalisation of the standard network alignment method, equivalent to the one used by [57]. For simplicity, we describe our algorithm under LCS score; using the technique of Section 2.4, the algorithm can be generalised to an arbitrary rational-weighted score or edit distance metric.

Algorithm 12. *Sparse spliced alignment.*

Input: strings a, b of length m, n, respectively, where $m = \Theta(n)$; a set of k endpoint index pairs for the prescribed substrings in a.

Output: the chain of prescribed substrings in a, giving the highest LCS score against string b.

Description. The algorithm runs in two phases.

First phase. By running Algorithm 11, we compute the implicit highest-score matrix for every prescribed substring of a against b.

Second phase. We represent the problem by a *dag* (directed acyclic graph) on the set of nodes u_i, where $i \in [0 : m]$. For each prescribed substring $a\langle i : j\rangle$, the dag contains the edge $u_{i-1} \to u_j$. Overall, the dag contains $k = O(n)$ edges.

The problem can now be solved by dynamic programming on the representing dag as follows. Let $s(i, j)$ denote the highest LCS score for a chain of prescribed substrings in prefix string $a \restriction i$ against prefix string $b \restriction j$. With each node u_i, we associate the integer vector s_i, where $s_i(j) = s(i, j)$. The nodes are processed in increasing order of their indices. For the node u_0, vector s_0 is initialised by all zeros. For a node u_j, we consider every edge $u_{i-1} \to u_j$, and compute the highest-score matrix-vector product between vector s_{i-1} and the highest-score matrix $H_{a\langle i:j\rangle,\backsim b\sim}$ by the algorithm of Theorem 5. Vector s_j is now obtained by taking the elementwise maximum between vector s_{j-1} and all the above highest-score matrix-vector products.

The solution score is given by the value $s_m(n) = s(m, n)$. The solution chain of prescribed substrings can now be obtained by tracing the dynamic programming sequence backwards from node u_m to node u_0.

Cost analysis.

First phase. Algorithm 11 runs in time $O(nk \log^2 n)$.

Second phase. For each of the k edges in the representing dag, the algorithm of Theorem 5 runs in time $O(n \log n)$. Therefore, the total running time of this phase is $k \cdot O(n \log n) = O(nk \log n)$.

Total. The overall running time of the algorithm is dominated by the first phase, and is therefore $O(nk \log^2 n)$. □

Similarly to Algorithm 11, a sharper analysis for $k \approx \binom{m}{2}$ leads to a smooth transition to the running time $O(n^3)$ in the dense case $k = \binom{m}{2}$,

which is asymptotically equal to the running time of the dense spliced algorithm of [39].

Chapter 9

Conclusions

We have surveyed a number of existing and new algorithmic techniques and applications related to semi-local string comparison. Our approach unifies a substantial number of previously unrelated problems and techniques, and in many cases allows us to match or improve existing algorithms. It is likely that further development of this approach will give it even more scope and power.

A number of questions related to the semi-local string comparison framework remain open. In particular, it is not yet clear whether the framework can be extended to arbitrary real costs, or to sequence alignment with non-linear gap penalties.

In summary, semi-local string comparison turns out to be a useful algorithmic plug-in, which unifies, and often improves on, a number of previous approaches to various substring- and subsequence-related problems.

Chapter 10

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Bibliography

[1] A. Aggarwal, M. M. Klawe, S. Moran, P. Shor, and R. Wilber. Geometric applications of a matrix-searching algorithm. *Algorithmica*, 2(1):195–208, 1987.

[2] A. V. Aho, J. E. Hopcroft, and J. D. Ullman. *The Design and Analysis of Computer Algorithms*. Addison-Wesley, 1976.

[3] A. V. Aho, D. S.Hirschberg, and J. D. Ullman. Bounds on the complexity of the longest common subsequence problem. *Journal of the ACM*, 23:1–12, 1976.

[4] M. H. Albert, R. E. L. Aldred, M. D. Atkinson, H. P. van Ditmarsch, B. D. Handley, C. C. Handley, and J. Opatrny. Longest subsequences in permutations. *Australasian Journal of Combinatorics*, 28:225–238, 2003.

[5] M. H. Albert, M. D. Atkinson, D. Nussbaum, J.-R. Sack, and N. Santoro. On the longest increasing subsequence of a circular list. *Information Processing Letters*, 101:55–59, 2007.

[6] M. H. Albert, A. Golynski, A. M. Hamel, A. López-Ortiz, S. S. Rao, and M. A. Safari. Longest increasing subsequences in sliding windows. *Theoretical Computer Science*, 321:405–414, 2004.

[7] C. E. R. Alves, E. N. Cáceres, and S. W. Song. An all-substrings common subsequence algorithm. *Discrete Applied Mathematics*, 156(7):1025–1035, 2008.

[8] A. Amir, G. Benson, and M. Farach. Let sleeping files lie: Pattern matching in Z-compressed files. *Journal of Computer and System Sciences*, 52(2):299–307, 1996.

[9] A. Apostolico, M. J. Atallah, and S. E. Hambrusch. New clique and independent set algorithms for circle graphs. *Discrete Applied Mathematics*, 36:1–24, 1992.

[10] A. Apostolico and C. Guerra. The longest common subsequence problem revisited. *Algorithmica*, 2(1):315–336, 1987.

[11] V. L. Arlazarov, E. A. Dinic, M. A. Kronrod, and I. A. Faradzev. On economical construction of the transitive closure of an oriented graph. *Soviet Mathematical Doklady*, 11:1209–1210, 1970.

[12] A. N. Arslan and Ö. Eğecioğlu. Approximation algorithms for local alignment with length constraints. *International Journal of Foundations of Computer Science*, 13(5):751–767, 2002.

[13] A. N. Arslan, Ö. Eğecioğlu, and P. A. Pevzner. A new approach to sequence comparison: Normalized sequence alignment. *Bioinformatics*, 17(4):327–337, 2001.

[14] G. Benson. A space efficient algorithm for finding the best nonoverlapping alignment score. *Theoretical Computer Science*, 145:357–369, 1995.

[15] G. Benson. Tandem cyclic alignment. *Discrete Applied Mathematics*, 146(2):124–133, 2005.

[16] J. L. Bentley. Multidimensional divide-and-conquer. *Communications of the ACM*, 23(4):214–229, 1980.

[17] L. Bergroth, H. Hakonen, and T. Raita. A survey of longest common subsequence algorithms. In *Proceedings of the 7th SPIRE*, pages 39–48, 2000.

[18] P. Bille and I. L. Gørtz. Matching subsequences in trees. *Jounal of Discrete Algorithms*. To appear.

[19] H. Bunke and U. Bühler. Applications of approximate string matching to 2D shape recognition. *Pattern Recognition*, 26(12):1797–1812, 1993.

[20] R. E. Burkard, B. Klinz, and R. Rudolf. Perspectives of Monge properties in optimization. *Discrete Applied Mathematics*, 70(2):95–161, 1996.

[21] S. Cabello and E. W. Chambers. Multiple-source shortest paths in a genus g graph. In *Proceedings of the 18th ACM-SIAM SODA*, pages 89–97, 2007.

[22] P. Cégielski, I. Guessarian, Y. Lifshits, and Y. Matiyasevich. Window subsequence problems for compressed texts. In *Proceedings of CSR*, volume 3967 of *Lecture Notes in Computer Science*, pages 127–136, 2006.

[23] P. Cégielski, I. Guessarian, and Y. Matiyasevich. Multiple serial episodes matching. *Information Processing Letters*, 98(6):211–218, 2006.

[24] E. Chen, L. Yang, and H. Yuan. Longest increasing subsequences in windows based on canonical antichain partition. *Theoretical Computer Science*, 378(3):223–236, 2007.

[25] CLC bio. *CLC Protein Workbench: User Manual*, 2006.

[26] G. Cormode and S. Muthukrishnan. The string edit distance matching problem with moves. *ACM Transactions on Algorithms*, 3(1), 2007.

[27] M. Crochemore, G. M. Landau, B. Schieber, and M. Ziv-Ukelson. Reuse dynamic programming for sequence alignment: An algorithmic toolkit. In *String Algorithmics*, volume 2 of *Texts in Algorithmics*. King's College Publications, 2004.

[28] M. Crochemore, G. M. Landau, and M. Ziv-Ukelson. A subquadratic sequence alignment algorithm for unrestricted score matrices. *SIAM Journal on Computing*, 32(6):1654–1673, 2003.

[29] M. Crochemore and W. Rytter. *Text Algorithms*. Oxford University Press, 1994.

[30] G. Das, R. Fleischer, L. Gasieniec, D. Gunopulos, and J. Kärkkäinen. Episode matching. In *Proceedings of CPM*, volume 1264 of *Lecture Notes in Computer Science*, pages 12–27, 1997.

[31] E. Davydov and S. Batzoglou. A computational model for RNA multiple structural alignment. *Theoretical Computer Science*, 368(3):205–216, 2006.

[32] M. Demange, T. Ekim, and D. de Werra. A tutorial on the use of graph coloring for some problems in robotics. *European Journal of Operational Research*, 192(1):41–55, 2009.

[33] S. Deorowicz. An algorithm for solving the longest increasing circular subsequence problem. *Information Processing Letters*. To appear.

[34] A. Dress, J. H. Koolena, and V. Moulton. On line arrangements in the hyperbolic plane. *European Journal of Combinatorics*, 23(5):549–557, 2002.

[35] S. Even and A. Itai. Queues, stacks and graphs. In *Theory of Machines and Computations*, pages 71–86. Academic Press, 1971.

[36] G. Fertin, D. Hermelin, R. Rizzi, and S. Vialette. Common structured patterns in linear graphs: Approximation and combinatorics. In *Proceedings of CPM*, volume 4580 of *Lecture Notes in Computer Science*, pages 241–252, 2007.

[37] V. A. Fischetti, G. M. Landau, P. H. Sellers, and J. P. Schmidt. Identifying periodic occurrences of a template with applications to protein structure. *Information Processing Letters*, 45(1):11–18, 1993.

[38] F. Gavril. Algorithms for a maximum clique and a maximum independent set of a circle graph. *Networks*, 3:261–273, 1973.

[39] M. S. Gelfand, A. A. Mironov, and P. A. Pevzner. Gene recognition via spliced sequence alignment. *Proceedings of the National Academy of Sciences of the USA*, 93(17):9061–9066, 1996.

[40] R. Giancarlo. Dynamic programming: Special cases. In A. Apostolico and Z. Galil, editors, *Pattern Matching Algorithms*, chapter 7, pages 201–236. Oxford University Press, 1997.

[41] A. J. Gibbs and G. A. McIntyre. The diagram, a method for comparing sequences. *European Journal of Biochemistry*, 16(1):1–11, 1970.

[42] M. C. Golumbic. *Algorithmic Graph Theory and Perfect Graphs*. Number 57 in Annals of Discrete Mathematics. Elsevier, second edition, 2004.

[43] M. Gondran and M. Minoux. *Graphs, Dioids and Semirings*. Springer, 2008.

[44] O. Gotoh. An improved algorithm for matching biological sequences. *Journal of Molecular Biology*, 162(3):705–708, 1982.

[45] D. Gusfield. *Algorithms on Strings, Trees, and Sequences: Computer Science and Computational Biology*. Cambridge University Press, 1997.

[46] D. Hermelin, G. M. Landau, S. Landau, and O. Weimann. A unified algorithm for accelerating edit-distance computation via text-compression. In *Proceedings of the 26th STACS*, pages 529–540, 2009.

[47] D. S. Hirschberg. A linear space algorithm for computing maximal common subsequences. *Communications of the ACM*, 18(6):341–343, 1975.

[48] W.-L. Hsu. Maximum weight clique algorithms for circular-arc graphs and circle graphs. *SIAM Journal on Computing*, 14(1):224–231, 1985.

[49] Yue Huang and Ling Zhang. Rapid and sensitive dot-matrix methods for genome analysis. *Bioinformatics*, 20(4):460–466, 2004.

[50] J. W. Hunt and T. G. Szymanski. A fast algorithm for computing longest common subsequences. *Communications of the ACM*, 20(5):350–353, 1977.

[51] Y. Ishida, S. Inenaga, A. Shinohara, and M. Takeda. Fully incremental LCS computation. In *Proceedings of FCT*, volume 3623 of *Lecture Notes in Computer Science*, pages 563–574, 2005.

[52] B. N. Jackson and S. Aluru. Pairwise sequence alignment. In *Handbook of Computational Molecular Biology*, Chapman and Hall/CRC Computer and Information Science Series, chapter 1, pages 1–1 – 1–31. Chapman and Hall/CRC, 2006.

[53] J. JáJá, C. Mortensen, and Q. Shi. Space-efficient and fast algorithms for multidimensional dominance reporting and counting. In *Proceedings of the 15th ISAAC*, volume 3341 of *Lecture Notes in Computer Science*, pages 558–568, 2004.

[54] N. C. Jones and P. A. Pevzner. *An introduction to bioinformatics algorithms*. Computational Molecular Biology. The MIT Press, 2004.

[55] S. K. Kannan and E. W. Myers. An algorithm for locating non-overlapping regions of maximum alignment score. *SIAM Journal on Computing*, 25(3):648–662, 1996.

[56] A. Karzanov. Combinatorial methods to solve cut-determined multiflow problems. In *Combinatorial Methods for Flow Problems*, volume 3, pages 6–69. VNIISI, 1979. In Russian.

[57] C. Kent, G. M. Landau, and M. Ziv-Ukelson. On the complexity of sparse exon assembly. *Journal of Computational Biology*, 13(5):1013–1027, 2006.

[58] S.-R. Kim and K. Park. A dynamic edit distance table. *Journal of Discrete Algorithms*, 2(2):303–312, 2004.

[59] P. N. Klein. Multiple-source shortest paths in planar graphs. In *Proceedings of the 16th ACM-SIAM SODA*, pages 146–155, 2005.

[60] A. Kosowski. An efficient algorithm for the longest tandem scattered subsequence problem. In *Proceedings of the 11th SPIRE*, volume 3246 of *Lecture Notes in Computer Science*, pages 93–100, 2004.

[61] J. Krumsiek, R. Arnold, and T. Rattei. Gepard: A rapid and sensitive tool for creating dotplots on genome scale. *Bioinformatics*, 23(8):1026–1028, 2007.

[62] G. Landau. Can DIST tables be merged in linear time? An open problem. In *Proceedings of the Prague Stringology Conference*, page 1. Czech Technical University in Prague, 2006.

[63] G. M. Landau, E. Myers, and M. Ziv-Ukelson. Two algorithms for LCS consecutive suffix alignment. *Journal of Computer and System Sciences*, 73(7):1095–1117, 2007.

[64] G. M. Landau, E. W. Myers, and J. P. Schmidt. Incremental string comparison. *SIAM Journal on Computing*, 27(2):557–582, 1998.

[65] G. M. Landau and U. Vishkin. Fast parallel and serial approximate string matching. *Journal of Algorithms*, 10(2):157–169, 1989.

[66] G. M. Landau and M. Ziv-Ukelson. On the common substring alignment problem. *Journal of Algorithms*, 41(2):338–359, 2001.

[67] V. Levenshtein. Binary codes capable of correcting spurious insertions and deletions of ones. *Problems of Information Transmission*, 1:8–17, 1965.

[68] Y. Lifshits. Processing compressed texts: A tractability border. In *Proceedings of CPM*, volume 4580 of *Lecture Notes in Computer Science*, pages 228–240, 2007.

[69] Y. Lifshits and M. Lohrey. Querying and embedding compressed texts. In *Proceedings of MFCS*, volume 4162 of *Lecture Notes in Computer Science*, pages 681–692, 2006.

[70] M. Maes. On a cyclic string-to-string correction problem. *Information Processing Letters*, 35:73–78, 1990.

[71] J. V. Maizel and R. P. Lenk. Enhanced graphic matrix analysis of nucleic acid and protein sequences. *Proceedings of the National Academy of Sciences of the USA*, 78(12):7665–7669, 1981.

[72] A. Marzal and S. Barrachina. Speeding up the computation of the edit distance for cyclic strings. In *Proceedings of the 15th ICPR, part 2*, pages 891–894, 2000.

[73] W. J. Masek and M. S. Paterson. A faster algorithm computing string edit distances. *Journal of Computer and System Sciences*, 20:18–31, 1980.

[74] S. Masuda, K. Nakajima, T. Kashiwabara, and T. Fujisawa. Efficient algorithms for finding maximum cliques of an overlap graph. *Networks*, 20:157–171, 1990.

[75] C. Mueller, M. M. Dalkilic, and A. Lumsdaine. High-performance direct pairwise comparison of large genomic sequences. *IEEE Transactions on Parallel and Distributed Systems*, 17(8):764–772, 2006.

[76] E. W. Myers and W. Miller. Approximate matching of regular expressions. *Bulletin of Mathematical Biology*, 51(1):5–37, 1989.

[77] G. Myers. Approximately matching context-free languages. *Information Processing Letters*, 54:85–92, 1995.

[78] G. Navarro. A guided tour to approximate string matching. *ACM Computing Surveys*, 33(1):31–88, 2001.

[79] S. B. Needleman and C. D. Wunsch. A general method applicable to the search for similarities in the amino acid sequence of two proteins. *Journal of Molecular Biology*, 48(3):443–453, 1970.

[80] S. Ott, S. Gunawardana, M. Downey, and G. Koentges. Loss-free identification of alignment-conserved CRMs. In preparation.

[81] M. S. Paterson and V. Dančík. Longest common subsequences. In *Proceedings of MFCS*, volume 841 of *Lecture Notes In Computer Science*, pages 127–142, 1994.

[82] F. P. Preparata and M. I. Shamos. *Computational Geometry: An Introduction*. Texts and Monographs in Computer Science. Springer, 1985.

[83] C. Putonti, Yi Luo, C. Katili, S. Chumakov, G. E. Fox, D. Graur, and Y. Fofanov. A computational tool for the genomic identification of regions of unusual compositional properties and its utilization in the detection of horizontally transferred sequences. *Molecular Biology and Evolution*, 23(10):1863–1868, 2006.

[84] P. Rice, I. Longden, and A. Bleasby. EMBOSS: The European molecular biology open software suite. *Trends in Genetics*, 16(6):276–277, 2000.

[85] G. Rote. Path problems in graphs. *Computing Supplementum*, 7:155–189, 1990.

[86] D. Rotem and J. Urrutia. Finding maximum cliques in circle graphs. *Networks*, 11:269–278, 1981.

[87] W. Rytter. Algorithms on compressed strings and arrays. In *Proceeedings of SOFSEM*, volume 1725 of *Lecture notes in Computer Science*, pages 48–65, 1999.

[88] J. P. Schmidt. All highest scoring paths in weighted grid graphs and their application to finding all approximate repeats in strings. *SIAM Journal on Computing*, 27(4):972–992, 1998.

[89] P. H. Sellers. The theory and computation of evolutionary distances: Pattern recognition. *Journal of Algorithms*, 1(4):359–373, 1980.

[90] T. F. Smith and M. S. Waterman. Identification of common molecular subsequences. *Journal of Molecular Biology*, 147(1):195–197, 1981.

[91] E. L. L. Sonnhammer and R. Durbin. A dot-matrix program with dynamic threshold control suited for genomic DNA and protein sequence analysis. *Gene*, 167(1–2):GC1–GC10, 1995.

[92] A. Tiskin. Faster subsequence recognition in compressed strings. *Journal of Mathematical Sciences*. To appear.

[93] A. Tiskin. All semi-local longest common subsequences in subquadratic time. In *Proceedings of CSR*, volume 3967 of *Lecture Notes in Computer Science*, pages 352–363, 2006.

[94] A. Tiskin. Longest common subsequences in permutations and maximum cliques in circle graphs. In *Proceedings of CPM*, volume 4009 of *Lecture Notes in Computer Science*, pages 271–282, 2006.

[95] A. Tiskin. Semi-local longest common subsequences in subquadratic time. *Journal of Discrete Algorithms*, 6(4):570–581, 2008.

[96] A. Tiskin. Semi-local string comparison: Algorithmic techniques and applications. *Mathematics in Computer Science*, 1(4):571–603, 2008.

[97] R. A. Wagner and M. J. Fischer. The string-to-string correction problem. *Journal of the ACM*, 21(1):168–173, 1974.

[98] B. W. Watson and G. Zwaan. A taxonomy of sublinear multiple keyword pattern matching algorithms. *Science of Computer Programming*, 27(2):85–118, 1996.

[99] T. A. Welch. A technique for high-performance data compression. *Computer*, 17(6):8–19, 1984.

[100] S. Wu, U. Manber, and G. Myers. A subquadratic algorithm for approximate limited expression matching. *Algorithmica*, 15:50–67, 1996.

[101] G. Ziv and A. Lempel. A universal algorithm for sequential data compression. *IEEE Transactions on Information Theory*, 23:337–343, 1977.

[102] G. Ziv and A. Lempel. Compression of individual sequences via variable-rate coding. *IEEE Transactions on Information Theory*, 24:530–536, 1978.

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