Finding Diverse Strings and Longest Common Subsequences in a Graph

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Seminar for the course of Bioinformatics

Structure of the Presentation

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- Exact Algorithms for Bounded Number of Diverse Strings
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Longest Common Subsequence (LCS)

Definition

Given a set of m strings $S = \{S_1, S_2, \dots, S_m\}$, a **common subsequence** (CS) is a sequence that appears in all m strings. A **longest common subsequence** LCS is a common subsequence of maximum length. We denote the set of all LCSs of S as LCS(S).

Goal

The goal is to find a diverse set of solutions to the LCS problem under the Hamming distance.

Definition

Given two strings $X, Y \in \Sigma^r$, the **Hamming distance** between X and Y, denoted with $d_H(X, Y)$, is the number of positions at which the corresponding symbols differ.

A simple example

Table: Longest common subsequences of two input strings X = ABABCDDEE and Y = ABCBAEEDD. over $\Sigma = \{A, B, C, D, E\}$

E, A, B, C, D, E,
 AA, AB, AC, AD, AE, BA, ..., CD, CE, DD, EE,
 ABA, ABB, ABC, ABD, ..., CEE,
 ABAD, ABAE, ABBD, ..., BCEE,
 ABADD, ABAAE, ABBDD,
 ABBEE, ABCDD, ABCEE

Efficient methods for finding a diverse set of solutions

More formally, let's consider the following two diversity measures for a multiset $\mathcal{X} = \{X_1, X_2, \dots, X_K\} \subseteq \Sigma^r$ of solutions, allowing repetitions:

$$D_{d_H}^{\text{sum}}(\mathcal{X}) = \sum_{1 \le i < i \le K} d_H(X_i, X_j)$$
 Max-Sum Diversity (1)

$$D_{d_H}^{\min}(\mathcal{X}) = \min_{i < j} d_H(X_i, X_j) \qquad \text{Max-Min Diversity} \qquad (2)$$

Notation

A subset $\mathcal{X} \subseteq \Sigma^r$ is Δ -diverse w.r.t. $D_{d_H}^{\tau}$ if $D_{d_H}^{\tau}(\mathcal{X}) \geq \Delta$ for some $\Delta \geq 0$.

Where for $\tau \in \{sum, min\}$, $D_{d_H}^{\tau}$ denotes one of the two diversity measures.

Two problems

Problem 1: DIVERSE LCSs WITH DIVERSITY MEASURE $D_{d_H}^{ au}$

Input: A set $S = \{S_1, S_2, \dots, S_m\}$ of $m \ge 2$ strings over Σ , an integer $K \ge 1$ and $\Delta \ge 0$.

Question: Is there some set $\mathcal{X} \subseteq LCS(S)$ such that $\mathcal{X} = K$ and

 $D_{d_H}^{\tau}(\mathcal{X}) \geq \Delta$?

Problem 2: DIVERSE STRING SET

Input: $K, r, \Delta \in \mathbb{Z}$ and a Σ -DAG G for a set $L(G) \subseteq \Sigma^r$ of strings. Question: Decide if there exists some subset $\mathcal{X} \subseteq L(G)$ such that $|\mathcal{X}| = K$ and $D^T(\mathcal{X}) > \Delta$

and $D_{d_H}^{\tau}(\mathcal{X}) \geq \Delta$.

Σ -Labeled Directed Acyclic Graphs (Σ -DAGs)

Definitions

- Alphabet (Σ) : Set of symbols.
- String Set (Language): $L = \{X_1, X_2, \dots, X_n\} \subseteq \Sigma^*$, with:
 - ▶ Total Length: $||L|| = \sum_{X \in L} |X|$
 - Max Length: $\max_{L \in \mathcal{L}} |X| = \max_{X \in \mathcal{L}} |X|$
- **r-String**: Any string X where |X| = r

Σ-DAG Structure

A graph G = (V, E, s, t) with:

- V: vertices, E: labeled edges (v, c, w) with $c \in \Sigma$
- Source s and Sink t such that paths exist from s to all vertices
- **Size**: size(*G*), the number of its labeled edges

Σ -Labeled Directed Acyclic Graphs (Σ -DAGs)

Any path $P = (e_1, e_2, \dots, e_n)$ of outgoing edges *spells out* a string $str(P) = c_1 c_2 \dots c_n \in \Sigma^n$ where c_i is the label of edge e_i .

Language Representation

A Σ -DAG represents $L(G) \subset \Sigma^*$: all strings spelled from paths $s \to t$. Equivalent to an NFA over Σ with initial s, final t, and no ϵ -edges.

Remarks

- For any set L of strings, a Σ -DAG G exists s.t. L(G) = L and size $(G) \leq ||L||$. Construction time: $O(||L|| \log |\Sigma|)$.
- If G represents a set L of r-strings ($L \subseteq \Sigma^r, r \ge 0$), all paths $s \to v$ have the same length $d \le r$.

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Σ -DAGs for LCSs and Diverse String Sets

Lemma (Σ -DAG for LCSs)

For any constant $m \ge 1$ and set $S = \{S_1, \dots, S_m\} \subseteq \Sigma^*$ of m strings, there exists a Σ -DAG G of polynomial size in $\ell := \text{maxlen}(S)$ such that L(G) = LCS(S) and can be computed in polynomial time ℓ

Consequence of the Lemma

- If MAX-MIN (or MAX-SUM) DIVERSE STRING SET solvable in $f(M, K, r, \Delta)$,
- Then MAX-MIN (or MAX-SUM) DIVERSE LCSs on $S \subseteq \Sigma^r$ solvable in $O(|\Sigma| \cdot \ell^m + f(\ell^m, K, r, \Delta))$ time.

where $\ell = \max \text{len}(S)$

Exact Algorithms for Bounded Number of Diverse Strings

Algorithm for MAX-MIN DIVERSE STRING SET problem

Dynamic Programming Approach

Pattern of Path Tuple: For each $d \le r$ and K-tuple of length-d paths $P = (P_1, \dots, P_K)$, define pattern Pattern $(P) = (\mathbf{w}, \mathbf{Z})$, where:

- $\mathbf{w} = (w_1, \dots, w_K)$: *K*-tuple of vertices representing endpoints of P_i paths.
- **Z** = $(Z_{i,j})$: Upper triangular matrix of Hamming distances, where $Z_{i,j} = \min\{\Delta, d_H(\text{str}(P_i), \text{str}(P_j))\}.$

DP Table of Weights

Weights:
$$V^K \times (\Delta \cup \{0\})^{K \times K} \to \{0, 1\}$$
 (3)

Boolean matrix where Weights(\mathbf{w}, \mathbf{Z}) = 1 iff (\mathbf{w}, \mathbf{Z}) matches pattern Pattern(P) for some K-tuple of paths of length d from s to \mathbf{w} .

Algorithm for MAX-MIN DIVERSE STRING SET problem

Algorithm 1

```
1: Set Weights(\mathbf{s}, Z) = 0 for all Z \in (\Delta \cup \{0\})^{K \times K} and Weights(\mathbf{s}, \mathbf{0}) \leftarrow 1
 2: for d \leftarrow 1, \ldots, r do
 3:
           for \mathbf{v} \leftarrow (v_1, \dots v_K) \in (V_d)^K do
                for (v_1, c_1, w_1) \in E^+(v_1), \dots, (v_K, c_K, w_K) \in E^+(v_K) do
 4:
 5:
                     Set \mathbf{w} = (w_1, \dots, w_K)
                     for U \in (\Delta \cup \{0\})^{K \times K} such that Weights(\mathbf{v}, U) = 1 do
 6:
 7:
                           Set Z = (Z_{i,i})_{i < i} with Z_{i,i} \leftarrow \min\{\Delta, U_{i,i} + \mathbb{1}\{c_i \neq c_i\}\}\ \forall i, j \in K
 8:
                          Set Weights(\mathbf{w}, Z) \leftarrow 1
                                                                                                                    ▶ Update
 9:
                     end for
                end for
10:
11:
           end for
12: end for
13: Answer Yes if Weights(\mathbf{t}, Z) = 1 and D_{du}^{\min}(Z) > \Delta for some Z, else No
```

For any $K \geq 1$ and $\Delta \geq 0$, it solves the MAX-MIN DIVERSE STRING SET problem in $O(\Delta^{K^2}K^2M^K(\log |V| + \log \Delta))$ time and space when an input string set L is represented by a Σ -DAG G with size(G) = M

Example Run of the Algorithm

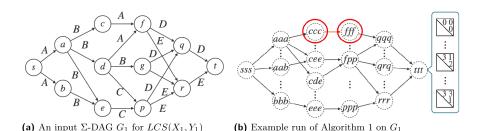


Figure: (a) An input Σ -DAG G_1 over $\Sigma = \{A,B,C,D,E\}$ for the set of all longest common subsequences of two strings $X_1 = \mathsf{ABABCDDEE}$ and $Y_1 = \mathsf{ABCBAEEDD}$ and (b) an example run of Algorithm 1 based on dynamic programming with K = 3 on an input G_1

Algorithm for MAX-SUM DIVERSE STRING SET problem

Modify the Max-Sum Diverse String Set problem

Instead of the entire $K \times K$ weight matrix Z, only the sum $z = \sum_{i < j} d_H(\text{str}(P_i), \text{str}(P_j))$ is needed for computing Max-Sum diversity.

New DP Table Weights

For $\mathbf{w} = (w_1, \dots, w_K)$ of depth $0 \le d \le r$ and integer $0 \le z \le rK$, define:

$$Weights(\mathbf{w},z)=1$$

if and only if there exists a K-tuple of length-d prefix paths (P_1, \ldots, P_K) from s to w_1, \ldots, w_K with sum of pairwise Hamming distances z.

Algorithm for MAX-SUM DIVERSE STRING SET problem

Algorithm 2

```
1: Set Weights(\mathbf{s}, Z) = 0 for all Z \in (\Delta \cup \{0\})^{K \times K} and Weights(\mathbf{s}, \mathbf{0}) \leftarrow 1
 2: for d \leftarrow 1, \ldots, r do
           for \mathbf{v} \leftarrow (v_1, \dots, v_K) \in (V_d)^K do
 3:
 4:
                for (v_1, c_1, w_1) \in E^+(v_1), \dots, (v_K, c_K, w_K) \in E^+(v_K) do
 5:
                     Set \mathbf{w} = (w_1, \ldots, w_K)
                     for u \leftarrow (0, ..., rK) such that Weights(\mathbf{v}, U) = 1 do
 6:
 7:
                           Set Z = (Z_{i,j})_{i < j} with Z_{i,j} \leftarrow \min\{\Delta, u + \sum_{i < i} \mathbb{1}\{c_i \neq c_j\}\}
                           Set Weights(\mathbf{w}, Z) \leftarrow 1
 8:

▷ Update

 9:
                     end for
                end for
10:
           end for
11:
12: end for
13: Answer Yes if Weights(\mathbf{t}, Z) = 1 and D_{du}^{\min}(Z) \geq \Delta for some Z, else No
```

For any $K \geq 1$, 15 solves the MAX-SUM DIVERSE STRING SET under Hamming Distance in $O(\Delta K^2 M^K (\log |V| + \log \Delta))$ time and space, where M is the size of the input Σ -DAG G

Approximation Algorithms for Unbounded Number of Diverse Strings

MAX-SUM DIVERSE STRING SET problem

Use a local search algorithm for computing approximate solutions $\mathcal{X} \subseteq \mathcal{L}$ with $|\mathcal{X}| = K$ on a finite metric space (\mathcal{L}, d) , where $d : \mathcal{L} \times \mathcal{L} \to \mathbb{R}_{\geq 0}$.

Algorithm 3 LocalSearch $(\mathcal{L}, \mathcal{K}, d)$

```
1: \mathcal{X} \leftarrow arbitrary set of K solutions in \mathcal{L}

2: for i \leftarrow 1, \dots, \lceil \frac{K(K-1)}{K+1} \log \frac{(K+2)(K-1)^2}{4} \rceil do

3: for X \in \mathcal{X} s.t \mathcal{L} \setminus \{X\} \neq \emptyset do

4: Y \leftarrow \operatorname{argmax}_{Y \in \mathcal{L} \setminus \{X\}} \sum_{X' \in \mathcal{X} \setminus \{X\}} d(X', Y)

5: \mathcal{X} \leftarrow \mathcal{X} \setminus \{X\} \cup \{Y\}

6: end for

7: end for

8: return \mathcal{X}
```

Theorem

When the distance d is a semi-metric of negative type over \mathcal{X} , then LocalSearch has improved approximation ratio $(1-\frac{2}{K})$ for any $K \geq 2$. The Hamming distance d_H over the set of r-strings is a semi-metric of negative type.

MAX-SUM FARTHEST r-STRING problem

How do we solve efficiently the subproblem at line 4 of the ${\it LocalSearch}$ algorithm?

$$Y \leftarrow \mathsf{argmax}_{Y \in \mathcal{L} \setminus \{X\}} \sum_{X' \in \mathcal{X} \setminus \{X\}} d(X', Y)$$

The following algorithm can be modified to compute such Y by reordering the parent pair (v, y) of each (w, z) and then tracking back

Algorithm 4 Decisional Max-Sum Farthest r-String

- 1: Set Weights(s,z):=0 for all $z\in [\Delta]_+$, and Weights(s,0):=1
- 2: **for** d := 1, ..., r **do**
- 3: **for** $0 \le u \le \Delta$ such that Weights(v, u) := 1 **do**
- 4: Set Weights(w, z) := 1 for $z := u + \sum_{i \in [K]} \mathbb{1}\{c \neq X_i[d]\}$

▷ Update

- 5: end for
- 6: end for
- 7: Answer YES if $Weights(t, \Delta) = 1$, and NO otherwise

▷ Decide

MAX-SUM FARTHEST r-STRING problem

Lemma (Max-Sum Farthest *r*-String)

For any $K \geq 1$ and $\Delta \geq 0$, ALGORITHM 3 computes the farthest r-string $Y \in L(G)$ that maximizes $D^{sum}_{d_H}(Y \cup \mathcal{X})$ over all r-strings in L(G) in $O(K\Delta M)$ time and space, where M is the size of the input Σ -DAG G.

Theorem (Polynomial Time Approximation Scheme for unbounded K)

When K i part of an input, MAX-SUM DIVERSE STRING SET problem on a Σ -DAG admits a PTAS

The corresponding result for the $\operatorname{Max-Sum}$ DIVERSE LCSs follows immediately.

Fixed-Parameter Tractable (FPT)
Algorithms for Bounded Number and
Length of Diverse Strings

FPT Algorithms for Max-Min and Max-Sum Diverse String Set problems

Definition (Fixed-Parameter Tractable (FPT) Algorithm)

A problem parametrized with κ is said to be *fixed-parameter tractable* (FPT) if there exists an algorithm for the problem running on an input x in time $f(\kappa(x) \cdot |x|^c)$, where f is a computable function and c > 0 is a constant.

Proposed FPT Algorithm

We use the *color-coding* technique with dynamic programming to solve these problems efficiently. Assign a random color to the edges of the Σ -DAG G, creating a colored graph called C-DAG.

Computation of Reduced C-DAG

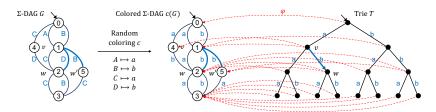


Figure: Computation of reduced C-DAG H from an input Σ -DAG G over alphabet $\Sigma = \{A, B, C, D\}$, which shows G (left), a random coloring C on $C = \{a, b\}$, a colored C-DAG C(G) (middle), and a reduced C-DAG C in the form of trie C (right)

An analogous FPT algorithm can be designed for the MAX-SUM DIVERSE STRING SET problem with a small modification in the research phase, that, in this case, is $O(\Delta K^2 M^K)$

Complexity Results for Diverse String Problems

Negative Results

- NP-hard for unbounded K (MAX-MIN, MAX-SUM) in Σ -graphs for r-strings, $r \geq 3$.
- W[1]-hard parameterized with K for MAX-MIN and MAX-SUM in Σ -DAGs.

Reduction to Diverse LCSs

MAX-MIN and MAX-SUM problems are FPT-reducible to DIVERSE LCSs for m=2 strings.

Corollaries

NP-hard and W[1]-hard results extend to DIVERSE LCSs for two r-strings.

Conclusion

- Polynomial-Time Solutions: When K is bounded, both the MAX-SUM and MAX-MIN versions of DIVERSE STRING SET and DIVERSE LCSs can be solved in polynomial time using dynamic programming (DP).
- PTAS for Input-Based K: For input-dependent K, the MAX-SUM versions of both DIVERSE STRING SET and DIVERSE LCSs admit a PTAS using local search due to the Hamming distance being a metric of negative type.
- **Fixed-Parameter Tractability (FPT)**: Both versions are FPT when parameterized by *K* and *r*, combining the color coding technique and DP.
- NP-Hardness for Constant $r \ge 3$: When K is part of the input, both the MAX-SUM and MAX-MIN versions are NP-hard for any constant $r \ge 3$.
- **W[1]-Hard for Parameterized** *K*: Parameterized by *K*, both versions are W[1]-hard.