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Artificial Intelligence and Data Engineering

Master Degree Thesis

A New Compressing Technique for Labeled Trees

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Contents

Chapter 1

Introduction

The aim of this thesis is to study a new technique for the compression of labeled trees. The aim of the project is to implement and experiment with the technique, and to compare it with other state-of-the-art techniques for tree compression such as the Extended Burrows-Wheeler Transform (XBWT) [6].

1.1 The idea

Let T be an ordered tree of arbitrary fan-out, depth, and shape. T consists of n internal nodes and ℓ leaves, for a total of $t = n + \ell$ nodes. Every node of T is labeled with a symbol drawn from an alphabet Σ. We assume that Σ is the set of labels effectively used in T's nodes and that these labels are encoded with the integers in the range $[1, |\Sigma|]$. Then we need to define the array π where, for each node u, $\pi(u)$ is the string obtained by concatenating the labels on the **upward path** from u's parent to the root of the tree (root has an empty π component).

The following pipeline is used to compress the tree T:

1. Initially the array π is computed for the tree T by traversing the tree in a pre-order fashion. Then the nodes are stably sorted by the lexicographic order of their π strings. In order to sort the nodes, the **Path Sort** algorithm introduced in [6] is used, allowing to sort the nodes in linear time and $O(t \log t)$ space.
2. Then, using Hopcroft algorithm for minimization of DFA [12] the nodes are partitioned into equivalence classes where two nodes are equivalent if they have the same subtree rooted at them.
3. Given a width p, the nodes previously sorted are then divided into p chains with the aim to minimize the run length encoding of each chain (by considering the equivalence classes). In order to do so we reduced this problem to the **Minimum Perfect Bipartite Matching** problem, which can be solved in polynomial time.
4. Lastly, the resulting DFA or NFA can be indexed using the indexing scheme introduced by Cotumaccio et al. [3]. Also, the chains can be compressed using some techniques that will be discussed in the next chapters.

1.2 The structure of the thesis

The thesis is structured as follows:

Chapter 2

Hopcroft Algorithm for Minimization of DFA

2.1 Introduction

The process of automata minimization is the process of reducing the number of states in a DFA while preserving the language accepted by the DFA. The minimization of DFA is crucial for a variety of applications, such model checking, hardware design, and compilers, as it produces a more effective and compact representation of the automata.

The minimization of DFA is a well-studied problem in automata theory, and there are several algorithms available for this purpose. One of the most popular algorithms for DFA minimization is the Hopcroft algorithm, which was proposed by John Hopcroft in 1971 [12]. The Hopcroft algorithm is an efficient and simple algorithm that can minimize a DFA in $O(n \log n)$ time, where n is the number of states in the DFA.

Before we delve into the details of the Hopcroft algorithm, let us first introduce the concept of DFA.

2.1.1 Deterministic Finite Automata (DFA)

A deterministic finite automaton (DFA) is a 5-tuple $M = (Q, \Sigma, \delta, q_0, F)$ where:

- Q is a finite set of states
- Σ is a finite set of input symbols (alphabet)
- $\delta : Q \times \Sigma \to Q$ is the transition function
- $q_0 \in Q$ is the initial state
- $F \subseteq Q$ is the set of final (accepting) states

The DFA processes an input string by starting from the initial state q_0 and following transitions based on the input symbols. The string is accepted if the DFA ends in an accepting state after processing all input symbols.

2.2 Hopcroft's Minimization Algorithm

Minimization of deterministic finite automata (DFA) is a classical and widely studied problem in Theory of Automata and Formal Languages. It consists in finding the unique (up to isomorphism) finite automaton with the minimal number of states, recognizing the same regular language of a given DFA.

The Hopcroft algorithm works by iteratively refining partitions of states until no further refinement is possible. The algorithm is the following:

Algorithm 1 Hopcroft's Algorithm: DFA Minimization ($\mathcal{A} = (Q, \Sigma, \delta, q_0, F)$)

$\Pi \leftarrow \{F, Q \setminus F\}$
for all $a \in \Sigma$ **do**
    $\mathcal{W} \leftarrow \{(\min(F, Q \setminus F), a)\}$
end for
while $\mathcal{W} \neq \emptyset$ **do**
    choose and delete any (C, a) from $\mathcal{W}$
    for all $B \in \Pi$ **do**
        if B is split from (C, a) **then**
            $B' \leftarrow \delta_a^{-1}(C) \cap B$
            $B'' \leftarrow B \setminus \delta_a^{-1}(C)$
            $\Pi \leftarrow \Pi \setminus \{B\} \cup \{B', B''\}$
            for all $b \in \Sigma$ **do**
                if $(B, b) \in \mathcal{W}$ **then**
                    $\mathcal{W} \leftarrow \mathcal{W} \setminus \{(B, b)\} \cup \{(B', b), (B'', b)\}$
                else
                    $\mathcal{W} \leftarrow \mathcal{W} \cup \{(\min(B', B''), b)\}$
                end if
            end for
        end if
    end for
end while

The algorithm enables to compute equivalence classes of nodes in $O(n \log n)$, in particular, the Myhill-Nerode equivalence classes. The Myhill-Nerode theorem states that a language is regular if and only if it has a finite number of Myhill-Nerode equivalence classes. This theorem provides a powerful tool for determining the regularity of languages and is a cornerstone of automata theory. Let's formalize the concept of equivalence classes and the Myhill-Nerode theorem.

Definition 1 (Equivalence Relation)**.** *For a language $L \subseteq \Sigma^*$ and any strings $x, y \in \Sigma^*$, we say x is equivalent to y with respect to L (written as $x \approx_L y$) if and only if for all strings $z \in \Sigma^*$:*

$$xz \in L \Leftrightarrow yz \in L$$

That is, strings x and y are equivalent if they have the same behavior with respect to the language L - either they both lead to acceptance or both lead to rejection when any suffix z is appended.

Theorem 1 (Myhill-Nerode theorem)**.** *Let L be a language over an alphabet Σ. Then L is regular if and only if there exists a finite number of Myhill-Nerode equivalence classes for L. Specifically, the number of equivalence classes is equal to the number of states in the minimal DFA recognizing L.*

2.3 Minimization of acyclic DFA in linear time

For our purpose, we will focus on a specific type of finite automaton: an acyclic deterministic finite automaton (or DAWG). An acyclic DFA is one where there are no cycles within the transitions. This property simplifies the minimization process since it ensures that every state can be reached from the start state through a unique path.

Let's start by giving the notion of directed acyclic word graph (DAWG):

Definition 2 (DAWG)**.** *A **DAWG** (directed acyclic word graph) or automaton $\mathcal{A}$ is defined by the following 5-uple:*

$$\mathcal{A} = (Q, \Sigma, F, T, q_0),$$

where

- *Q is a set of states;*
- *Σ is an alphabet of finite cardinal denoted by $|\Sigma|$;*
- *q_0 is the initial state;*
- *T is the subset of terminal states of Q;*
- *F is a function of $Q \times \Sigma$ into Q defining the transitions (arcs) of the automaton.*

In this section, we will discuss an efficient algorithm for minimizing acyclic deterministic finite automata in linear time on the number of states [19]. The minimization process involves identifying and merging equivalent states. Two states are considered equivalent if they have the same set of reachable final states, meaning that from any state q, there is a path to a final state in both states. This equivalence relation partitions the DAWG into disjoint sets of states, each representing an equivalence class. The purpose of using this approach is then to apply it to the input tree for our pipeline since the problem can directly be applied to trees where the leaf nodes are considered as final states, the root as the initial state and the edges of the tree are considered directed from node to its children.

2.3.1 The minimization algorithm

The minimization algorithm introduced in [19] operates by labeling each state with a unique identifier that represents the structure of the automaton from that state onward. It proceeds in the following steps:

1. **Height Computation:** The height of each state is determined, where the height of a state is the length of the longest path from that state to a final state.
2. **State Labeling:** Each state is labeled based on the structure of its transitions. The label consists of:
   - Whether the state is final or not.
   - The transitions, recorded as ordered pairs of symbols and target state identifiers.

3. **Lexicographic Sorting:** States at each height level are sorted lexicographically based on their labels using a bucket sort technique.
4. **Merging Equivalent States:** After sorting, states with identical labels are merged, ensuring that equivalent states are unified.

Chapter 3

Wheeler Graphs

3.1 Definition of Wheeler Graph

Definition 3. *A Wheeler graph $G = (V, E)$ is defined as a directed graph with labeled edges, equipped with a total order $<_\pi$ on the nodes in V, which satisfies the following three axioms:*

(i) All vertices with in-degree 0 must precede those with a greater in-degree in the ordering;

For every pair of edges (u_1, v_1, k_1) and (u_2, v_2, k_2):

(ii) $k_1 < k_2 \Rightarrow v_1 <_\pi v_2$;

(iii) $(k_1 = k_2) \wedge (u_1 <_\pi u_2) \Rightarrow v_1 \leq_\pi v_2$.

3.2 Examples of Wheeler Graphs

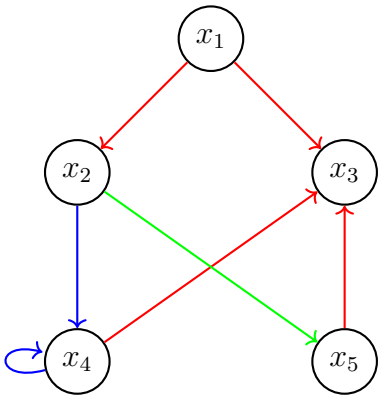

Figure 3.1: Example of a Wheeler graph with $\sigma = 3$. The label order is as follows: red < blue < green. The resulting total order of nodes is: $x_1 < x_2 < x_3 < x_4 < x_5$.

Consider Figure 3.1. Axiom (i) states that nodes with no incoming edges (in-degree 0) must be positioned at the beginning of the total order and never after nodes with a greater in-degree. In the example, node x_1 is the only node with in-degree 0, so it is placed as the first element in the resulting total order.

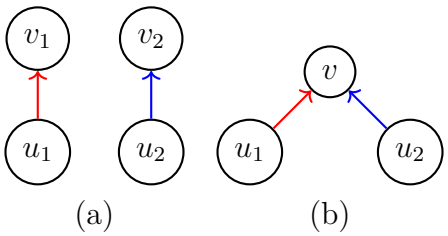

Figure 3.2: Examples for Axiom (ii).

To better understand Axiom (ii), consider Figure 3.2. In example (a), we have two edges (u_1, v_1, red) and $(u_2, v_2, blue)$ with $red < blue$. According to the axiom, since the edges have different labels, the destination node of the edge with the smaller label (in this case v_1) must precede the destination node of the edge with the larger label, so we obtain v_1 before v_2 in the total order.

In example (b), we instead have two edges (u_1, v, red) and $(u_2, v, blue)$ with $red < blue$, but they share the same destination node. This case is not accepted by the second axiom because, if the labels are different, their order must be reflected in the destination nodes, which thus cannot be the same.

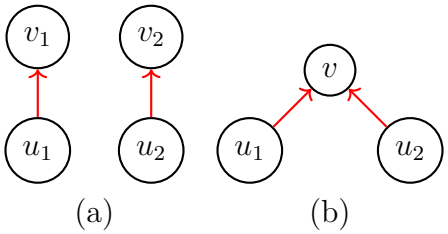

Figure 3.3: Examples for Axiom (iii).

To better understand Axiom (iii), consider Figure 3.3. In example (a), we have two edges (u_1, v_1, red) and (u_2, v_2, red) with $u_1 < u_2$. The axiom applies here because the edges share the same label. Consequently, the order of the source nodes propagates to the destination nodes of the two edges. Specifically, the destination node of the edge whose source node is smaller in the total order must not be larger than the destination node of the edge whose source node is larger. In this case, since $u_1 < u_2$, we obtain $v_1 \leq v_2$.

In example (b), we consider the case where the two edges (u_1, v, red) and (u_2, v, red) with $u_1 < u_2$ have the same label and share the same destination node. Again, the axiom applies, requiring that $v_1 \leq v_2$. In this case, we obtain $v_1 = v_2$.

3.3 Properties of Wheeler Graphs

The following is a list of some properties of Wheeler graphs that can be derived from the axioms (Definition 3).

Lemma 1. *All incoming edges to a node v must have the same label. This property makes it equivalent to label either the nodes or the edges of the graph.*

Proof. Lemma 1 is a natural derivation of the second Wheeler axiom (Definition 3). It states that given two edges (u_1, v_1, k_1) and (u_2, v_2, k_2) with $k_1 < k_2$, the order of the

edge labels propagates to the destination nodes, implying $v_1 < v_2$. This means that the destination nodes v_1 and v_2 cannot be the same if they receive incoming edges with different labels; otherwise, the considered graph would not be Wheeler. □

Lemma 2. *A node v may have multiple outgoing edges with the same label.*

Proof. Assume, for contradiction, that the statement does not hold and that a node v cannot have multiple outgoing edges with the same label if the graph is Wheeler. The graph in Figure 3.1 is a valid counterexample demonstrating the opposite, as node x_1 has two outgoing edges labeled *red*, and the graph is Wheeler. This leads to a contradiction. □

Lemma 3. *Consider a Wheeler graph $G = (V, E)$ with labeling defined over a set $\Sigma = \{a, b, c\}$, where the label order is $a < b < c$. Let $V_a \subseteq V$ be the set of vertices with label a (i.e., those with incoming edges labeled a), $V_b \subseteq V$ the set of vertices with label b, and $V_c \subseteq V$ the set of vertices with label c. Also, let $u_a \in V_a$, $u_b \in V_b$, and $u_c \in V_c$. Then, in the context of vertex ordering in the graph, it holds that $u_a < u_b < u_c$. More generally, all vertices in V_k for a certain label k will be consecutive in the ordering, with no nodes of other labels interspersed among them in the total order.*

Proof. Lemma 3 follows naturally from the second Wheeler axiom (Definition 3). Consider a Wheeler graph $G = (V, E)$ with labeling over a set $\Sigma = \{a, b\}$, where the order of labels is $a < b$. Let $V_a \subseteq V$ be the set of vertices labeled a and $V_b \subseteq V$ be the set of vertices labeled b. Suppose, for contradiction, that there exist two nodes $u_a \in V_a$ and $u_b \in V_b$ such that $u_b < u_a$ in the Wheeler ordering.

Since $u_a \in V_a$ and $u_b \in V_b$, by the definition of sets V_a and V_b, there must exist two edges (v_1, u_a, a) and (v_2, u_b, b). However, this leads to a contradiction because the second axiom states that for two edges (u_1, v_1, k_1) and (u_2, v_2, k_2) with $k_1 < k_2$, the order of edge labels must be reflected in the destination nodes, meaning $v_1 < v_2$. In our case, $a < b$, but $u_b < u_a$, implying the graph is not Wheeler. □

Lemma 4. *Consider a total Wheeler order. Let V_k be the set containing all nodes with the same label k. Let V_k^1 and V_k^2 be two partitions of V_k, where V_k^1 contains all nodes v_1 with incoming edges from nodes preceding v_1 in the total order, while V_k^2 contains all nodes v_2 with incoming edges from nodes following v_2 in the total order. Consequently, the intersection of V_k^1 and V_k^2 contains at most one vertex u, and all vertices in $V_k^1 \setminus \{u\}$ precede those in V_k^2 in the ordering. Moreover, given a vertex $v \in V_k^1$, there cannot exist an edge (v, z, k) with $z < v$, and similarly, given a vertex $v \in V_k^2$, there cannot exist an edge (v, z, k) with $z > v$ (see [8]).*

3.3.1 Path Coherence

The following defines *path coherence* and a related property of Wheeler graphs introduced and proven in [22].

Definition 4 (Path Coherence)**.** *A labeled directed graph G is said to be path coherent if there exists a total order of nodes such that, for every consecutive interval $[i, j]$ of nodes and a string α, the nodes reachable from those in $[i, j]$ in $|\alpha|$ steps,*

following edges whose labels form α when concatenated, themselves form an interval in the total order.

Lemma 5. *A Wheeler graph is path coherent with respect to any possible Wheeler order of the nodes.*

Thanks to this crucial property, it was proven in [22] that if the state diagram of a finite-state automaton is a Wheeler graph, then, due to Lemma 5, the nodes can be ordered so that for any string, the nodes reachable from the initial state(s) by processing that string are consecutive. This means that even if the automaton is non-deterministic, it can still be stored compactly and used to process strings efficiently.

3.3.2 Topological Ordering for $\sigma = 1$

The following defines *topological ordering* and a related property of Wheeler graphs introduced and proven in [8].

Definition 5 (Topological Ordering)**.** *A topological ordering is a linear ordering of all vertices of a directed graph. The nodes of a graph are said to be topologically ordered if they are arranged such that each node precedes all nodes connected to its outgoing edges. The topological ordering of a graph may not be unique. In the worst case, there can be $n!$ different topological orderings corresponding to all possible permutations of the n nodes. A topological ordering is possible if and only if the graph has no directed cycles, meaning it is a directed acyclic graph (DAG) [21].*

Lemma 6. *For $\sigma = 1$, every Wheeler order also represents a topological ordering, except for vertices with self-loops, which must be placed at the end of the order since a cyclic graph cannot have a valid topological ordering.*

This property follows from Lemma 4 and the first axiom (Definition 3). Finally, it is important to highlight that this result is used in [8] to prove that the Wheeler graph recognition problem can be solved in linear time when $\sigma = 1$.

3.4 Bipartite Representation of Wheeler Graphs

The following section explains a simple and intuitive technique used to graphically check whether a directed labeled graph, along with its total node ordering, satisfies the three Wheeler axioms (Definition 3). More specifically, the technique involves representing the graph as a bipartite graph with useful properties related to the three Wheeler axioms. Additionally, later in the text, we will see how this idea is also useful for the Wheelerization problem of a graph.

3.4.1 Construction of the Bipartite Graph

Consider a directed labeled graph on the edges $G = (V, E)$ where $V = \{x_1, \ldots, x_n\}$ and a total ordering of V (in the example, consider $x_1 < x_2 < \cdots < x_n$). The bipartite graph $B = (V_1, V_2, E_B)$ is constructed as follows:

- $V_1 = \{x_i^s : i \in [1, n]\}$. Where the node $x_i^s \in V_1$ corresponds to the node $x_i \in V$ for $1 < i < n$. This set is thus composed of the nodes in V, and is ordered according to the given ordering.
- $V_2 = \{x_i^d : i \in [1, n]\}$. Where the node $x_i^d \in V_2$ corresponds to the node $x_i \in V$ for $1 < i < n$. This set is also composed of the nodes in V, and is ordered according to the given ordering.
- $E_B = \{(u, v) : u \in V_1 \wedge v \in V_2 \wedge (u, v) \in E\}$. Therefore, for every edge $(x_i, x_j) \in E$, a corresponding edge is created in the bipartite graph such that $x_i = x_i^s \in V_1$ and $x_j = x_j^d \in V_2$ with $i, j \in [1, n]$. For example, given the edge (x_1, x_4), an edge is created between x_1^s and x_4^d (edge (x_1^s, x_4^d) in the bipartite graph).

The following explanation assumes a vertical construction of the bipartite graph. As a result, since the nodes in V_1 and V_2 are ordered according to the total ordering of V (in the example, we have $x_1^s < x_2^s < \cdots < x_n^s$ and $x_1^d < x_2^d < \cdots < x_n^d$), a node $x_i^s \in V_1$ is positioned graphically above a node $x_j^s \in V_1$ if and only if $i < j$ in the ordering, and similarly, a node $x_i^d \in V_2$ is positioned graphically above a node $x_j^d \in V_2$ if and only if $i < j$ in the ordering.

This vertical construction implies that the nodes in the set V_1 will be arranged in ascending order downward, maintaining the total ordering. Similarly, the nodes in the set V_2 will be arranged in ascending order downward, respecting the established ordering. In this way, the vertical position of the nodes reflects the ordering of the nodes within the graph. See the example in Figure 3.4-(a), which shows the bipartite representation of the graph in Figure 3.1.

3.4.2 Properties of the Bipartite Graph

As introduced earlier, the bipartite representation allows us to easily verify whether the three Wheeler axioms (Definition 3) are satisfied by the graph G and the ordering on V (consider the graph and ordering defined in the previous section). The properties related to the axioms are as follows:

- Axiom (i) is satisfied if for every pair of nodes $u, v \in V$ it holds that if $indegree(u) = 0 \wedge indegree(v) > 0$, then $u < v$ in the ordering.
- Axiom (ii) is satisfied if every node in the bipartite graph has all incoming edges with the same label, and moreover, the order of the labels respects the node ordering. Formally, let $\lambda(u)$ be a function that returns the label of a given node $u \in V$. It must hold that $\lambda(x_1) \leq \lambda(x_2) \leq \cdots \leq \lambda(x_n)$.
- Axiom (iii) is satisfied if there are no edges with the same label crossing in the bipartite graph. Formally, a crossing is defined as follows: let (x_i^s, x_j^d, k_1), (x_k^s, x_w^d, k_2) be two edges of the bipartite graph labeled k_1 and k_2, respectively, a crossing occurs if $(i < k \wedge j > w) \vee (i > k \wedge j < w)$, where the subscripts of the nodes indicate their position in the ordering.

3.4.3 Examples of Bipartite Representation of Wheeler Graphs

Consider the Wheeler graph shown in Figure 3.1, and the resulting bipartite graph shown in Figure 3.4-(a).

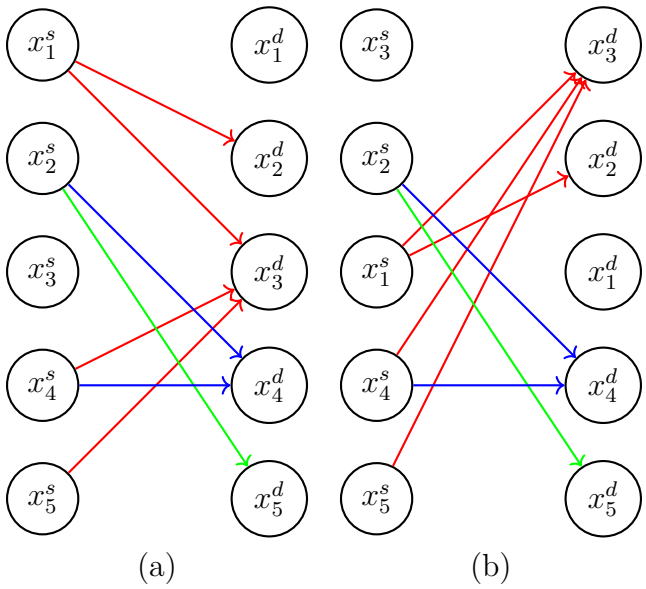

Figure 3.4: Example of bipartite representation of the graph in Figure 3.1, useful for verifying that it satisfies the three Wheeler axioms. (a) respects the correct ordering, while (b) does not.

As we can observe, the three axioms are satisfied, because:

- x_1 is the only node with in-degree 0 and is at the beginning of the ordering;
- all nodes have all incoming edges with the same label[1];
- starting from the top, the sequence of labels assigned to the incoming edges on each node is as follows: red, red, blue, green, which respects the ordering of the alphabet considered (red $<$ blue $<$ green);
- there are no crossings between edges with the same color in the bipartite graph.

Therefore, we can confidently assert that the graph in question is a Wheeler graph for the given node order.

The example in Figure 3.4-(b), however, is constructed using the graph from Figure 3.1, but considering the following node order: $x_3 < x_2 < x_1 < x_4 < x_5$. The resulting bipartite graph shows that the graph from Figure 3.1 with the order $x_3 < x_2 < x_1 < x_4 < x_5$ is not a Wheeler graph, because:

- the first axiom is not satisfied since node x_1 is not at the beginning of the ordering;

[1]In the image, the colors represent the labels.

- the third axiom is not satisfied because there are red edges that cross in the bipartite graph.

Chapter 4

Extended Burrows-Wheeler Transform

4.1 Introduction

The Extended Burrows-Wheeler Transform (XBWT) is a data structure designed to efficiently compress and index labeled trees. A labeled tree is a data structure where each node is assigned a label from a given alphabet, and the tree can have an arbitrary shape and degree.

XBWT works by linearizing a labeled tree into two coordinated arrays: one capturing the structural properties of the tree and the other storing its labels. This transformation allows for efficient representation, navigation, and querying of the tree. The key advantage of XBWT lies in its ability to compress labeled trees while supporting a wide range of operations, such as parent-child navigation and sophisticated path-based searches, in (near-)optimal time and space.

One of the primary applications of XBWT is in the compression and indexing of hierarchical data formats, such as XML documents. It provides significant improvements in both compression ratio and query performance compared to traditional tools, making it an invaluable resource for data-intensive applications in fields like bioinformatics, information retrieval, and big data analytics.

This project aims to implement the XBWT data structure and explore its applications in the context of labeled trees. We will start by providing an overview of the theoretical foundations of the XBWT. Finally, we will describe and compare the algorithms for constructing the XBWT and demonstrate its use in compressing and indexing labeled trees.

Let's start with a quick overview of the XBWT and its theoretical foundations.

How XBWT Works

The transformation process of XBWT is as follows:

1. **Path Sorting:** The labeled tree is linearized by sorting its nodes based on the *paths* from each node's parent to the root. The resulting order groups nodes with similar upward paths together, clustering related labels.
2. **Array Construction:** Two arrays, S_{last} and S_α, are generated:
    - S_{last} stores structural information, such as whether a node is the last child of its parent. This encodes the tree's structure without the need for explicit pointers.
    - S_α stores the labels of the nodes in the sorted order determined by their upward-path sorting.

3. **Compression:** Both S_{last} and S_α are highly compressible due to the clustering of similar labels and structural redundancy.

Key Properties of XBWT

The XBWT has several key properties that make it an effective tool for labeled tree compression and indexing:

- **Succinctness:** The XBWT representation of a labeled tree uses space close to the *information-theoretic lower bound*, which is $2t - \Theta(\log t) + t \log |\Sigma|$ bits for a tree with t nodes and an alphabet of size $|\Sigma|$.
- **Efficient Querying:** XBWT supports a range of navigational operations, such as finding the parent, child, or subtree of a node in near-optimal time.
- **Scalability:** XBWT is particularly useful for large-scale hierarchical data, such as XML documents or phylogenetic trees, where both compression and fast querying are critical.

4.1.1 Project implementation

The XBWT data structure will be implemented in C++ using the Succinct Data Structure Library 2.0 (SDSL) for efficient representation and manipulation of compressed data structures. We will develop two algorithms for constructing the XBWT: one efficient linear-time recursive algorithm and one more straightforward iterative algorithm. Also, we will implement the necessary data structures and algorithms for navigating and querying the XBWT, such as parent-child navigation and path-based searches.

The code is available on GitHub at `https://github.com/davide-tonetto-884585/XBWT`. The project will be structured as follows:

- **XBWT.hpp**: File containing the class definition and implementation for the generic XBWT data structure.
- **LabeledTree.hpp**: File containing the class definition and implementation for the generic labeled tree data structure used to feed and test the XBWT.
- **main.cpp**: Main file containing the test cases and examples for the XBWT implementation.
- **experiments.cpp**: File containing the experiments and performance evaluation of the XBWT construction algorithms and compression efficiency.
- **CMakeLists.txt**: CMake configuration file for building the project.

The project will be developed and tested on a Linux environment using the GCC compiler and the CMake build system.

4.2 Theoretical Background on Labeled Trees

4.2.1 Labeled Trees

A **labeled tree** is a rooted, ordered, hierarchical data structure in which every node is assigned a label from a predefined alphabet Σ. The structure consists of nodes connected by edges, forming a directed acyclic graph. Formally, a labeled tree T with t nodes can be defined as $T = (V, E, \ell)$, where:

- V is the set of nodes,
- $E \subseteq V \times V$ is the set of directed edges, and
- $\ell : V \to \Sigma$ is a labeling function that assigns a label $\ell(u) \in \Sigma$ to each node u.

In the case of ordered labeled tree, the children of a node in the tree are ordered, meaning their positions relative to each other matter. A labeled tree can have arbitrary degrees and shapes, and the alphabet Σ used for labels can be of arbitrary size.

Applications of Labeled Trees

Labeled trees are widely used in computer science and data representation due to their hierarchical structure and flexibility in modeling relationships. Prominent applications include:

1. **XML Data Representation:** XML documents are often modeled as labeled trees, where each element is a node labeled by its tag, and hierarchical nesting represents parent-child relationships.
2. **JSON Data Representation:** JSON objects can be viewed as labeled trees, with keys as labels and values as children.
3. **Bioinformatics:** Labeled trees are used to represent phylogenetic trees, genome annotations, and hierarchical clustering.
4. **Compiler Design:** Abstract Syntax Trees (ASTs) for programming languages are labeled trees that capture the structure of code.
5. **File Systems:** The directory structure of file systems can be viewed as labeled trees.

Efficient representation, navigation, and querying of labeled trees are essential for many applications, motivating the development of specialized data structures and algorithms.

4.2.2 Compressing and Indexing Labeled Trees

The goal of compressing and indexing labeled trees is to design a compressed storage scheme for a labeled tree T with t nodes that allows for efficient navigation operations in T, as well as fast search and retrieval of subtrees or paths within T. To be effective, the compressed representation should minimize the space required to store the tree while supporting a wide range of operations in (near-)optimal time.

Let u be a node in the labeled tree T and let $c \in \Sigma$. We define the following navigation operations on T:

- **Navigational queries:** ask for the parent of u, the i-th child of u, or the label of u. The last two operations might be restricted to the children of u with a specific label c.
- **Path queries:** retrieve the nodes in the subtree rooted at u (any possible order should be implemented).
- **Subpath queries:** ask for the (number of occurrences of) nodes of T that descend from a labeled subpath P. Which may be anchored anywhere in the tree (i.e., not necessarily in its root).

A naive solution to index labeled trees is to store the tree in a straightforward manner, such as a list of nodes with their labels and parent-child relationships using pointer in $O(tlogt)$. However, this representation is not space-efficient and does not support fast navigation or query operations.

Many data structures have been proposed to compress and index labeled trees, each with its trade-offs in terms of space usage, query performance, and supported operations. One of the most successful approaches is the Extended Burrows-Wheeler Transform (XBWT), which extends the classical Burrows-Wheeler Transform (BWT) to handle labeled trees efficiently.

Before the advent of XBWT, Kosaraju [15] proposed a method to index labeled trees by extending the concept of prefix sorting, which is commonly applied to strings, to work with labeled trees by leveraging the structure of tries (prefix trees). To achieve this, he introduced the idea of constructing a suffix tree for a reversed trie allowing subpath queries in $O(|P| \log |\Sigma| + occ)$ time, where occ is the number of occurrences of P in T but still requiring $O(t \log t)$ space and so not being compressed.

4.2.3 Succinct Data Structures for Trees

In order to compress the index of labeled trees, we need to avoid the use of pointers and store the tree in a space-efficient manner. Succinct data structures are a class of compressed data structures that support efficient navigation and query operations on the compressed data. These structures are designed to use close to the information-theoretic lower bound on space while providing fast access to the original data. They were first introduced by Jacobson [13] and have been applied to various problems in string processing, graph theory, and data compression.

Information-Theoretic Lower Bound for Trees

The information-theoretic lower bound for storing an unlabeled tree with t nodes is given by:

- The number of binary unlabeled trees with t nodes is given by the Catalan number $C_t = \frac{1}{t+1}\binom{2t}{t}$ that can can be approximated as $C_t \approx \frac{4^t}{t^{3/2}\sqrt{\pi}}$ using Stirling's approximation.
- The entropy (or the information-theoretic minimum number of bits to encode the structure of the tree) is the logarithm (base 2) of the total number of trees,

which is $-\log_2 C_t \approx 2t - \frac{1}{2}\log_2 \pi t^3$.

- The correction term $\frac{1}{2}\log_2 \pi t^3$ grows slower that the linear term $2t$, we can say that $-\frac{1}{2}\log_2 \pi t^3 = -\Theta(\log t)$.
- The information-theoretic lower bound for storing an unlabeled tree with t nodes is $2t - \Theta(\log t)$ bits.

Then for labeled trees, the labels assigned to each node must be stored, which requires an additional space:

- Let Σ denote the alphabet of labels, and let $|\Sigma|$ be the size of the alphabet.
- Each node in the tree requires $\log_2 |\Sigma|$ bits to store its label.
- Therefore, for t nodes, the total space required to store the labels is $t \log_2 |\Sigma|$ bits.

Combining the structural representation and the labeling, the information-theoretic lower bound for storing a labeled tree is:

$$2t - \Theta(\log t) + t \log_2 |\Sigma| \text{ bits}$$

4.3 Extended Burrows-Wheeler Transform

In 2005, Ferragina et al. [6] observed that succinctness could be achieved for labeled trees by exploiting an index scheme that fit into a space proportional to the entropy-compressed edge labels plus the succinct tree's topology. This observation was the starting point for the development of the Extended Burrows-Wheeler Transform (XBWT). Let's start by defining the XBWT.

4.3.1 Definition of XBWT

The **Extended Burrows-Wheeler Transform (XBWT)** is a data structure designed to efficiently compress and index *labeled trees*. Inspired by the classical Burrows-Wheeler Transform (BWT) [1] for strings, the XBWT extends these principles to hierarchical structures, enabling efficient storage, navigation, and querying of trees. It is particularly effective for trees where each node has a label drawn from an alphabet Σ and the tree structure has an arbitrary shape and degree.

Given an ordered labeled tree T of arbitrary fan-out, depth and shape, with n internal nodes and l leaves (t nodes in total) and alphabet Σ. Let u be a node in T, we define the following information:

- $last[u]$: is a binary value that is 1 if u is the last (rightmost) child of its parent, and 0 otherwise.
- $\alpha[u]$: denotes the label of node u plus one bit that is 1 if u is a leaf and 0 otherwise.
- $\pi(u)$: is the string obtained by concatenating the labels of the nodes on the path from u's parent to the root of T (the root has an empty π component).

Then, to define the XBWT, a sorted multi-set S consisting of t triplets (one per node of T) is built, where each triplet is of the form $(last[u], \alpha[u], \pi(u))$ for some node u in T. S is built by traversing T in a pre-order fashion, for each visited node u, the triplet $(last[u], \alpha[u], \pi(u))$ is added to S, then S is stably sorted in accordance with the lexicographic order of the π component of the triplets.

Theorem 2. *The XBWT of a labeled tree T consist of the two arrays $\{S_{last}, S_\alpha\}$ after sorting, and takes $2t + t \log |\Sigma|$ bits of space.*

4.3.2 Properties of XBWT

The following two properties of the ordered multi-set S are crucial for the indexing scheme, they immediately follow from the composition of the transform and from the way S is built.

Property 1

1. S_{last} has n 1s (one for each internal node) and l 0s (one for each leaf).
2. S_α is a permutation of the labels of the nodes in T.
3. S_π contains all the upward labeled paths of T consisting internal node labels only. Also, each path is repeated a number of times equal to the number of its offsprings.

Property 2

1. The first triplet of S refers to the root of T.
2. The triplet of node u precedes the triplet of node v in S iff either $\pi[u] < \pi[v]$ or $\pi[u] = \pi[v]$ and u precedes v in the pre-order traversal of T.
3. Let $u_1, \ldots, u_z$ be the children of node u in T, then the triplets of $u_1, \ldots, u_z$ are consecutive in S following this order. Moreover, the subarray $S_{\text{last}}[u_1 \ldots u_z]$ provides the unary encoding of u's degree, namely $S_{\text{last}}[u_z] = 1$ and $S_{\text{last}}[u_i] = 0$ for $1 \leq i < z$.
4. Let u, v be two nodes in T having the same label $\alpha[u] = \alpha[v]$, then if the triplets of u precedes the triplets of v in S, then the contiguous block of children of u in S precedes the contiguous block of children of v in S.

Property 3

Let $c \in \Sigma$ be an internal node label, and let $S[j_1, j_2]$ be all triplets whose π-components are prefixed by c. If u is the i-th node labeled c in S_α, its children occur contiguously within $S[j_1, j_2]$ and delimited by the $i-1$-th and i-th bit set to 1 in $S_{\text{last}}[j_1, j_2]$.

4.3.3 XBWT Construction

A naive approach to build the XBWT would be to explicitly construct S through the concretization of π-strings and then sort it using a stable sorting algorithm.

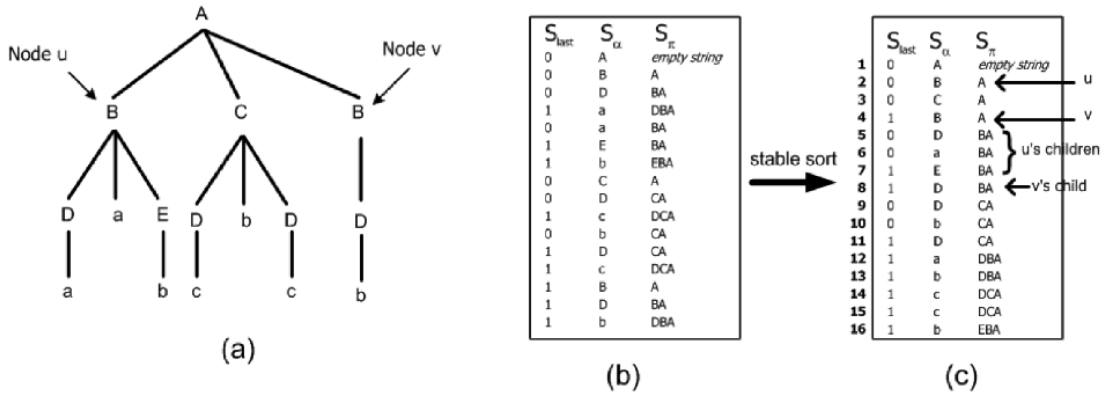

Figure 4.1: (a) A labeled tree T where $\Sigma_N = \{A, B, C, D, E\}$ and $\Sigma_L = \{a, b, c\}$. Notice that $\alpha[u] = \alpha[v] = B$ and $\pi[u] = \pi[v] = A$. (b) The multi-set S obtained after the pre-order visit of T. (c) The final multi-set S after the stable sort based on the π's component of its triplets.

However, this approach would require $\Theta(t^2)$ space in the worst case, which is not feasible for large deep trees. To overcome this issue, Ferragina et al. [6] proposed a more efficient algorithm that builds S in linear time and $O(t \log t)$ space.

The linear time algorithm is called **pathSort**, it is based on a generalization of the Skew algorithm for suffix array construction of strings [14]. Let's see briefly how the Skew algorithm works.

Skew Algorithm

The Skew algorithm is an efficient method for constructing the suffix array of a string in linear time. A suffix array is a data structure that lists the starting indices of all the suffixes of a string in lexicographical order, and it is widely used in various string processing algorithms.

Algorithm Overview

1. Divide the String

The algorithm begins by partitioning the indices of the string into three groups based on their modulo 3 value:

- S_0: Indices congruent to 0 mod 3.
- S_1: Indices congruent to 1 mod 3.
- S_2: Indices congruent to 2 mod 3.

The suffixes starting at positions in S_1 and S_2 are combined into a single group called S_{12}.

2. Sort Suffixes in S_{12}

To sort the suffixes in S_{12}, the algorithm considers the triplets of characters starting at each position in S_{12}. These triplets are sorted using a linear-time sorting algorithm, such as radix sort, and then renamed by assigning each triplet an integer value representing its rank in the sorted order. If all triplets are unique, the sorting

is complete; otherwise, the same procedure is applied recursively to the sequence of ranks obtained.

3. Sort Suffixes in S_0

Once the suffixes in S_{12} are sorted, the algorithm proceeds to sort the suffixes in S_0. To compare two suffixes starting at positions i and j in S_0, it compares the first characters of their respective substrings. If these are equal, it compares the suffixes starting at positions $i+1$ and $j+1$, whose ranks are already known from the sorting of S_{12}.

4. Merge the Sorted Orders

Finally, the sorted orders of the suffixes in S_0 and S_{12} are merged to obtain the complete suffix array of the original string. This merging process can be performed in linear time, ensuring the overall efficiency of the algorithm.

PathSort Algorithm

The pseudocode of the pathSort algorithm is shown in Algorithm 2. As we can see the algorithm is based on the Skew algorithm, but it is adapted to work on labeled trees. The main idea is to recursively sort the upward subpaths of the tree starting at nodes in levels $\not\equiv j \pmod 3$, then sort the upward subpaths starting at nodes in levels $\equiv j \pmod 3$ using the result of the previous step, and finally merge the two sets of sorted subpaths by exploiting their lexicographic names. The value of j is chosen in such a way that the number of nodes in `IntNodes` whose level is $\equiv j \pmod 3$ is at least $t/3$ so that a constant fraction of upward paths are ensured to be dropped at each recursive step. Is important to note that:

1. The height of the new (contracted) tree shrinks by a factor three, hence the node naming requires the radix sort over triples of names;
2. given the choice of j, the number of nodes of the new (contracted) tree will be at most $2t/3$, thus ensuring that the running time of the algorithm satisfies the recurrence $R(t) = R(2t/3) + \Theta(t) = \Theta(t)$;
3. following an argument similar to [14], the names of the dropped subpaths can be computed in $O(t)$ time from the names of the non dropped subpaths, by radix sorting.

Recursive Step of PathSort

At each recursive step, the algorithm constructs the array `IntNodes` (as shown in Figure 4.1-(b)), which stores the triplets $(\alpha[u], \text{level}(u), \text{parent}(u))$ for every internal node u in the given tree T.

Next, the algorithm selects a value j such that the number of nodes in `IntNodes` with depth $\equiv j \pmod 3$ is at least $t/3$. Based on this choice, two separate arrays are created:

- `IntNodesAtPosJ`, containing nodes at levels $\equiv j \pmod 3$,
- `IntNodesNotAtPosJ`, containing nodes at levels $\not\equiv j \pmod 3$

Algorithm 2 PathSort(T)

1: Create the array `IntNodes`$[1, t]$, initially empty.
2: Visit the internal nodes of T in pre-order. Let u denote the i-th visited node.
3: Write in `IntNodes`$[i]$ the symbol $\alpha[u]$, the level of u in T, and the position in `IntNodes` of u's parent.
4: Let $j \in \{0, 1, 2\}$ be such that the number of nodes in `IntNodes` whose level is $\equiv j \pmod 3$ is at least $t/3$. Sort recursively the upward subpaths starting at nodes in levels $\not\equiv j \pmod 3$.
5: Sort the upward subpaths starting at nodes in levels $\equiv j \pmod 3$ using the result of Step 3.
6: Merge the two sets of sorted subpaths by exploiting their lexicographic names.

For each node u in `IntNodesNotAtPosJ`, the algorithm extracts the upward path consisting of the first three ancestors of u. These paths are then sorted using radix sort. If the sorted upward paths contain duplicates, the algorithm recursively calls the PathSort function on a new contracted tree, where nodes are renamed according to their sorted paths. Otherwise, if all upward paths are unique, the nodes in `IntNodesAtPosJ` are sorted and subsequently merged with `IntNodesNotAtPosJ` using lexicographic ordering, following the same merging strategy as in the Skew algorithm.

4.3.4 Inverting the XBWT

Property 3 4.3.2 ensures that the two array S_{last} and S_α of the XBWT can be used to reconstruct the original tree T. The algorithm to invert the XBWT is linear in time and requires $O(t \log t)$ bits of space.

The algorithm 3 initially builds the array F that stores the first entry in S whose π-component is prefixed by a symbol x (F approximates S_π at its first symbol). Then, it exploits the array F to efficiently build the array J that stores the position in S of the first child of each node in T. Finally, the algorithm deploys the array J to simulate a depth-first visit of T, creates its labeled nodes, and properly connects them to their parents.

Algorithm 3 RebuildTree(`xbw[`T`]`)

```
1: F = BuildF(xbw[T]); ▷ F[x] = first entry in S whose π-component is prefixed by symbol x
2: J = BuildJ(xbw[T], F); ▷ J[i] = position in S of the first child of S[i]; J[i] = −1 if leaf
3: Create node r and set Q = {(1, r)}; ▷ Q is a stack
4: while Q ≠ ∅ do ▷ We still have nodes to create in T
5:     ⟨i, u⟩ = pop(Q);
6:     j = J[i]; ▷ Take the block of u's children in S
7:     if j = −1 then ▷ u is a leaf of T
8:         continue;
9:     end if
10:    Find first j′ ≥ j such that S_last[j′] = 1; ▷ S[j, j′] are the children of u in T
11:    for h = j′ downto j do ▷ Recall that Q is a stack
12:        Create the node v labeled S_α[h];
13:        Attach v as first child of u;
14:        push(⟨h, v⟩, Q);
15:    end for
16: end while
17: return node r.
```

Algorithm 4 BuildF(`xbw[`T`]`)

```
1: for i = 1, ..., |Σ_N| do
2:     C[S_α[i]] ← C[S_α[i]] + 1; ▷ Count the occurrences of node labels
3: end for
4: F[1] = 2; ▷ S_π[1] is the empty string
5: for i = 1, ..., |Σ_N| − 1 do ▷ Consider just the internal-node labels
6:     s = 0; j = F[i];
7:     while s ≠ C[i] do ▷ Not all blocks of children have been passed
8:         if S_last[j++] = 1 then s++; ▷ One further block of children has passed
9:         end if
10:    end while
11:    F[i + 1] = j;
12: end for
13: return F.
```

Algorithm 5 BuildJ(`xbw[`T`]`, F)

```
1: for i = 1, ..., t do
2:     if S_α[i] ∈ Σ_L then
3:         J[i] = −1;                                  ▷ S_α[i] is a leaf label
4:     else
5:         z = J[S_α[i]];
6:         while S_last[z] ≠ 1 do z++;                 ▷ Reach the last child of S_α[i]
7:         end while
8:         F[S_α[i]] = z + 1;
9:     end if
10: end for
11: return J.
```

4.3.5 Compressing Labeled Trees

Let the k-context of a node u in a tree T be defined as the first k symbols of the π-component of the triplet associated with u. We denote this k-long prefix as $\pi_k[u]$. Thus, $\pi_k[u]$ represents the subpath of length k leading to u in T, or equivalently, the node u descends from a subpath labeled as $\pi_k[u]$, where the nodes in $\pi_k[u]$ are encountered in an upward direction.

The XBW[T] exhibits a local homogeneity property on the string S_α, which can be demonstrated through the concept of k-contexts on trees. This property mirrors the strong local homogeneity exhibited by strings under the Burrows-Wheeler Transform [Burrows and Wheeler 1994] when applied to labeled trees. Specifically, node labels in T are distributed across S_α in a manner that clusters together those labels originating from "similar" upward paths that share long prefixes.

To illustrate this, let us consider two arbitrary nodes u and v in T, and examine their contexts $\pi[u]$ and $\pi[v]$. Given the sorting of S, the greater the length of the shared prefix between $\pi[u]$ and $\pi[v]$, the closer the corresponding labels $\alpha[u]$ and $\alpha[v]$ will be in the string S_α. These closely spaced labels are expected to be few in number, resulting in S_α exhibiting local homogeneity. As a consequence, we can leverage the advanced algorithmic techniques developed for BWT-based compression methods to achieve efficient compression.

At the end, the XBWT is used for turning the labeled tree compression problem into a string compression problem. To this aim, two string compressors C_α and C_{last} are used to squeeze the two strings that compose XBW[T], by exploiting their fine specialties. Of course, many choices are possible for C_{last} and C_α, each having implications on the algorithmic time and compression bounds.

In general, let C_α be a k-th order string compressor that compresses any string w into $|w|H_k(w) + |w| + o(|w|)$ bits, taking $O(|w|)$ time; and let C_{last} be an algorithm that stores S_{last} without compression. With this simple instantiation, the labeled tree T can be compressed within $tH_k(S_\alpha) + 2t + o(t)$ bits and takes $O(t)$ optimal time.

4.3.6 Indexing a compressed labeled tree

In order to implement the efficient operations listed in 4.2.2 using the compressed arrays S_{last} and S_α of XBWT, we need that the chosen compressors C_α and C_{last} support the following operations:

Given a string $S[1,t]$ over alphabet Σ

- $rank_c(S,q)$: gives the number of times the symbol $c \in \Sigma$ appears in $S[1,q]$.
- $select_c(S,i)$: gives the position of the i-th occurrence of the symbol $c \in \Sigma$ in S.

The compressed indexing of XBWT$[T]$ will be based on three compressed data structures that support rank and select queries over the two strings S_α and S_{last}, and over an auxiliary binary array $A[1,t]$ defined as: $A[1] = 1$, $A[j] = 1$ if and only if the first symbol of $S_\pi[j]$ differs from the first symbol of $S_\pi[j-1]$. Hence, A contains at most $|\Sigma|+1$ bits set to 1 out of t positions. It is also easy to see that, by means of rank and select operations over A, we can succinctly implement the array F deployed in the algorithms 3 and 4.

The following methods are supported by the compressed index:

- **GetRankedChild(i, k)**: returns the position in S of the k-th child of u; the output is -1 if this child does not exist. As an example, `GetRankedChild(2, 2) = 6` in Figure 4.1.
- **GetCharRankedChild(i, c, k)**: returns the position in S of the triplet representing the k-th child of u among the ones whose label is c. The output is -1 if this child does not exist. As an example, `GetCharRankedChild(1, B, 2) = 4` in Figure 4.1.
- **GetDegree(i)**: returns the number of children of u.
- **GetCharDegree(i, c)**: returns the number of children of u labeled c.
- **GetParent(i)**: returns the position in S of the triplet representing the parent of u. The output is -1 if $i = 1$ (the root). As an example, `GetParent(8) = 4` in Figure 4.1.
- **GetSubtree(i)**: returns the node labels of the subtree rooted at u. Any possible order (i.e., pre, in, post) may be implemented.
- **SubPathSearch(P)**: determines the range $S[\text{First}, \text{Last}]$ of nodes, which are immediate descendants of each occurrence of the labeled path $P = c_1 c_2 \cdots c_k$ in T. Note that all strings in $S_\pi[\text{First}, \text{Last}]$ are prefixed by P^R. As an example, `SubPathSearch(BD) = [12, 13]` and `SubPathSearch(AB) = [5, 8]` in Figure 4.1.

It is important to note that their time complexity is dependent on the specific implementation for rank and select over the compressed strings S_α and S_{last}.

Let's now see how to implement some of the above methods (from which the others can be derived) using the rank and select operations over the compressed strings S_α and S_{last}.

GetChildren(i)

Algorithm 6 GetChildren(i)

1: **if** $S_\alpha[i] \in \Sigma_L$ **then**
2: **return** -1 ▷ $S[i]$ is a leaf
3: **end if**
4: $c \leftarrow S_\alpha[i]$ ▷ $S[i]$ is labeled c
5: $r \leftarrow \text{rank}_c(S_\alpha, i)$
6: $y \leftarrow \text{select}_1(A, c)$ ▷ $y = F[c]$
7: $z \leftarrow \text{rank}_1(S_{\text{last}}, y - 1)$
8: $\text{First} \leftarrow \text{select}_1(S_{\text{last}}, z + r - 1) + 1$
9: $\text{Last} \leftarrow \text{select}_1(S_{\text{last}}, z + r)$
10: **return** (First, Last)

The algorithm exploits directly the properties described before, in particular the Property 3 (4.3.2). The rank operation at line 5 is used to get the number r of nodes labeled c up to position i in S_α. Then, the position $F[c]$through a select operation on A (line 6). By Property 3, the children of $S[i]$ are located at the r-th block of children following position $F[c]$. Lines $8 - 9$ identify this block.

GetParent(i)

Algorithm 7 GetParent(i)

1: **if** $i == 1$ **then**
2: **return** -1 ▷ $S[i]$ is the root of $\mathcal{T}$
3: **end if**
4: $c \leftarrow \text{rank}_1(A, i)$
5: $y \leftarrow \text{select}_1(A, c)$
6: $k \leftarrow \text{rank}_1(S_{\text{last}}, i - 1) - \text{rank}_1(S_{\text{last}}, y - 1)$
7: $p \leftarrow \text{select}_c(S_\alpha, k + 1)$
8: **return** p

Algorithm 7 is based on the Property 3 (4.3.2) and it is the inverse of the GetChildren method. At line 4 the algorithm computes the label c of the parent of $S[i]$ that prefixes the upward path leading to $S[i]$. Then, the parent of $S[i]$ is searched among the nodes labeled c in S_α by exploiting Property 3 in a reverse manner. Namely, the number k of children-blocks in the range $S[y, i]$ is computed, these are children of nodes labeled c and preceding i in the stable sort of S. Then, the k-th occurrence of c in S_α is selected, which is properly the parent of $S[i]$.

SubPathSearch(P)

Algorithm 8 SubPathSearch(P)

```
1: First ← F(c_1); Last ← F(c_1 + 1) − 1
2: if First > Last then
3:     return "P is not a subpath of T"
4: end if
5: for i ← 2, ..., k do
6:     k_1 ← rank_{c_i}(S_α, First − 1); z_1 ← select_{c_i}(S_α, k_1 + 1)        ▷ first entry in S_α[First, t] labeled c_i
7:     k_2 ← rank_{c_i}(S_α, Last); z_2 ← select_{c_i}(S_α, k_2)        ▷ last entry in S_α[1, Last] labeled c_i
8:     if z_1 > z_2 then
9:         return "P is not a subpath of T"
10:    end if
11:    First ← GetRankedChild(z_1, 1)        ▷ get the first child of S[z_1]
12:    Last ← GetRankedChild(z_2, GetDegree(z_2))        ▷ get the last child of S[z_2]
13: end for
14: return (First, Last)
```

We assume that $P = c_1 c_2 \cdots c_k$ algorithm SubPathSearch computes the range $[First, Last]$ in $|P| = l$ phases, each one preserving the following invariant:

- Invariant of Phase i. At the end of the phase, $S_\pi[First]$ is the first entry prefixed by $P[1,i]^R$, and $S_\pi[Last]$ is the last entry prefixed by $P[1,i]^R$, where s^R is the reversal of string s.

At the beginning (i.e., $i = 1$), First and Last are easily determined via the entries $F[c_1]$ and $F[c_1 + 1] - 1$, which point to the first and last entry of S_π prefixed by c_1 (by definition of array F). Since we do not have the F array, we implement these operations via rank and select queries over array A. Let us assume that the invariant holds for Phase $i - 1$, and prove that the i-th iteration of the for-loop in algorithm SubPathSearch preserves the invariant. More precisely, let $S_\pi[First, Last]$ be all entries prefixed by $P[1, i-1]^R$. So $S[First, Last]$ contains all nodes descending from $P[1, i-1]$. SubPathSearch determines $S[z_1]$ (respectively $S[z_2]$) as the first (respectively last) node in $S[First, Last]$ that descends from $P[1, i-1]$ and is labeled c_i, if any. Then it jumps to the first child of $S[z_1]$ and the last child of $S[z_2]$. From Property 2 (item 2), and the correctness of algorithms GetChildren and GetDegree, we infer that the positions of these two children are exactly the first (respectively last) entry in S whose π-component is prefixed by $P[1,i]^R$.

The time complexity of the SubPathSearch algorithm is $O(l)$, where l is the length of the input path P.

4.4 Implementation of the XBWT

The implementation of the XBWT is based on what has been described in the previous chapters. The implementation is written in C++ and is available on GitHub

at the following link: `https://github.com/davide-tonetto-884585/XBWT`.

4.4.1 Implementation choices

Follows a list of the main choices made during the implementation of the XBWT:

- The implementation is not focused on working for a specific kind of data such as XML documents or JSON files, but it is designed to work with any kind of labeled tree.
- The construction method of the XBWT class takes as input a labeled tree, and construct directly a compressed indexing scheme for it based on the Extended Burrows-Wheeler Transform of the tree as described in the previous chapters.
- In order for the XBWT to work we assume that the labels of the leaf nodes of the given labeled tree are lexicographically greater than the labels of the internal nodes. This is necessary to ensure that the navigational and search operations work correctly.
- The implementation is based on the Succinct Data Structure Library (SDSL) to handle the compressed data structures generated by the XBWT. The SDSL library provides efficient implementations of various compressed data structures and algorithms, which are essential for representing and querying the XBWT efficiently.
- The labels of the alphabet are encoded as integers, starting from 0 to $|\Sigma| - 1$, where $|\Sigma|$ is the cardinality of the alphabet. This encoding respect the order of the labels in the alphabet and allows simplifying and reduce the space needed to store the labels in the compressed data structures. For this reason the constructor of the XBWT class takes as input a generic labeled tree.

Succinct Data Structure Library (SDSL)

The Succinct Data Structure Library (SDSL) is a C++ library that provides efficient implementations of various compressed data structures and algorithms. It is used in this project to handle the compressed data structures generated by the XBWT. The SDSL library provides a wide range of succinct data structures, such as bit vectors, wavelet trees, and compressed suffix arrays, which are essential for representing and querying the XBWT efficiently. The library is available at `https://github.com/simongog/sdsl-lite` [10]. Let's see the implementation details of the SDSL data structures used in the XBWT implementation.

sdsl::rrr_vector

The `sdsl::rrr_vector` is a class of the Succinct Data Structure Library (SDSL), designed to provide space-efficient representations of bit vectors while supporting efficient rank and select operations. This data structure implements the RRR (Raman, Raman, and Rao) encoding method, which compresses bit vectors by partitioning them into fixed-size blocks and encoding each block based on its population count (the number of 1s) and specific configuration [18].

The space needed by `sdsl::rrr_vector` for a bit vector of length n with m set bits is $nH_0+o(n)$ ($\approx \lceil \log \binom{n}{m} \rceil$). The rank support is provided by `sdsl::rank_support_rrr` adding 80 bits and requiring $O(\log k)$ time for rank queries, where k is the number of set bits. The select support is provided by `sdsl::select_support_rrr` adding 64 bits and requiring $O(\log n)$ time for select queries.

sdsl::wt_int

The `sdsl::wt_int` is a class of the Succinct Data Structure Library (SDSL) that implements wavelet trees designed to efficiently handle sequences over large alphabets, such as integer sequences. It provides a space-efficient representation while supporting fast access, rank, and select operations. The wavelet tree is a balanced binary tree that recursively partitions the alphabet into two equal-sized subsets and encodes the sequence based on the partitioning [11]. The `sdsl::wt_int` uses the RRR compressed bit vectors or other succinct representations for storing the bit vectors in each node of the wavelet tree. This makes the structure space-efficient.

In the case of RRR compressed bit vectors the space needed by `sdsl::wt_int` for a sequence of length n over an alphabet of size σ is $nH_0(S)+o(n \log \sigma)+\Theta(\sigma \log n)$ bits, where $H_0(S)$ is the zero-order empirical entropy of the sequence S. Also supports query access, rank and select operations in $O(\log \sigma)$ time.

Details of the XBWT Class Elements

The XBWT class utilizes several data structures from the SDSL library to efficiently represent and query the compressed data. Below are the details of the main elements used in the class:

- `sdsl::rrr_vector<> SLastCompressed`: This is a compressed bit vector that stores the S_{last} array of the XBWT.
- `sdsl::wt_int<sdsl::rrr_vector<» SAlphaCompressed`: This is a wavelet tree built on top of a compressed bit vector. The wavelet tree is used to compress and index the S_α array of the XBWT.
- `sdsl::rrr_vector<> SAlphaBitCompressed`: Another compressed bit vector used to store the additional bit of S_α needed to distinguish between internal and leaf nodes.
- `sdsl::rrr_vector<> ACompressed`: A compressed bit vector representing the A array of the XBWT used to in the F array of the XBWT.
- `sdsl::rrr_vector<>::rank_1_type SLastCompressedRank`: A rank support structure for the `SLastCompressed` bit vector, allowing efficient rank queries.
- `sdsl::rrr_vector<>::select_1_type SLastCompressedSelect`: A select support structure for the `SLastCompressed` bit vector, allowing efficient select queries.
- `sdsl::rrr_vector<>::rank_1_type ACompressedRank`: A rank support structure for the `ACompressed` bit vector.

- `sdsl::rrr_vector<>::select_1_type ACompressedSelect`: A select support structure for the `ACompressed` bit vector.
- `std::unordered_map<T, unsigned int> alphabetMap`: An hash map that maps each label in the alphabet to a unique integer.
- `unsigned int cardSigma`: The cardinality of the alphabet Σ.
- `unsigned int cardSigmaN`: The cardinality of the Σ_N alphabet. Where Σ_N is the set of labels that appear in the internal nodes of the labeled tree.
- `unsigned int maxNumDigits`: The maximum number of digits that has the integer code associated to the greater label in the alphabet (needed to sort the labels in the alphabet).

The overall space complexity of the XBWT class can be derived from the space complexity of the compressed data structures used in the class.

4.4.2 Construction of the XBWT

The construction of the XBWT is done by the constructor of the XBWT class. The constructor takes as input a generic labeled tree and constructs the compressed indexing scheme using the linear pathSort (also the naive construction method can be used by passing the boolean flag `usePathSort = false`). The construction process is divided into the following steps:

1. **Alphabet Encoding**: The first step is to encode the labels of the alphabet as integers. The labels are sorted in lexicographical order and assigned a unique integer code starting from 1 to $|\Sigma|$. Two hash maps are used to map each label to a unique integer and vice versa.
2. **Construct `intNodes` array**: The next step is to construct the `intNodes` array as described in the previous chapters. `intNodes` is an array of triplets of length t in which node is represented as a triplet containing the node's label, its level, and the index of its parent node in the array (from 1 to t, root has parent 0). The nodes are inserted in preorder traversal of the labeled tree.
3. **Sort `intNodes` array:** Call the `pathSort` or `upwardStableSortConstruction` (naive method) method to get the sorted array of nodes `intNodes`.
4. **Construct S_{last} array**: Construct the S_{last} array by iterating over the sorted `intNodes` array.
5. **Construct S_α array**: Construct the S_α array by iterating over the sorted `intNodes` array, along with the additional bit array to distinguish between internal and leaf nodes.
6. **Construct A array**: Construct the A array by iterating over the sorted `intNodes` array.
7. **Construct rank and select support structures**: Construct the rank and select support structures for the compressed bit vectors.

4.4.3 Navigational Operations

The XBWT class provides several navigational operations to traverse the labeled tree and retrieve information about the nodes. The navigational operations implemented are:

- `getChildren(unsigned int i)`: This method returns a pair of integers representing the indices of the leftmost and rightmost children of the node at index `i`.
- `getRankedChild(unsigned int i, unsigned int k)`: This method returns the index of the `k`-th child of the node at index `i`.
- `getCharRankedChild(unsigned int i, T label, unsigned int k) const`: This method returns the index of the `k`-th child of the node at index `i` with the specified label.
- `getDegree(unsigned int i)`: This method returns the degree (number of children) of the node at index `i`.
- `getCharDegree(unsigned int i, T label)`: This method returns the number of children of the node at index `i` with the specified label.
- `getParent(unsigned int i)`: This method returns the index of the parent of the node at index `i`.
- `getSubtree(unsigned int i, unsigned int order = 0)`: This method returns a vector containing the labels of the nodes in the subtree rooted at index `i`. The `order` parameter specifies the traversal order (e.g., preorder, post-order).

All the methods refer to the index of the nodes in S_{last} and S_α arrays.

4.4.4 Search Operations

The XBWT class provides search operation `subPathSearch(const std::vector<T> &path)` that searches for a subpath in the XBWT structure. It uses the compressed vectors to determine the range of positions corresponding to the nodes whose upward path is prefixed by a given vector reversed.

4.5 Experiments and Conclusions

The experiments have been run on a machine with an AMD Ryzen 9 5600Hs CPU with 24 GB of RAM. The results are shown in Table 4.1 and Table 4.2. The source code for the experiments can be found in the `experiments.cpp` file.

4.5.1 Experiments

Construction Performance of the XBWT

To evaluate the performance of the implemented algorithms, we conducted a series of experiments on randomly generated trees created using the Python library `networkx`. The trees were generated with sizes ranging from 100 to 900,000 nodes.

For each tree, we executed the construction algorithms 10 times, measuring the average execution time for both the linear *PathSort* (P.S.) algorithm and the naive *UpwardStableSort* (N.S.) algorithm used for constructing the XBWT. This approach allowed us to compare their performance across different tree sizes and assess their scalability.

The results are shown in Table 4.1.

Nodes	Depth	P.S. Time (s)	N.S. Time (s)
100	22	0.002	0.001
500	45	0.004	0.002
1000	74	0.006	0.003
5000	175	0.028	0.015
10000	288	0.056	0.053
50000	486	0.31	0.35
100000	754	0.69	1.25
500000	2246	4.7	16.46
900000	2658	8.51	34.2

Table 4.1: Performance comparison between PathSort and Naive Sort algorithms.

Space Analysis of the XBWT

To evaluate the space savings achieved through XBWT compression, we conducted experiments on the same set of randomly generated trees used for the construction performance tests. For each tree, we compared the memory usage (in bytes) of three representations: the plain tree, the uncompressed XBWT, and the compressed XBWT.

The plain tree representation consists of the simple balanced parenthesis encoding of the tree structure combined with the edge labels. For example for tree in Figure 4.1, the plain tree representation would be:

`(A(B(D(a))(a)(E(b)))(C(D(c))(b)(D(c)))(B(D(b)))).`

By *uncompressed XBWT*, we refer to the XBWT arrays S_{last} and S_α (including the additional bit) stored without any compression. Specifically, S_{last} is represented as a plain bitvector (`sdsl::bit_vector`), and S_α is stored as a wavelet tree (`sdsl::wt_int`) with plain bitvectors (`sdsl::bit_vector`). In contrast, the *compressed XBWT* representation stores S_{last} and S_A as compressed RRR bitvectors (`sdsl::rrr_vector`), and S_α as a wavelet tree with RRR bitvectors, as described in the previous chapter.

Table 4.2 reports the sizes (in bytes) for each representation of the trees across different sizes. The last column highlights the space savings achieved by the compressed XBWT compared to the plain tree representation, expressed as a percentage. These results illustrate the substantial space reductions achieved through compression, especially as the tree size increases.

Nodes	Plain tree (B)	U. XBWT (B)	C. XBWT (B)	Saving (%)
100	390	424	496	-27.18
500	2390	1112	1136	52.47
1000	4890	2242	2056	57.96
5000	28890	12911	10400	64
10000	58890	45625	21848	62.90
50000	338890	175146	123216	63.64
100000	688890	349478	259376	62.35
500000	3888890	1850850	1451570	62.67
900000	7088890	3480190	2718570	61.65

Table 4.2: Space analysis of the XBWT. Plain tree is the size in bytes of the tree in the simple balanced parenthesis representation plus the edge labels, U. XBWT is the size in bytes of the tree in the uncompressed XBWT, and C. XBWT is the size in bytes of the tree in the compressed XBWT. The last column shows the space-saving percentage between plain tree and compressed XBWT.

4.5.2 Conclusions

From the results shown in Table 4.1, we can draw several conclusions about the performance of the PathSort (P.S.) algorithm compared to the Naive Sort (N.S.) algorithm and the space savings achieved by compressing the XBWT.

Firstly, the PathSort algorithm consistently outperforms the Naive Sort algorithm in terms of execution time, especially as the number of nodes increases. For smaller trees, the difference in execution time between the two algorithms is minimal. However, as the number of nodes grows, the PathSort algorithm demonstrates significantly better scalability. For instance, with 900,000 nodes, the PathSort algorithm takes 8.51 seconds, whereas the Naive Sort algorithm takes 34.2 seconds.

Secondly, the depth of the tree appears to increase with the number of nodes, which is expected in randomly generated trees. This increase in depth does not seem to adversely affect the performance of the PathSort algorithm as much as it does the Naive Sort algorithm.

For small trees, the compressed XBWT does not always provide immediate savings due to the overhead of succinct data structures. For instance, for 100 nodes, the compressed representation is larger than the plain tree, showing a -27.18% increase in space. However, as the number of nodes increases, the compression becomes more effective, achieving savings of over 60% for large trees.

The space reduction becomes particularly evident for trees with more than 500 nodes. These results confirm that the compressed XBWT provides a scalable and space-efficient alternative for storing and indexing labeled trees. The efficiency gains are particularly beneficial for applications requiring large-scale tree processing, such as bioinformatics and text indexing.

In conclusion, the PathSort algorithm is a more efficient choice for constructing the XBWT, especially for larger trees, and the compression method provides significant space savings, making the overall process more efficient in terms of both time and space.

Future Work

There are several directions for future work that could be explored to further improve the performance of the algorithm. One possible avenue is to investigate the impact of different tree structures on the performance of the algorithm. For instance, it would be interesting to see how the algorithm performs on trees with different branching factors or depths.

Also, the algorithm could be parallelized in order to take advantage of multicore processors and further improve the scalability of the algorithm. This could potentially reduce the execution time even further, especially for very large trees.

Chapter 5

Min-Weight Perfect Bipartite Matching

5.1 Problem definition

Given a weighted bipartite graph $G = (V, E)$ (remember that a bipartite graph is a graph whose vertices can be divided into two disjoint sets V_1 and V_2 such that every edge connects a vertex in V_1 to a vertex in V_2), let's define the concept of a matching.

Definition 6 (Matching)**.** *A matching $M \in E$ is a collection of edges such that every vertex of V is incident to at most one edge of M. In other words, a matching is a set of edges such that no two edges share a common vertex.*

If a vertex v has no edge of M incident to it then v is said to be exposed (or unmatched). A matching is perfect if no vertex is exposed; in other words, a matching is perfect if its cardinality is equal to $|V_1| = |V_2|$ [9].

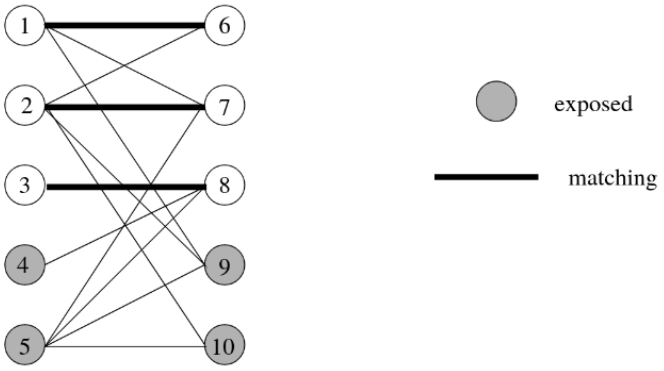

Figure 5.1: Example of a perfect matching in a bipartite graph.

The problem of finding a minimum weight perfect matching in a bipartite graph is a well-known problem in combinatorial optimization. The problem can be formulated as follows:

Definition 7 (Minimum weight perfect matching in bipartite graphs (MWPBM))**.** *Given a weighted bipartite graph $G = (V, E)$, where $V = V_1 \cup V_2$ and $V_1 \cap V_2 = \emptyset$, find a perfect matching M such that the sum of the weights of the edges in M is minimized. The weight of a matching is the sum of the weights of the edges in the matching. The weight of an edge $e = (u, v)$ is denoted by $w(e)$. This problem is also called* ***the assignment problem****.*

5.1.1 The existence of perfect matchings in bipartite graphs

In this subsection a theorem is introduced that states a condition for the existence of perfect matchings in bipartite graphs. This theorem will be useful in the following chapter to proof our reduction [17].

Let's start with the definition of the **Tutte matrix** of a bipartite graph.

Definition 8 (Tutte matrix)**.** *The Tutte matrix of bipartite graph $G = (U, V, E)$ is an $n \times n$ matrix M with the entry at row i and column j*

$$M_{i,j} = \begin{cases} 0, & \text{if } (u_i, u_j) \notin E \\ x_{i,j}, & \text{if } (u_i, u_j) \in E \end{cases} \tag{5.1}$$

The determinant of the Tutte matrix is useful in testing whether a graph has a perfect matching or not, as the following theorem shows.

Theorem 3 (Existence of perfect matchings in bipartite graphs)**.** *Given a bipartite graph G and the Tutte matrix M for G then the following equivalence holds:*

$$Det(M) \neq 0 \iff \text{There exists a perfect matching in } G$$

Proof. We have the following expression for the determinant:

$$\mathrm{Det}(M) = \sum_{\pi \in S_n} (-1)^{sgn(\pi)} \prod_{i=1}^{n} M_{i,\pi(i)}$$

where S_n is the set of all permutations on $[n]$, and $sgn(\pi)$ is the sign of the permutation π. There is a one-to-one correspondence between a permutation $\pi \in S_n$ and a (possible) perfect matching

$$\{(u_1, v_{\pi(1)}), (u_2, v_{\pi(2)}), \cdots, (u_n, v_{\pi(n)})\} \text{ in } G.$$

Note that if this perfect matching does not exist in G (i.e., some edge $(u_i, v_{\pi(i)}) \notin E$), then the term corresponding to π in the summation is 0. So we have

$$\mathrm{Det}(M) = \sum_{\pi \in P} (-1)^{sgn(\pi)} \prod_{i=1}^{n} x_{i,\pi(i)}$$

where P is the set of perfect matchings in G. This is clearly zero if $P = \emptyset$, i.e., if G has no perfect matching. If G has a perfect matching, there is a $\pi \in P$ and the term corresponding to π is

$$\prod_{i=1}^{n} x_{i,\pi(i)} \neq 0.$$

Additionally, there is no other term in the summation that contains the same set of variables. Therefore, this term is not cancelled by any other term. So in this case, $\mathrm{Det}(M) \neq 0$. □

5.1.2 Problem formulation

The problem of finding a minimum weight perfect matching in a bipartite graph can be formulated as an integer linear program (ILP), i.e.an optimization problem in which the variables are restricted to integer values and the constraints and the objective function are linear as a function of these variables. Given a matching M, let x be its incidence vector where $x_{ij} = 1$ if edge (i, j) is in the matching, and $x_{ij} = 0$ otherwise. Then, the problem can be formulated as follows:

$$\begin{aligned} \text{minimize} \quad & \sum_{(i,j)\in E} w_{ij}x_{ij} \\ \text{subject to} \quad & \sum_{j\in V_2} x_{ij} = 1, \quad \forall i \in V_1 \\ & \sum_{i\in V_1} x_{ij} = 1, \quad \forall j \in V_2 \\ & x_{ij} \in \{0, 1\}, \quad \forall (i, j) \in E \end{aligned} \tag{5.2}$$

Notice that any solution to this integer program corresponds to a matching and therefore this is a valid formulation of the minimum weight perfect matching problem in bipartite graphs.

The linear program relaxation of the above integer program is as follows:

$$\begin{aligned} \text{minimize} \quad & \sum_{(i,j)\in E} w_{ij}x_{ij} \\ \text{subject to} \quad & \sum_{j\in V_2} x_{ij} = 1, \quad \forall i \in V_1 \\ & \sum_{i\in V_1} x_{ij} = 1, \quad \forall j \in V_2 \\ & 0 \le x_{ij} \le 1, \quad \forall (i, j) \in E \end{aligned} \tag{5.3}$$

The set of feasible solutions to the constraints in (P) forms a polytope. When optimizing a linear constraint over a polytope, the optimum will be achieved at one of the "corners" or extreme points of the polytope. An extreme point x of a set Q is an element $x \in Q$ that cannot be expressed as $\lambda y + (1 - \lambda)z$ with $0 < \lambda < 1$, $y, z \in Q$, and $y \neq z$. (This concept will be formalized and discussed in more detail when we cover polyhedral theory.)

In general, even if all the coefficients of the constraint matrix in a linear program are either 0 or 1, the extreme points of a linear program are not guaranteed to have all coordinates integral. This is not surprising since the general integer programming problem is NP-hard, while linear programming is solvable in polynomial time. Consequently, there is no guarantee that the value Z_{IP} of an integer program is equal to the value Z_{LP} of its LP relaxation. However, since the integer program is more constrained than the relaxation, we always have $Z_{IP} \geq Z_{LP}$, implying that Z_{LP} is a lower bound on Z_{IP} for a minimization problem. Moreover, if an optimal solution to a linear programming relaxation is integral, then it must also be an optimal solution to the integer program.

In our problem, the constraint matrix has a special form that lead to the following result:

Theorem 4. *Any extreme point of (P) is a* $0-1$ *vector and, hence, is the incidence vector of a perfect matching.*

Consequently, the polytope

$$\begin{aligned} P = \{x : \sum_{j \in V_2} x_{ij} = 1, \quad & \forall i \in V_1, \\ \sum_{i \in V_1} x_{ij} = 1, \quad & \forall j \in V_2, \\ 0 \leq x_{ij} \leq 1, \quad & \forall (i,j) \in E\} \end{aligned} \tag{5.4}$$

is called the bipartite perfect matching polytope.

5.2 Solutions to the problem

There are several algorithms to solve the problem of finding a minimum weight perfect matching in a bipartite graph. The first algorithm to solve this problem was proposed by Kuhn in 1955 [16]. The algorithm is based on the Hungarian method, which is a combinatorial optimization algorithm that solves the assignment problem in polynomial time. In the original paper the complexity of the algorithm was $O(n^4)$, but later Dinic and Kronrod [4] showed that the algorithm can be implemented in $O(n^3)$ time.

The Hungarian method is a powerful algorithm, however, the algorithm is not very intuitive and can be difficult to implement. In recent years, several other algorithms have been proposed to solve the problem of finding a minimum weight perfect matching in a bipartite graph. In 1970, Edmonds and Karp [5] proposed an algorithm that solves the problem in $O(nm + n^2 \log n)$ time. In 1989 Gabow and Tarjan [7] proposed an algorithm that solves the problem in $O(\sqrt{n}m \log(nW))$ time, where n, m and W denote the number of vertices, number of edges, and largest magnitude of a cost; costs are assumed to be integral. The algorithms work by scaling. Lastly, in 2009, Sankowski and Piotr [20] introduced a randomized algorithm that solves the problem in $O(Wn^w)$ time, where w is the exponent of matrix multiplication, and W is the highest edge weight in the graph.

In 2022, Chen, Li, et al. [2] proposed a new solution to the Minimum-Cost Flow problem that woks in almost-linear time, precisely in $O(m^{1+o(1)})$ time. The minimum-cost flow problem is a classic combinatorial graph problem that find numerous applications in engineering and scientific computing. This result is important also for our problem, since the maximum weight perfect matching problem can be reduced to the minimum-cost flow problem, allowing to solve the problem in almost-linear time.

5.3 Implementation used in this work

In this section, we will present an implementation of the Gabow and Tarjan algorithm to solve the problem of finding a minimum weight perfect matching in a bipartite graph. The algorithm is based on scaling and is a generalization of the Hungarian method. The algorithm works by scaling the edge weights and then finding a perfect matching in the scaled graph.

Chapter 6

Reduction to the assignment problem

6.1 Introduction

In this chapter, we will show how we can reduce the problem of finding the optimal partition of the nodes of a tree T given their equivalence classes into p with $p \leq |E| \leq t$ chains to the Minimum Weight Perfect Bipartite Matching problem, where E is the set of equivalence classes of the nodes of T and t is the number of nodes of the tree. This reduction will allow us to solve the problem in polynomial time as shown in the previous chapter.

Then we will show how to optimize the reduction by introducing some constraints that will allow us to reduce the number of edges in the bipartite graph, and we will also show how to move from the Minimum Weight Perfect Bipartite Matching problem to the more studied Maximum Weight Perfect Bipartite Matching problem without losing generality.

6.2 The reduction

6.2.1 Bipartite graph construction

Let T be a tree with t nodes and p, which is the number of chains we want to partition the nodes into. Let E be the set of equivalence classes of the nodes of T. We can construct a bipartite graph $G = (V, E)$ such that vertices are divided in two disjoint sets $V = V_1 \cup V_2$ in the following way:

Definition 9. *The two sets V_1 and V_2 of the bipartite graph G are constructed in the following way:*

- *V_1 contains $t + p$ nodes composed by p source nodes $s_1, s_2, \ldots, s_p$ and the t elements of E ordered.*
- *V_2 contains $t + p$ nodes composed by the t elements of E ordered and p destination nodes $d_1, d_2, \ldots, d_p$.*

Then the edges of the graph G will be constructed in the following way:

1. *The sources nodes $s_i \in V_1$ for $i = 1, 2, \ldots, p$ are connected to the first p nodes with distinct equivalence class in V_2 with weight 1.*
2. *Each of the t nodes of the tree in V_1 is connected to the first p (at most) nodes with distinct class in V_2 (and without the same class of the considered node) coming after it in the ordering of the nodes with weight 1.*

3. *Each of the t nodes of the tree in V_1 is also connected to the first node with its same class in V_2 coming after it in the ordering of the nodes of t with weight 0 iff there is one, otherwise p edges with weight 0 are added to each of the destination nodes $d_i \in V_2$ for $i = 1, 2, \ldots, p$.*

Notice that it is important to consider the order of the nodes of the two sets V_1 and V_2 as stated above, because we will need to connect the source nodes to the destination nodes in a way that will allow us to find the optimal partition of the nodes of the tree. In Figure 6.4 the nodes are ordered from top to bottom. An example of the node structure is shown in Figure 6.1.

Notice also that when we talk about the same V_1 node placed in V_2 we are referring to the corresponding node in V_2 that derives from the same node in the original tree T since the nodes of the tree are placed ordered in both sets V_1 and V_2. In Figure 6.1, 6.4 and 6.2 the node's correspondence is achieved by putting the two nodes at the same level.

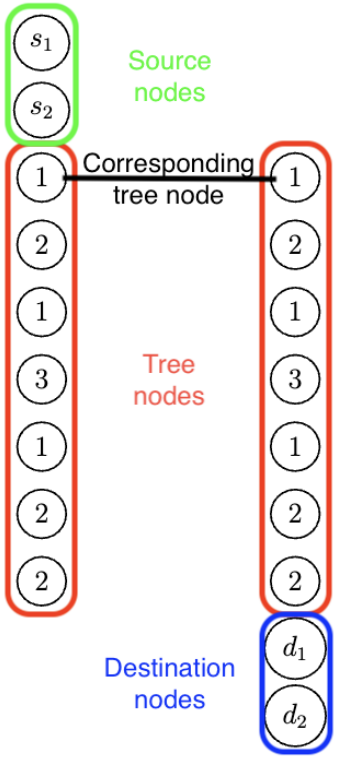

Figure 6.1: Example of a bipartite graph nodes constructed from a tree with the following equivalence classes $E = \{1, 2, 1, 3, 1, 2, 2\}$. The nodes are ordered from top to bottom.

Definition 10 (Bipartite graph properties)**.** *The resulting bipartite graph G will have $2t + 2p$ nodes and $O(t(p + 1) + p^2 + tp)$ edges, where the $O(t(p + 1))$ edges come from the tree nodes, the $O(p^2)$ edges come from the sources since each source node is connected to p nodes, and the $O(tp)$ edges come from the destination nodes since in the worst case we have t distinct equivalence class and so all the nodes are connected to the destination nodes. The weight of the edges will be 0 or 1.*

Let's see a small example for each case, consider $p = 2$. In Figure 6.2-(a) there is an example for the sources' edges, as stated before, for each source p nodes with weight

1 are created and connected to the first p nodes with distinct equivalence class in V_2.

In Figure 6.2-(b) there is an example for the tree nodes' edges, for each node in the tree T edges with weight 1 are created and connected to the first p nodes with distinct equivalence class in V_2 after the corresponding node in V_2 (coming after the node itself in the ordering), and edges with weight 0 are created and connected to the first node with the same class in V_2 after the corresponding node in V_2. As we can see from the image, we consider the first node in V_1 labelled 1 that is connected to the node 2 with weight 1 and to the node 3 with weight 1, and to the second node labelled 1 in V_2 with weight 0.

Lastly, in Figure 6.2-(c) there is an example for the destination nodes' edges, we start by considering the first node in V_1 that is labelled 1, it is connected to the node 2 with weight 1, then since there is no node with the same class in V_2 we connect it to the destination nodes d_1 and d_2 with weight 0. The same is done for the second node in V_1 that is labelled 2 since no nodes are coming after it in the order it is connected to the destination nodes d_1 and d_2 with weight 0.

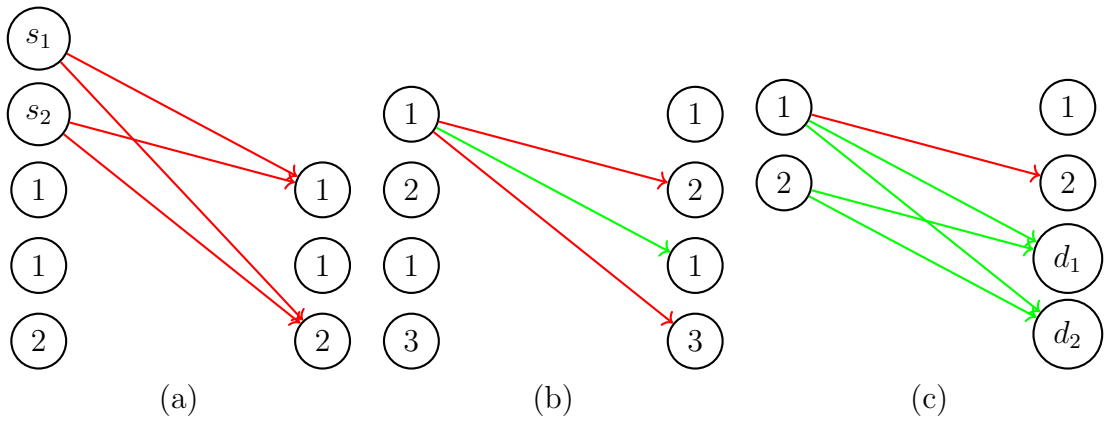

Figure 6.2: Considering $p = 2$ these three examples show how to connect nodes in the bipartite graph in the case of sources (a), tree nodes (b), and destinations (c).

6.2.2 Proof of correctness

In order to prove the correctness of the reduction, it is important to start by defining the problem we want to solve.

Definition 11 (CHAINS-DIVISION problem)**.** *Given a tree T with t nodes, and given the equivalence classes E coming from the Hopcroft algorithm applied to the tree T, the sorted order of the nodes in T according to the upward path π, and the number of chain $p \leq t$, we want to find the optimal partition of the nodes of T into p chains with $p \leq t$ such that the run length encoding of each chain is minimized.*

Let's give a formal definition of run length encoding.

Definition 12 (Run length encoding)**.** *Given a sequence $S = \{s_1, s_2, \ldots, s_n\}$, the run length encoding of S is the sequence $R = \{r_1, r_2, \ldots, r_m\}$ where r_i is the number of times the element s_i is repeated in S. It allows us to represent the sequence S in a more compact way.*

So, we aim to divide the nodes of the tree into p chains such that the run length encoding of the chains is minimized meaning that we want to minimize the number of distinct equivalence classes in each chain. Follows the definition of chain.

Definition 13 (Chains)**.** *Given a tree T with t nodes and p chains, a chain C is a sequence of nodes $C = \{c_1, c_2, \ldots, c_m\}$ such that c_i is a node of T for $i = 1, 2, \ldots, m$ and $m \leq t$. Also, Each node of T is in exactly one chain and the nodes of the chain are ordered according to the upward path π of the tree.*

Let's start by stating the following lemma.

Lemma 7. *Exactly $|E|$ nodes of the tree T of the set V_1 are connected each to all the destination nodes $d_i \in V_2 \quad \forall i = 1, 2, \ldots, p$ with weight 0. Where E is the set of equivalence classes of the nodes of T coming from the Hopcroft algorithm applied to the tree T.*

Proof. Since the destination nodes $d_i \in V_2$ are connected to the nodes of the tree T with weight 0 only if there is no other node with the same class in V_2 coming after the node in the ordering, then for sure there are $|E|$ nodes of the tree T in V_1 that have no other node with the same class in V_2 coming after the node in the ordering. □

Lemma 8. *The optimal solution of the CHAINS-DIVISION problem for an instance $\mathcal{I}$ for a tree T is always greater or equal to the number of equivalence classes coming from the Hopcroft algorithm applied to the tree T.*

Proof. Since we aim to minimize the run length encoding of the chains, and the minimum cost of a chain is 1, then the optimal cost of the *CHAINS-DIVISION* problem for the tree T is always greater or equal to the number of equivalence classes since if we dispose them in $|E|$ chains we will have a cost of $|E|$ since each chain contains only nodes with the same class, and if we dispose them in $p < |E|$ chains we will have a cost greater or equal to $|E|$ since we will have to put at least two nodes with the same class into one chain or more than one. □

Lemma 9. *The solutions for the CHAINS-DIVISION problem for the instances where the number p of chains is greater than $|E|$ are not better than the solutions for the instances where $p \leq |E|$.*

Proof. The proof comes directly from lemma 8. □

Lemma 10. *A perfect matching for a bipartite graph G constructed as stated in Definition 9 exist for each possible instance of the CHAINS-DIVISION problem.*

Proof. The proof comes from the construction of the bipartite graph G and from theorem 3. We are going to proof that the bipartite graph G constructed as stated in Definition 9 has a Tutte matrix (definition 8) with determinant different from 0 and so a perfect matching for G exists.

We know that a $n \times n$ matrix M has $Det(M) \neq 0$ if and only if it has full rank ($rank(M) = n$), or equivalently if it has n linearly independent rows or columns. We can see that the bipartite graph G has $2t + 2p$ nodes and $O(t(p + 1) + p^2 + tp)$

	1	2	1	3	1	2	2	d_1	d_2
s_1	1	1	0	0	0	0	0	0	0
s_2	1	1	0	0	0	0	0	0	0
1	0	1	1	1	0	0	0	0	0
2	0	0	1	1	0	1	0	0	0
1	0	0	0	1	1	1	0	0	0
3	0	0	0	0	1	1	0	1	1
1	0	0	0	0	0	1	0	1	1
2	0	0	0	0	0	0	1	0	0
2	0	0	0	0	0	0	0	1	1

Figure 6.3: Example of a Tutte matrix for a bipartite graph in figure 6.4-(a). As we can see the matrix has full rank and so a perfect matching exists.

edges, and so the Tutte matrix of G will have $2t + 2p$ rows and $2t + 2p$ columns. The columns of M are all independent since each node of G in V_1 is connected only to nodes in V_2 that are greater than u in the ordering. Also each node is connected to at least one node in V_2 and at most $p + 1$ distinct nodes with distinct class in V_2. Those conditions on the edges are sufficient to get a full rank matrix and so a perfect matching for G exists. □

In figure 6.3 the Tutte matrix for the bipartite graph in Figure 6.4-(a) is shown.

Lemma 11. *Given a bipartite graph G constructed as stated in Definition 9 from a tree T, for each node $u \in V_1$ coming from the nodes of T it is impossible for u to be connected to node $v \in V_2$ coming from the nodes of T such as $v < u$ in the order of the nodes of the tree T.*

Proof. The proof comes from the construction of G where the nodes of V_1 are always connected to the nodes of V_2 coming after them in the ordering of the nodes of the tree T. □

Now we can prove the correctness of the reduction.

Theorem 5. *An optimal solution of an instance $\mathcal{I}$ with $p \leq |E|$ of the problem defined in Definition 11 is equivalent to an optimal solution of the Minimum Weight Perfect Bipartite Matching for the instance $r(\mathcal{I})$ where $r : \mathcal{I}_{CHAINS-DIVISION} \rightarrow \mathcal{I}_{MWPBM}$ is the reduction function that maps an instance of the problem defined in Definition 11 to an instance of the Minimum Weight Perfect Bipartite Matching problem defined in Definition 7 constructed as stated in Definition 9.*

Proof. Let $p \leq t$ be the number of chains we want to partition the nodes of a given tree T into. Let E be the set of equivalence classes of the nodes of T, from lemma 9 we consider that $p \leq |E|$. We can construct a bipartite graph $G = (V, E)$ such that vertices are divided in two disjoint sets $V = V_1 \cup V_2$ as stated in Definition 9. We will show that the optimal solution of the Minimum Weight Perfect Bipartite Matching problem for the graph G is equivalent to the optimal solution of the CHAINS-DIVISION problem for the tree T.

From definition 9 we know that V_1 contains $t + p$ nodes including $s_1, s_2, \ldots, s_p$ and the t elements of E ordered, and V_2 contains $t + p$ nodes including the t elements of E ordered and $d_1, d_2, \ldots, d_p$.

The source nodes are necessary to distinguish the chains, by starting from each source node we can follow the edges of the nodes and reach the destination nodes in order to retrieve the nodes of a chain. The source nodes are all connected to the first p nodes with distinct equivalence class in V_2 with weight 1 since each chains has at least one node and a minimum cost of 1.

The destination nodes are necessary to close the chains, by connecting the nodes of the tree to the destination nodes we can ensure that the chains are closed and allows to get a perfect matching otherwise we would have $|V_1| > |V_2|$ and so we would have unmatched nodes. From lemma 7 we know that exactly $|E|$ nodes of the tree T in V_1 are connected to all the destination nodes $d_i \in V_2 \quad \forall i = 1, 2, \ldots, p$ with weight 0. This is done in order to ensure that the chains are closed and that the nodes of the tree are connected to the destination nodes in order to have a perfect matching. The weight of the edges is 0 since if we conclude a chain no additional cost is needed.

We know from definition 13 that the order of the nodes of each chain must follow the order given by the upward path π of each node in the tree T. This is ensured by lemma 11 that states that it is impossible for a node $u \in V_1$ coming from the nodes of T to be connected to a node $v \in V_2$ coming from the nodes of T such as $v < u$ in the order of the nodes of the tree T. This is done in order to ensure that the nodes are connected in the right order.

Given the construction of the bipartite graph G we can see that the optimal solution of the Minimum Weight Perfect Bipartite Matching problem for the graph G is equivalent to the optimal solution of the CHAINS-DIVISION problem for the tree T since the chains are closed and the nodes are connected in the right order. The weight of the edges 0 allow the problem to chain subsequent nodes with the same class without adding additional cost. Also from the definition of matching (6) no node of G is exposed and so the matching is perfect as proved in lemma 10. The fact that each node in V_1 is connected to at least p edges allow the problem to compare all the possible chains and so to find the optimal solution. □

6.2.3 Full example

Consider The example in Figure 6.4 where we have a tree T with $t = 7$ nodes, $p = 2$ chains and the equivalence classes $E = \{1, 2, 1, 3, 1, 2, 2\}$ sorted accordingly to the upward path π of each node of the tree. We can construct the two distinct sets V_1 and V_2 of the bipartite graph G as follows: $V_1 = \{s_1, s_2, 1, 2, 1, 3, 1, 2, 2\}$ and $V_2 = \{1, 2, 1, 3, 1, 2, 2, d_1, d_2\}$. The edges of the graph G will be constructed as stated in Definition 9. In Figure 6.4-(a) we have the resulting bipartite graph, and in Figure 6.4-(b) we have one of the possible minimum perfect matchings for the graph in (a) having weight 4. A the end we can see that the optimal partition of the nodes of the tree T is $C_1 = \{1, 1, 1, 2, 2\}$ and $C_2 = \{2, 3\}$ with a total cost of 4, this can be obtained starting from the sources and by following the edges of the nodes, jumping to the corresponding node in V_1 and following the edges again until we reach the destination nodes.

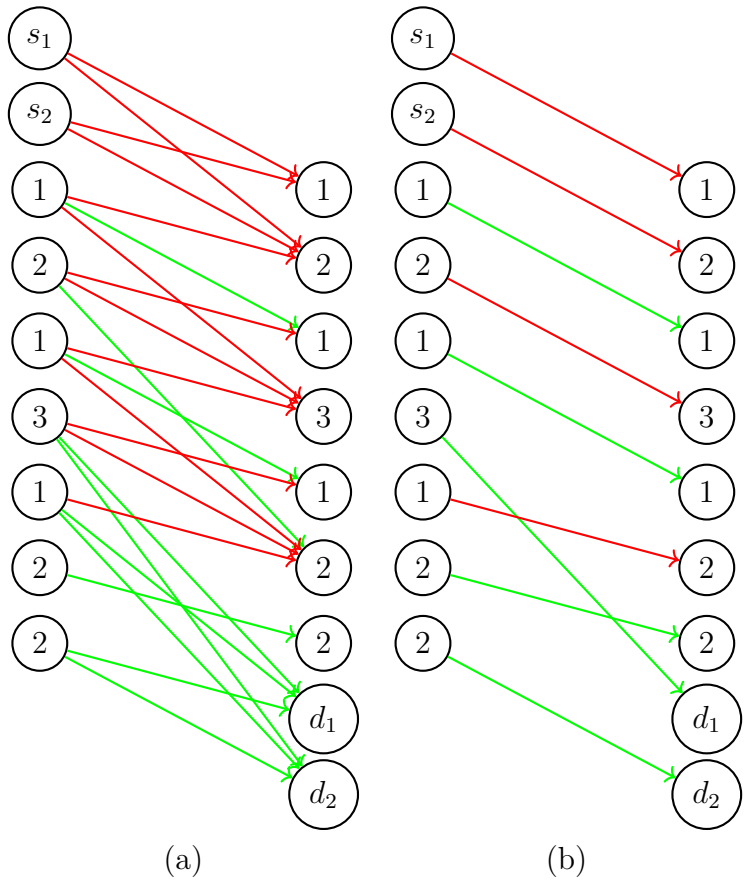

Figure 6.4: Example of a reduction for the sorted nodes' equivalency classes $E = \{1, 2, 1, 3, 1, 2, 2\}$. In (a), we have the resulting bipartite graph constructed from E. In (b), we have the resulting perfect matching for the graph in (a) having weight 4. Green edges weigh 0, while red edges weigh 1.

6.3 Heuristics and Improvements

Some changes can be made to the reduction in order to optimize it and to reduce the number of edges in the bipartite graph. Here are some of the improvements that can be made.

- **Sources' edges optimization**:

  Lemma 12. *The sources' edges can be optimized by connecting each source only to the smaller node (considering the order of the nodes) in V_2 coming from the tree T that is not connected to any other source.*

  Proof. Since the source nodes are needed to distinguish the chains as starting points, we need that each source is connected to at least one node in V_2 coming from the tree T. Having the sources connected to the first p nodes with distinct equivalence class in V_2 is not necessary since allows us just to invert the chains starting from each source and so it is redundant. We can connect each source to the smaller node in V_2 coming from the tree T that is not connected to any other source since we need to connect each source to at least one node in V_2 coming from the tree T and this will allow us to distinguish the chains. □

  This will reduce the number of edges coming from the sources from $O(p^2)$ to $O(p)$. In Figure 6.5-(a) the removed edges are shown in green.

- **Tree nodes' edges optimization 1**:

  Lemma 13. *The tree nodes' edges can be optimized by removing the edges of tree nodes that are connected to nodes in V_2 already linked to a source node in V_1.*

  Proof. From definition 6 we know that a matching $M \in E$ is a collection of edges such that every vertex of V is incident to at most one edge of M. In other words, a matching is a set of edges such that no two edges share a common vertex. Given that, in all the solutions to the problem all sources will be connected to exactly one node in V_2 coming from the tree T and so we can remove the edges of the tree nodes that are connected to nodes in V_2 already linked to a source node in V_1 since they will not be part of the final matching. □

  This will reduce the number of edges by a factor of $O(p-1)$. In Figure 6.5-(a) the removed edges are shown in blue.

- **Tree nodes' edges optimization 2**:

  Lemma 14. *The tree nodes' edges can be optimized by removing the edges with weight* 1 *starting from a node $u \in V_1$ to a node $v \in V_2$ if the node u has another edge with weight* 0 *connected to a node $z \in V_2$ such that $z < v$ in the ordering of the nodes.*

  Proof. To proof the lemma since every time we have an edge with weight 0 between two nodes of V_1 and V_2 it means that those two nodes have the same equivalence class and so there is no need to add additional cost trying to connect that node to nodes with different classes coming after in the ordering, as that would only increase the cost without providing any benefit to the solution. Also, we know that connecting nodes with the same class is always the best choice for optimizing the run length encoding of each chain. □

  In Figure 6.5-(a) the removed edges are shown in red.

In figure 6.5-(b) we can see the resulting bipartite graph for the example shown in previous section after the optimizations.

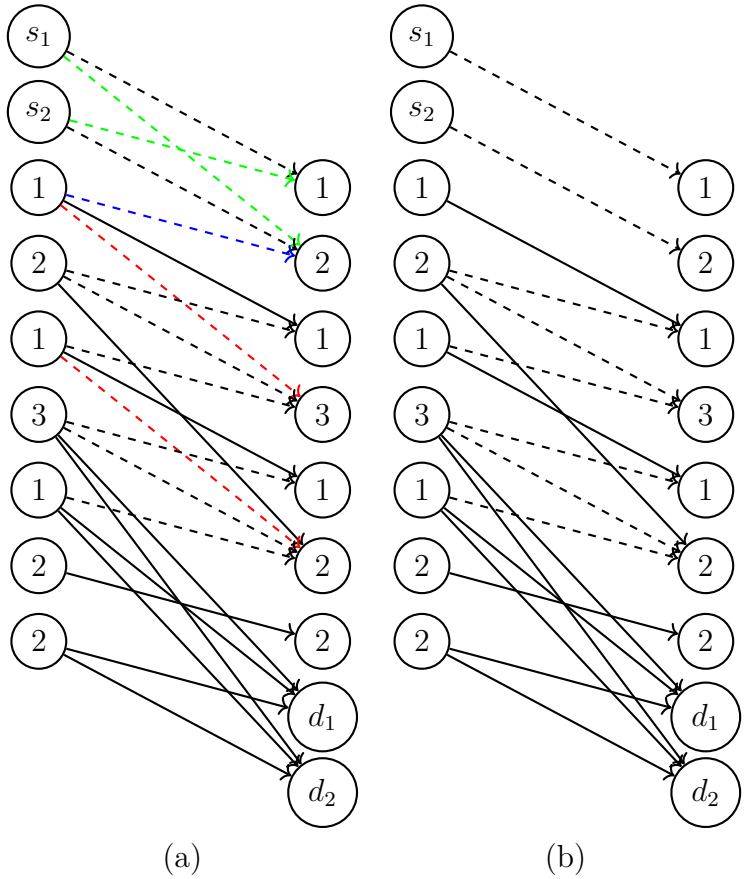

Figure 6.5: Example of a reduction for the sorted nodes' equivalency classes $E = \{1, 2, 1, 3, 1, 2, 2\}$ applying also the heuristics showed. In (a), the edges removed are shown in green for lemma 12, blue for lemma 13, and red for lemma 14. In (b), we have the resulting bipartite graph after the heuristics applied. Dashed edges weigh 1, while solid edges weigh 0.

6.4 Moving to Maximum weight perfect bipartite matching

In this section, we will discuss how to slightly modify the reduction process to move from a minimum weight perfect bipartite matching problem to a maximum weight perfect bipartite matching problem. This will be helpful in solving the problem more efficiently by using some known algorithms to solve the maximum weight perfect bipartite matching problem.

Theorem 6. *An optimal solution of an instance $\mathcal{I}$ with $p \leq |E|$ of the CHAINS-DIVISION problem is equivalent to an optimal solution of the Maximum Weight Perfect Bipartite Matching for the instance $r(\mathcal{I})$ where $r : \mathcal{I}_{CHAINS-DIVISION} \rightarrow \mathcal{I}_{MWPBM}$ is the reduction function that maps an instance of the CHAINS-DIVISION problem to an instance of the Maximum Weight Perfect Bipartite Matching problem constructed as stated in Definition 9 but with inverted weights (weight 0 becomes 1 and weight 1 becomes 0).*

Proof. Let M be a perfect matching in the bipartite graph G constructed as stated in Definition 9. Let $w(M)$ be the sum of the weights of the edges in the matching M. From the previous theorem, we know that the optimal solution of the

CHAINS-DIVISION problem is equivalent to finding a perfect matching M in G that minimizes $w(M)$.

Let G' be a bipartite graph constructed as G but with inverted weights (weight 0 becomes 1 and weight 1 becomes 0). Let M' be a perfect matching in G' and let $w'(M')$ be the sum of the weights of the edges in the matching M'. Let k be the number of edges in the matching.

We can see that for any matching M in G:

$$w'(M) = k - w(M)$$

This means that maximizing $w'(M)$ is equivalent to minimizing $w(M)$. Therefore, finding the maximum weight perfect matching in G' is equivalent to finding the minimum weight perfect matching in G, which in turn is equivalent to finding the optimal solution of the CHAINS-DIVISION problem. □

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