Complexity of Splits Reconstruction for Low-Degree Trees *

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Abstract. Given a vertex-weighted tree T, the split of an edge xy in T is $\min\{s_x, s_y\}$ where s_x (respectively, s_y) is the sum of all weights of vertices that are closer to x than to y (respectively, closer to y than to x) in x. Given a set of weighted vertices x0 and a multiset of splits x3, we consider the problem of constructing a tree on x4 whose splits correspond to x5. The problem is known to be NP-complete, even when all vertices have unit weight and the maximum vertex degree of x5 is required to be no more than 4. We show that

- the problem is strongly NP-complete when T is required to be a path. For this variant we exhibit an algorithm that runs in polynomial time when the number of distinct vertex weights is constant. We also show that
- the problem is NP-complete when all vertices have unit weight and the maximum degree of T is required to be no more than 3, and
- it remains NP-complete when all vertices have unit weight and T is required to be a caterpillar with unbounded hair length and maximum degree at most 3.

Finally, we shortly discuss the problem when the vertex weights are not given but can be freely chosen by an algorithm.

The considered problem is related to building libraries of chemical compounds used for drug design and discovery. In these inverse problems, the goal is to generate chemical compounds having desired structural properties, as there is a strong correlation between structural properties, such as the Wiener index, which is closely connected to the considered problem, and biological activity.

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1 Introduction

In this paper, we consider trees T=(V,E) where integer weights are associated to vertices by a function $\omega:V\to\mathbb{N}$, where \mathbb{N} denotes the set of natural numbers excluding 0.

Definition 1. Let T be a tree and $\omega: V \to \mathbb{N}$ be a function. The split of an edge e in T is the minimum of $\Omega(T_1)$ and $\Omega(T_2)$, where T_1 and T_2 are the two trees obtained by deleting e from T, and $\Omega(T_i) = \sum_{v \in T_i} \omega(v)$. We use $\mathcal{S}(T)$ to denote the multiset of splits of T.

We consider the problem of reconstructing a tree with a given multiset of splits and a given set of weighted vertices.

WEIGHTED SPLITS RECONSTRUCTION (WSR): Given a set V of n vertices, a weight function $\omega: V \to \mathbb{N}$, and a multiset \mathcal{S} of integers, is there a tree T whose multiset of splits is \mathcal{S} (i.e. $\mathcal{S}(T) = \mathcal{S}$)?

The Weighted Splits Reconstruction for Trees of Maximum Degree k problem (WSR $_k$) is defined in the same way, except that we restrict the tree T to have maximum degree at most k. When we require T to belong to a class of trees T, the problem is called Weighted Splits Reconstruction for T. When ω assigns unit weights to the vertices, the problem is simply called Splits Reconstruction (SR). The Splits Reconstruction for Trees of Maximum Degree k problem (SR $_k$) and the Splits Reconstruction for T are the obvious unweighted counterparts of the weighted variants defined above.

Related Work. In the field of Chemical Graph Theory [2, 3, 18], molecules are modeled by graphs in order to study the physical properties of chemical compounds. A chemical graph is a graph, where vertices represent atoms of a chemical compound and edges the chemical bonds between them. Within the area of quantitative structure-activity relationship (QSAR), several structural measures of chemical graphs were identified that quantitatively correlate with a well defined process, such as biological activity or chemical reactivity. Probably the most widely known example is the Wiener index (see [12]): the sum of the distances in a graph between each pair of vertices, where the distance between two vertices is the number of edges on a shortest path from one to the other. Wiener [19] found a strong correlation between the boiling points of paraffins and the Wiener index. From then on, many other topological (using the information of the chemical graph) and topographical (using the information of the chemical graph and the location of its vertices in space) indices were introduced and their correlation with various other biological activities was investigated.

In Combinatorial Chemistry, drug design is facilitated by building libraries of molecules that are structurally related (via the Wiener index or any of the other numerous indices). We face inverse problems where the goal is to design new compounds that have a prescribed structural information (see also [6]).

Goldman et al. [11] study problems related to the design of combinatorial libraries for drug design from an algorithmic and complexity-theoretic point of

view, following the heuristic approaches of [17] and [10]. They show that for every positive integer W, except 2 and 5, there exists a graph with Wiener index W. They also show that every integer, except a finite set, is the Wiener index of some tree. For constructing a tree (of unbounded or bounded maximum degree) with a given Wiener index, they devise pseudo-polynomial dynamic programming algorithms. Goldman et al. also introduce the Splits Reconstruction problem and recall a result due to Wiener [19]: the Wiener index of a tree T on n vertices with unit weights is $\sum_{s \in \mathcal{S}(T)} s \cdot (n-s)$. They show that SR is NP-complete and give an exponential-time algorithm without running time analysis.

As it is not reasonable to construct chemical trees with arbitrarily high vertex degrees, Li and Zhang [15] studied SR_4 and showed that it is also NP-complete. Their algorithm to construct a tree with maximum degree at most 4 to solve SR_4 runs in exponential time (no running time analysis is provided) and creates weighted vertices in intermediate steps.

In order to reconstruct glycans or carbohydrate sugar chains, Aoki-Kinoshita et al. [1] study the reconstruction of a node-labeled supertree from a set of node-labeled subtrees. They give a 6-approximation algorithm for this problem, which generalizes the smallest superstring problem. We refer to [4] surveying results on the Wiener index for trees.

Our Results. By the result of Li and Zhang [15], SR_4 is NP-complete, while SR_2 is trivially in P. We close this gap by showing that SR_3 is NP-complete by a reduction from NUMERICAL MATCHING WITH TARGET SUMS (defined below). It is even NP-complete for caterpillars with unbounded hair length. Identifying small classes of trees for which the problem is NP-complete may be important for future investigations in the spirit of the deconstruction of hardness proofs [14] which aim at identifying parameters for which the problem becomes tractable if these parameters are small.

Our main result proves that WSR₂ is strongly NP-complete by a reduction from a variant of NUMERICAL MATCHING WITH TARGET SUMS in which all integers of the input are distinct. For the case where the weights of the vertices are chosen from a small set of values, our dynamic-programming algorithm solves WSR₂ in time $O(n^{k+3} \cdot k)$, where k is the number of distinct vertex weights.

Definitions. A caterpillar is a tree consisting of a path, called its backbone, and paths attached with one end to the backbone. Its hair length is the maximum distance from a leaf to the closest vertex of the backbone. A star $K_{1,k}$ is a tree with k leaves and one internal vertex, called the center. In our hardness proofs, we reduce from the following problem (problem [SP17] in [9]).

NUMERICAL MATCHING WITH TARGET SUMS (NMTS): Given three disjoint multisets A,B, and $S = \{s_1, \ldots, s_m\}$, each containing m elements from \mathbb{N} , can $A \cup B$ be partitioned into m disjoint sets C_1, C_2, \ldots, C_m , each containing exactly one element from each of A and B, such that, for $1 \leq i \leq m$, $\sum_{c \in C_i} c = s_i$?

Due to space constraints, the proofs of the statements marked with (\star) have been moved to the appendix.

2 WSR₂ is strongly NP-complete

In this section, we show that WSR₂ is strongly NP-complete. First we introduce a new problem that is polynomial-time-reducible to WSR₂, and then show that this new problem is strongly NP-hard.

SCHEDULING WITH COMMON DEADLINES (SCD): Given n jobs with positive integer lengths j_1, \ldots, j_n and n deadlines $d_1 \leq \ldots \leq d_n$, can the jobs be scheduled on two processors P_1 and P_2 such that at each deadline there is a processor that finishes a job exactly at this time, and processors are never idle between the execution of two jobs?

To reinforce the intuition on this problem one may imagine that we want to satisfy delivery deadlines and avoid using any warehouse space to store a product between its fabrication and the delivery date. There is no restriction as to which product should be delivered at a given time. (Another possibility is imagining computer scientists scheduling paper production to fit conference deadlines.)

Given an instance $(j_1, \ldots, j_n, d_1, \ldots, d_n)$ for SCD, we construct an instance for WSR₂ as follows. For each job j_i , $1 \le i \le n$, create a vertex v_i with weight $\omega(v_i) = j_i$. For each deadline d_i , $1 \le i \le n-1$, create a split d_i . We may assume that $\sum_{i=1}^n j_i = d_{n-1} + d_n$, otherwise we trivially face a No-instance.

Suppose the path $P=(v_{\pi(1)},v_{\pi(2)},\ldots,v_{\pi(n)})$ is a solution to WSR₂. Say $\{v_{\pi(\ell)},v_{\pi(\ell+1)}\}$ is the edge associated to the split d_{n-1} . We construct a solution for SCD by assigning the jobs $j_{\pi(1)},j_{\pi(2)},\ldots,j_{\pi(\ell)}$ to processor P_1 , and the jobs $j_{\pi(n)},j_{\pi(n-1)},\ldots,j_{\pi(\ell+2)},j_{\pi(\ell+1)}$ to processor P_2 , in this order. Note that then, one of the jobs $j_{\pi(\ell)},j_{\pi(\ell+1)}$ ends at d_{n-1} , and the other at $-d_{n-1}+\sum_{i=1}^n j_i=d_n$, which is as desired.

On the other hand, if SCD has a solution, then WSR₂ has a solution as well, because the previous construction is easily inverted. Visually, the list of jobs of P_2 is reversed and appended to the list of jobs of P_1 . Job lengths correspond to vertex weights and deadlines correspond to splits (the last deadline where a job from P_1 finishes is merged with the last deadline where a job from P_2 finishes). Thus, SCD is polynomial-time-reducible to WSR₂.

Lemma 1. SCD $\leq_p WSR_2$.

In the remainder of this section, we show that dNMTS is polynomial-time-reducible to SCD. The dNMTS problem is equal to the NMTS problem, except that all integers in $A \cup B \cup S$ are pairwise distinct. This variant has been shown to be strongly NP-hard by Hulett et al. [13]. As the proof becomes somewhat simpler, we use dNMTS instead of NMTS for our reduction.

Let us first give a high level description of the main ideas of the reduction. For a dNMTS instance (A, B, S), the elements of $A \cup B$ will be encoded as jobs, and the elements of S will be encoded as deadlines. A convenient way to represent an element $s \in S$ is by introducing segments which are delimited to the left and the right by double deadlines, and whose distance is equivalent to s. The elements of $A \cup B \cup S$ are blown up by well-chosen additive factors that preserve solutions

and make sure that the length of each segment can only be met by the sum of exactly two job-lengths, one corresponding to an element of A and the other to an element of B.

Our reduction will create an instance whose solution assigns, in each segment, one x-job (a job corresponding to an A-element) and one y-job (a job corresponding to a B-element) to the same processor, such that these two jobs are the only jobs executed on this processor in this segment, thus providing a solution to dNMTS. W.l.o.g., the x-job is scheduled first. As we must not introduce any restriction which x-jobs can be assigned to which segments, we introduce a deadline for each length of an x-job; these are the real deadlines. We refer to the x- and y-jobs as green jobs. The job lengths were blown up such that in each segment, exactly one processor starts with a green x-job, and in each segment, exactly one processor ends by executing a green y-job. In each segment, the green jobs must not overlap; this is achieved by multiplying all deadlines created so far and the corresponding job lengths by a factor 2, and introducing fake deadlines at odd positions one unit before the real deadlines. If an x-job and a y-job overlapped, there would be no job ending at the fake deadline preceding the real deadline at which the x-job ends, as all green jobs have even length and all real deadlines and double deadlines are even. Blue, red, and black jobs are created to meet all deadlines on the processor that is not currently executing green jobs. The blow-up of the elements of $A \cup B \cup S$ ensures that these jobs cannot equate the green jobs (except the black jobs whose lengths might equal the lengths of green y-jobs, but, w.l.o.g., one can assign them to the last part of each segment of the processor not executing a green job). That none of these jobs is executed between two green jobs within a segment is ensured as the sum of all green job lengths equals the sum of the lengths of the segments. This summarizes the reduction and gives the reasons for the different elements of the construction. Let us now turn to the formal reduction.

Let (A,B,S) be an instance for dNMTS. We suppose, w.l.o.g., that $\sum_{i=1}^{m} s_i = \sum_{x \in A \cup B} x$, otherwise (A,B,S) is trivially a No-instance for dNMTS. Let $A = \{a_1,\ldots,a_m\}$ and $B = \{b_1,\ldots,b_m\}$. We also assume, w.l.o.g., that $a_i < a_{i+1}, b_i < b_{i+1}, s_i < s_{i+1},$ for all $i \in \{1,\ldots,m-1\}$, that $a_m < b_m$, and that $s_m \leq a_m + b_m$.

First, we construct an equivalent instance (X,Y,Z) for dNMTS. Each of $X:=\{x_1,\ldots,x_n\},\ Y:=\{y_1,\ldots,y_n\},$ and $Z:=\{z_1,\ldots,z_n\}$ has n:=m+1 elements:

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\begin{array}{ll} \text{for } i \in \{1, \dots, n-1\}, \\[1mm] x_i := 2 \cdot (a_i + (b_m + 2)), \\[1mm] y_i := 2 \cdot (b_i + 3 \cdot (b_m + 2)), \\[1mm] z_i := 2 \cdot (s_i + 4 \cdot (b_m + 2)), \text{ and} \end{array} \qquad \begin{array}{ll} x_n := 2 \cdot (a_m + 1 + (b_m + 2)), \\[1mm] y_n := 2 \cdot (b_m + 1 + 3 \cdot (b_m + 2)), \\[1mm] z_n := 2 \cdot (a_m + b_m + 2 + 4 \cdot (b_m + 2)). \end{array}
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The elements of X, Y, and Z have the following properties.

Proposition 1 Each element of $X \cup Y \cup Z$ is an even positive integer.

Proposition 2 For every $i \in \{1, ..., n-1\}$, we have that $x_i < x_{i+1}$, that $y_i < y_{i+1}$, and that $z_i < z_{i+1}$.

Proposition 3 For every $i \in \{1, ..., n\}$, we have

$$2 \cdot b_m + 4 \le x_i \le 4 \cdot b_m + 4,$$

 $6 \cdot b_m + 12 \le y_i \le 8 \cdot b_m + 14, \text{ and}$
 $8 \cdot b_m + 16 \le z_i \le 12 \cdot b_m + 18.$

In particular, Property 3 implies that $y_1 > x_n$, that $z_1 > y_n$, and that $2 \cdot y_1 > z_n$. Properties 1–3 easily follow by construction of X, Y, and Z.

Proposition 4 If k and ℓ are integers such that $x_k + y_\ell = z_n$, then $k = \ell = n$.

Property 4 holds because x_n and y_n are the only elements of X and Y, resp., that are large enough to sum to z_n .

Proposition 5 Let $p, q \in X \cup Y$, $p \leq q$, and $z \in Z$. If p + q = z, then $p \in X$ and $q \in Y$.

By Property 3, the sum of any two X-elements is smaller and the sum of any two Y-elements is larger than any element of Z.

For our SCD instance, we create the following deadlines:

- real deadlines: $r_{i,j} := x_i + \sum_{k=1}^j z_k$, for each $j \in \{0, \dots, n-1\}$ and each $i \in \{1, \dots, n\}$,
- fake deadlines: $f_{i,j} := r_{i,j} 1$, for each $j \in \{0, \ldots, n-1\}$ and each $i \in \{1, \ldots, n\}$, and
- sum deadlines: two deadlines $ds_{1,j} := ds_{2,j} := \sum_{k=1}^{j} z_k$, for each $j \in \{1,\ldots,n\}$.

The sum deadlines we just defined partition the interval $[0, ds_{1,n}]$ into n segments $I_j := [ds_{1,j-1}, ds_{1,j}], j = 1, \ldots n$, where for convenience, we let $ds_{1,0} = 0$. We create jobs with the following lengths, where $x_0 = 0$:

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- green x-jobs: x_i, for each i \in \{1, ..., n\},

- green y-jobs: y_i, for each i \in \{1, ..., n\},

- blue jobs: n \cdot (n-1) times a job of length 1,
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- red fill jobs: n-1 times a job of length x_i-1-x_{i-1} , for each $i \in \{1,\ldots,n\}$,
- red overlap jobs: $x_i x_{i-1}$, for each $i \in \{1, \ldots, n\}$,
- black fill jobs: $z_i x_n$ for $i \in \{1, \dots, n-1\}$, and
- a black overlap job: $z_n x_n + 1$.

To illustrate these definitions, we start by showing that if we have a YES-instance (X,Y,Z) for dNMTS, then we have an SCD YES-instance as well. Let C_1,C_2,\ldots,C_n be n couples such that $C_j=\{x_{\pi_1(j)},y_{\pi_2(j)}\}$ and $x_{\pi_1(j)}+y_{\pi_2(j)}=z_j,\ j\in\{1,\ldots,n\}$, for two permutations π_1 and π_2 of the set $\{1,\ldots,n\}$. We construct a solution for SCD. Let us construct the schedules for P_1 and P_2 . For each $j\in\{1,\ldots,n-1\}$,

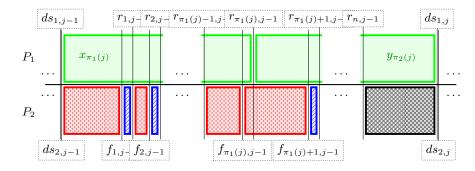


Fig. 1. How jobs are assigned to processors in the SCD instance in segment j < n.

- assign the green x-job $x_{\pi_1(j)}$ to the interval $[ds_{1,j-1}, r_{\pi_1(j),j-1}]$ of P_1 ,
- assign the green y-job $y_{\pi_2(j)}$ to the interval $[r_{\pi_1(j),j-1},ds_{1,j}]$ of P_1 , assign a red fill job of length x_1-1 to the interval $[ds_{1,j-1},f_{1,j-1}]$ of P_2 ,
- for every $i \in \{1, \dots, n-1\} \setminus \pi_1(j)$, assign a red fill job of length $x_{i+1} 1 x_i$ to the interval $[r_{i,j-1}, f_{i+1,j-1}]$ of P_2 ,
- for every $i \in \{1, \dots, n\} \setminus \pi_1(j)$, assign a blue job to the interval $[f_{i,j-1}, r_{i,j-1}]$
- assign a red overlap job of length $x_{\pi_1(j)+1} x_{\pi_1(j)}$ to the interval $[f_{\pi_1(j),j-1},$ $f_{\pi_1(j)+1,j-1}$] of P_2 , and
- assign a black fill job of length $z_j x_n$ to the interval $[r_{n,j-1}, ds_{1,j}]$ of P_2 .

It only remains to assign jobs to the last segment. The last segment of P_1 contains the green x-job x_n and the green y-job y_n , in this order. The last segment of P_2 contains a red fill job of length $x_1 - 1$, a blue job, a red fill job of length $x_2 - 1 - x_1$, a blue job, ..., a red fill job of length $x_n - 1 - x_{n-1}$, and the black overlap job, in this order. See Fig. 1 for an illustration.

Now suppose the SCD instance is a YES-instance. We will show some structural properties of any valid assignment of jobs to the processors, which will help to extract a solution for our original dNMTS instance. We will show that in each segment I_i , any valid solution for the SCD instance has exactly one green x-job x_k and exactly one green y-job y_ℓ , and x_k and y_ℓ sum to z_i .

Consider a valid assignment of the jobs to the processors P_1 and P_2 . As two jobs with the same length are interchangeable, when we encounter a job whose length belongs to more than one category (for example "black fill" and "green y") we may choose in this case, w.l.o.g., to which category the job belongs.

Claim 1 A black fill job is assigned to each interval $[r_{n,j}, ds_{1,j+1}], j \in \{0, \dots, n-1\}$ 2}.

Proof. Let $j \in \{0, ..., n-2\}$. Two jobs must finish at the double deadline $ds_{1,j+1}, ds_{2,j+1}$. One of these must start at $r_{n,j}$ and thus has length $ds_{1,j+1}$ $r_{n,j} = \sum_{k=1}^{j+1} z_k - x_n - \sum_{k=1}^{j} z_k = z_{j+1} - x_n$. So this job is, w.l.o.g., a black fill This uses up all black fill jobs.

Claim 2 (*) The green y-job y_n is assigned to the interval $[r_{n,n-1}, ds_{1,n}]$.

The proofs of claims 2, 3 and 5 are provided in appendix A.

Claim 3 (*) The black overlap job is assigned to the interval $[f_{n,n-1}, ds_{1,n}]$.

This uses up all black jobs. Now, the only jobs left whose length is between $6b_m + 12$ and $8b_m + 14$ are the green y-jobs y_1, \ldots, y_{n-1} .

Claim 4 For each $\ell \in \{1, \ldots, n-1\}$, the green y-job y_{ℓ} is assigned to an interval $[r_{i,j-1}, ds_{1,j}]$ for some $i \in \{1, \ldots, n-1\}$ and $j \in \{1, \ldots, n-1\}$.

Proof. Each job is assigned to an interval inside some segment, as the double deadlines prevent jobs to span more than one segment. Suppose the green y-job y_{ℓ} is assigned to segment p. As $ds_{1,p} + y_{\ell} > ds_{1,p} + x_n$, by Properties 2 and 3, and the deadline following $r_{n,p} = ds_{1,p} + x_n$ is $ds_{1,p+1}$, it must be that the green y-job y_{ℓ} finishes at $ds_{1,p+1}$. Moreover, $ds_{1,p+1} - y_{\ell}$ is equal to a real deadline as $ds_{1,p+1} - y_{\ell}$ is even.

Each of the 2n jobs that have been assigned so far finish at a double deadline $ds_{1,j}, ds_{2,j}$. Thus, no other jobs may end at a double deadline.

Claim 5 (*) A red fill job of length x_1-1 is assigned to each interval $[ds_{1,j}, f_{1,j}]$, $0 \le j \le n-1$.

This uses up all red fill jobs of length $x_1 - 1$.

Claim 6 For each $\ell \in \{1, ..., n\}$, the green x-job x_{ℓ} is assigned to an interval $[ds_{1,j}, r_{i,j}]$ for some $i \in \{1, ..., n\}$ and $j \in \{0, ..., n-1\}$.

Proof. Suppose the green x-job x_{ℓ} is assigned to segment p. Notice that $x_{\ell} > r_{n,p} - f_{1,p}$. Indeed $r_{n,p} - f_{1,p} = x_n - x_1 + 1$ and, by construction, $x_n - x_1 + 1 \le 2b_m$, whereas $x_{\ell} \ge 2b_m + 4$. Moreover, $r_{n,p}$ is the latest deadline in p. So the green x-job x_{ℓ} starts at $ds_{1,p}$. Notice that $ds_{1,p} + x_{\ell} < ds_{1,p+1}$ and that $ds_{1,p} + x_{\ell}$ corresponds to a real deadline as $ds_{1,p} + x_{\ell}$ is even, but all fake deadlines are odd.

By Claims 2, 4, and 6, and since we have the same amount of segments as green x-jobs, resp. green y-jobs, we obtain that each segment I_j , $1 \le j \le n$,, contains exactly one green x-job and exactly one green y-job.

Claim 7 For $j \in \{1, ..., n\}$, the green x-job and the green y-job in the segment I_j do not overlap.

Proof. Suppose otherwise, that is, suppose there is a $j \in \{1, ..., n\}$ such that I_j contains a green x-job, say x_ℓ , and a green y-job, say y_k , that overlap (i.e. the intervals they are assigned to overlap). Since x_ℓ ends at a real deadline by Claim 6 and y_k starts at a real deadline by Claim 4, no job ends at the fake deadline situated at $ds_{1,j-1} + x_\ell - 1$, which contradicts the validity of the SCD solution.

The last claim implies that in each segment I_j , $1 \le j \le n$, there is a green x-job x_{ℓ_j} and a green y-job y_{k_j} which together have the same size as the interval. Hence the couples $C_j = \{a_{\ell_j}, b_{k_j}\}, 1 \le j \le n$, form a solution of dNMTS. Thus, we have the following lemma.

Lemma 2. $dNMTS \leq_p SCD$.

Our main theorem follows from the strong NP-hardness of dNMTS, Lemmata 1 and 2, and the membership of WSR₂ in NP, which is easily verified as the certificate is a path and an assignment of the splits to its edges, all of which can be encoded in polynomial space.

Theorem 6. WSR₂ is strongly NP-complete.

Corollary 1 (*). Splits Reconstruction for Caterpillars of Unbounded Hair-Length and Maximum Degree 3 is NP-complete.

3 Algorithm for WSR₂ with few distinct vertex weights

Let $k = |\{\omega(v) : v \in V\}|$ denote the number of distinct vertex weights in an instance (V, ω, \mathcal{S}) for WSR₂. We exhibit a dynamic programming algorithm for WSR₂ that works in polynomial time when k is a constant. Moreover, standard backtracking can be used to actually construct a solution, if one exists.

Suppose |V| = n and the multiset of splits, S, contains the splits $s_1 \le s_2 \dots \le s_{n-1}$. Let $w_1 < w_2 \dots < w_k$ denote the distinct vertex weights and m_1, m_2, \dots, m_k denote their respective multiplicities, i.e. $m_i = |\{v \in V : \omega(v) = w_i\}|$ for all $i \in \{1, 2, \dots, k\}$.

Our dynamic programming algorithm computes the entries of a boolean table A. The table A has an entry $A[p, W_L, W_R, v_1, v_2, \ldots, v_k]$ for each integer p with $1 \leq p \leq n-1$, each two integers $W_L, W_R \in \mathcal{S}$, and each $v_i \in \{0, 1, \ldots, m_i\}$, where $i \in \{1, 2, \ldots, k\}$. The entry $A[p, W_L, W_R, v_1, v_2, \ldots, v_k]$ is set to true iff there is an assignment of the splits s_1, s_2, \ldots, s_p to the ℓ leftmost edges and the r rightmost edges of the path P_n on n vertices, such that

- $-\ p=\ell+r;$
- $-v_1$ weights w_1, v_2 weights w_2, \ldots , and v_k weights w_k are assigned to the ℓ leftmost and the r rightmost vertices of P_n such that each split assigned to the left (respectively to the right) part of the path corresponds to the sum of the vertex weights assigned to vertices to the left (respectively to the right) of this split; and
- W_L is equal to the value of the ℓ^{th} split from the left and W_R is equal to the r^{th} split from the right.

Intuitively, our algorithm assigns splits and weights by starting from both endpoints of the path and trying to meet these two sub-solutions. For the base case, set $A[0, W_L, W_R, v_1, v_2, \ldots, v_k]$ to true if $W_L = W_R = v_1 = v_2 = \ldots = v_k = 0$ and to false otherwise. We compute the remaining entries of A by increasing values of p using the following recurrence.

$$A[p,W_L,W_R,v_1,v_2,\ldots,v_k] = \bigvee_{i=1}^k \begin{cases} A[p-1,W_L-w_i,W_R,v_1,v_2,\ldots,v_{i-1},\\ v_i-1,v_{i+1},v_{i+2},\ldots,v_k]\\ \forall A[p-1,W_L,W_R-w_i,v_1,v_2,\ldots,v_{i-1},\\ v_i-1,v_{i+1},v_{i+2},\ldots,v_k] \end{cases}$$

In the previous recurrence, each table entry that does not exist has the value false.

The final result of the algorithm is computed by evaluating the expression

$$\bigvee_{\substack{W_L, W_R \in \mathcal{S} \\ i \in \{1, 2, \dots, k\} \\ (W_L \leq w_i + W_R) \ \land \ (W_R \leq w_i + W_L)}} A[|\mathcal{S}|, W_L, W_R, m_1, m_2, \dots, m_{i-1}, m_i - 1, m_{i-1}, m_{i+1}, m_{i+2}, \dots, m_k].$$

The correctness proof and the running-time analysis of our dynamic programming algorithm (see Appendix C) establish the following theorem.

Theorem 7 (*). WSR₂ can be solved in time $O(n^{k+3} \cdot k)$, where k is the number of distinct vertex weights of any input instance (V, ω, S) and n = |V|.

4 SR₃ is NP-complete

In this section we show that Splits Reconstruction with unit weights is NP-complete for trees with maximum degree 3. Our polynomial-time reduction is done from the strongly NP-complete NMTS problem recalled in Section 1. This problem remains NP-complete even if each integer of the NMTS instance is at most p(m), where p is a polynomial and m is the length of the description of the instance. Let us just mention that the next theorem does not immediately follow from Corollary 1.

Theorem 8. SR_3 is NP-complete.

Proof. Let $\tilde{A} = \{\tilde{a}_1, \tilde{a}_2, \dots, \tilde{a}_m\}$, $\tilde{B} = \{\tilde{b}_1, \tilde{b}_2, \dots, \tilde{b}_m\}$ and $\tilde{S} = \{\tilde{s}_1, \tilde{s}_2, \dots, \tilde{s}_m\}$ be an instance of NMTS. Let $C = \max\{x : x \in \tilde{A} \cup \tilde{B}\}$ be the maximum over $\tilde{A} \cup \tilde{B}$. W.l.o.g., we construct the following equivalent NMTS instance:

$$a_i := \tilde{a}_i + 2 + 3C, \quad 1 \le i \le m,$$

 $b_i := \tilde{b}_i + 3 + 5C, \quad 1 \le i \le m, \text{ and }$
 $s_i := \tilde{s}_i + 5 + 8C, \quad 1 \le i \le m.$

Let $A = \bigcup_{1 \leq i \leq m} \{a_i\}$, $B = \bigcup_{1 \leq i \leq m} \{b_i\}$, and $S = \bigcup_{1 \leq i \leq m} \{s_i\}$. Clearly, the instance $(\tilde{A}, \tilde{B}, \tilde{S})$ has a solution iff the instance (A, B, S) has a solution.

Now we describe an instance (V, S) of SR_3 , which is a YES-instance iff the

previous instance (A, B, S) of NMTS is a YES-instance (see also Figure 2). Let $n = 2m - 2 + \sum_{i=1}^{m} a_i + \sum_{i=1}^{m} b_i$ be the number of vertices in V; we recall that they have unit weight. The multiset $\mathcal S$ of splits is defined as follows.

- For each value s_i , $1 \le i \le m$, the value $1 + s_i$ is added to S and we refer to these splits as red splits.
- For each value s_i , $2 \le i \le m-2$, the value $(i-1) + \sum_{j=1}^{i} (1+s_j)$ is added to S and we refer to these splits as black splits.
- For each value a_i , $1 \le i \le m$, the values $\{1, 2, ..., a_i\}$ are added to S and we refer to these splits as green splits.
- For each value b_i , $1 \le i \le m$, the values $\{1, 2, ..., b_i\}$ are added to \mathcal{S} and we refer to these splits as blue splits.

Finally each value x of S is replaced by $\min(x, n - x)$.

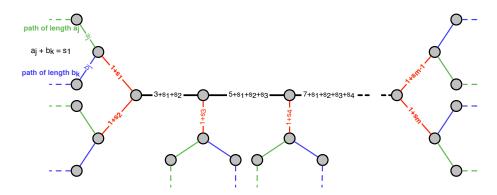


Fig. 2. A tree with maximum degree 3 representing a solution to a SR₃ instance constructed as described in the proof of Theorem 8.

Lemma 3 (*). (A, B, S) is a YES-instance for NMTS if and only if (V, ω) : $V \to \{1\}, \mathcal{S}$) is a YES-instance for SR₃.

As the certificate is a tree on n vertices, the membership in NP is obvious.

Freely choosable weights 5

We remark that the following modification of WSR makes any set of splits realizable in some tree. Suppose the weight function ω is not given, but freely choosable, that is, we ask whether, given a multiset S of integers, there exists a tree T = (V, E) and a weight function $\omega : V \to \mathbb{N}$, such that S is the multiset of splits of T. We call this problem CHWSR.

Theorem 9 (\star). CHWSR always admits a solution.

6 Conclusion

In Section 3, we have shown that, in the framework of parameterized complexity [5, 8, 16], WSR₂ is in XP when parameterized by the number of distinct vertex weights. A generalization of this problem is W[1]-hard [7], but it remains open whether this problem is fixed parameter tractable. For practical purposes, it would further be important to identify other quantities that are small in practice (e.g. the number of leaves, the diameter of the tree, or topological indices), and investigate the multivariate complexity of the considered problems parameterized by combinations of these quantities.

There is a large contrast between the complexities of WSR, where we are given n vertex weights, and CHWSR, where we can freely choose the vertex weights, or, alternatively, we can choose the vertex weights from an infinite multiset containing n times each element of N. It would be interesting to know some restrictions on the multiset of vertex weights such that the problem becomes tractable with respect to interesting parameterizations. Ideally, these restrictions should be consistent with the applications in drug design and discovery.

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A Proof of Claims 2, 3 and 5

Claim 2 (*) The green y-job y_n is assigned to the interval $[r_{n,n-1}, ds_{1,n}]$.

Proof. As in the previous proof, one job must be assigned to this interval, whose length is $\sum_{k=1}^{n} z_k - x_n - \sum_{k=1}^{n-1} z_k = z_n - x_n$, which is y_n by Property 4. Thus, the green y-job y_n is assigned to the interval $[r_{n,n-1}, ds_{1,n}]$.

Claim 3 (*) The black overlap job is assigned to the interval $[f_{n,n-1}, ds_{1,n}]$.

Proof. As $r_{n,n-1}$ is the only deadline between $f_{n,n-1}$ and $ds_{1,n}$, the processor that does not use this deadline needs to process a job finishing at $ds_{1,n}$ and starting before $r_{n,n-1}$. This is the black overlap job, since no other job is long enough. It is assigned to the interval $[f_{n,n-1}, ds_{1,n}]$ of length $ds_{1,n} - f_{n,n-1} = z_n - x_n + 1$.

Claim 5 (*) A red fill job of length x_1-1 is assigned to each interval $[ds_{1,j}, f_{1,j}]$, $0 \le j \le n-1$.

Proof. Since both processors finish a job at deadline $ds_{1,j}$ (resp., are initialized at time $ds_{1,0} = 0$) and one of them finishes a job at the following deadline, which is $f_{1,j}$, we need to assign a job of length $f_{1,j} - ds_{1,j} = x_1 - 1$ to the interval $[ds_{1,j}, f_{1,j}]$. W.l.o.g., this is one of the red fill jobs of length $x_1 - 1$.

B Proof of Corollary 1

Corollary 1 (*). Splits Reconstruction for Caterpillars of Unbounded Hair-Length and Maximum Degree 3 is NP-complete.

Proof. It is clear that this problem, abbreviated SRC, is in NP. To show that it is hard for NP, we reduce from WSR₂. Let $I_P' = (\omega_1', \ldots, \omega_{n-2}', s_1', \ldots, s_{n-3}')$ be an instance of WSR₂, where ω_i' , $1 \le i \le n-2$, are the vertex weights and s_j' , $1 \le j \le n-3$, are the splits. We assume that all vertex weights and splits are upper bounded by a polynomial in n; as WSR₂ is strongly NP-hard, it is still NP-hard with this restriction. Define $\Omega := 1+2 \cdot \max\{\omega_i' : 1 \le i \le n-2\}$. To simplify the argument, consider an auxiliary instance $I_P = (\omega_1, \ldots, \omega_n, s_1, \ldots, s_{n-1})$ of WSR₂ obtained from I_P' by:

- augmenting the values of s_i' , $1 \le j \le n-3$, by Ω ,
- adding $\omega_{n-1} = \omega_n = \Omega$ to the multiset of weights,
- adding $s_{n-2} = s_{n-1} = \Omega$ to the multiset of splits,
- and finally, multiplying each value in I_P by $n\Omega$ (so $\omega_i = \omega_i' n\Omega$, and $s_j = s_j' n\Omega$).

It is not difficult to see that I_P and I_P' are equivalent.

Now let us create an instance I_C of SRC in the following way.

- replace each weight ω_i , $1 \le i \le n$, by ω_i copies of weight 1,

- for each ω_i , $1 \le i \le n$, add auxiliary splits $s_{f,i} = f$, $1 \le f \le \omega_i 1$,
- keep the original splits (s_1, \ldots, s_{n-1}) .

Notice that there are $\sum_{i=1}^{n} \omega_i$ vertices and $(\sum_{i=1}^{n} \omega_i) - 1$ splits (i.e. edges) in total

As one easily checks, if I_P has a solution then I_C has a solution. Now suppose I_C has a solution C. Then, as C is an instance for SRC, it follows that C is a caterpillar of maximum degree 3 (with unbounded hair-length). Call B the backbone of C. Let $B' \subseteq B$ be maximal such that its endvertices have degree 3.

By construction $s_i > 1$, $1 \le i \le n - 1$, and only the splits $s_{1,i}$, $1 \le i \le n$, have value 1. There are exactly n such splits, and so, C must have exactly n leaves.

Since there is no split of value $n\Omega^2 + 1$, each hair of C has length at most $n\Omega^2$. So, as $s_i > n\Omega^2$ for $i = 1, \ldots, n-3$, we obtain that the splits s_1, \ldots, s_{n-3} are assigned to edges b_1, \ldots, b_{n-3} in E(B'). Observe that the edges b_1, \ldots, b_{n-3} induce a connected graph (i.e. a path), as all other splits are smaller than the minimum of the s_i , $i = 1, \ldots, n-3$.

Let P be the path formed by the edges b_1, \ldots, b_{n-3} and let u and v be the two endpoints of P. There is at most one vertex y such that if we look at the values of the splits of the edges from u to y (resp. from v to y), then they are strictly increasing. In addition, if two edges of P share a vertex $x \neq y$, then there must be hair attached to x, because the splits associated to these two edges differ by more than 1. Furthermore, there are hairs H_1 and H_2 of length $n\Omega^2$ attached to the first and to the last vertex on the backbone, as no two auxiliary splits are large enough to add up to one of the original splits s_i , $i = 1, \ldots n-3$. From the fact that C has exactly n leaves, it follows that the remaining hair has to be attached to y. As a consequence, $E(B') = \{b_1, \ldots, b_{n-3}\}$.

Hence, all edges outside B'' (that is, edges from hairs) belong to auxiliary splits, where B'' is equal to B' augmented with the two edges to which the splits of value $n\Omega^2$ are assigned. This means that the edges adjacent to B'' correspond to auxiliary splits $s_{\omega_i-1,i}$.

In order to find a solution for I_P , it thus suffices to take B'' and replace all hairs with the corresponding weight on their starting vertex on B''.

C Proof of Theorem 7

Theorem 7 (*). WSR₂ can be solved in time $O(n^{k+3} \cdot k)$, where k is the number of distinct vertex weights of any input instance (V, ω, S) and n = |V|.

Proof. The correctness of the base case is clear. For the correctness of the recurrence, let v_{pivot} be the vertex on P_n where the two sub-solutions corresponding to the left and to the right part of P_n meet. First note that the values of the splits increase from left to right until we encounter vertex v_{pivot} , from which point they decrease. Filling up the path from both ends, this means that reading the splits from s_1 to s_{n-1} , we can assign them to the path, each time only deciding whether we assign it to the left part or to the right part of the path

(in the SCD model, this would be equivalent to deciding whether to meet the next deadline on the processor P_1 or on the processor P_2). The first (respectively second) case of the recurrence corresponds to assigning the next split to the left (respectively right) part of the path by inserting a vertex of weight w_i , $i \in \{1, 2, ..., k\}$. The correctness of the final evaluation follows because it inserts the one missing vertex weight that has not been used between the left and the right part of the path.

The table has $|\mathcal{S}|^3 \cdot \Pi_{i=1}^k(m_i+1) \leq n^{k+3}$ entries, each entry can be computed in time O(k), and the final evaluation takes time $O(n \cdot k)$.

D Proof of Lemma 3

Lemma 3 (*). (A, B, S) is a YES-instance for NMTS if and only if $(V, \omega : V \to \{1\}, S)$ is a YES-instance for SR₃.

Proof. Throughout the proof, when we refer to a split of value x, we mean a split of value $\min(x, n - x)$.

" \Rightarrow " Assume that (A, B, S) is a YES-instance for NMTS. We will show that there is a solution to SR_3 . A tree T=(V,E) and a bijective function $b:E\to \mathcal{S}$ can be constructed as follows (see also Figure 2). Construct a path P with m-3 edges with the black splits such that the $(i-1)^{\text{th}}$ edge is associated to the black split $(i-1)+\sum_{j=1}^i(1+s_j), i\in\{2,3,\ldots,m-2\}$. Add two edges incident to the first vertex of P, that are associated to the red splits $1+s_1$ and $1+s_2$. Add two edges incident to the last vertex of P that are associated to the red splits $1+s_{m-1}$ and $1+s_m$. To the i^{th} vertex of P, $2\leq i\leq m-3$, add one incident edge associated to the red split $1+s_{i+1}$. Finally, for each $a_i\in A$ and each $b_i\in B$, construct the paths with a_i and b_i vertices respectively. To each edge of these 2m paths, we can associate a green or a blue split. It remains to attach one green path and one blue path to each endpoint of an edge associated to a red split (one endpoint is already involved in the path P and of degree 3). The way to attach these path is given by the solution to the (A, B, S) instance.

" \Leftarrow " Assume that there exists a solution (T,b) to SR_3 , where T=(V,E) is a tree of maximum degree 3 and b is a bijection from E to S. We show how a solution of the NMTS instance (A,B,S) can be derived from (T,b). Let us note that for any $i,j,k \in \{1,2,\ldots,m\}$, we have that $a_i+s_j>s_k$, that $a_i+a_j< s_k$, that $b_i+b_j>s_k$, and that $a_i+a_j>b_k$.

Claim 8 For every $i \in \{1, 2, ..., m\}$, there is a path on a_i edges, called the a_i -path, using the splits $1, 2, ..., a_i$ (w.l.o.g., they are green) and there is a path on b_i edges, called the b_i -path, using the splits $1, 2, ..., b_i$ (w.l.o.g., they are blue). All these a-paths and b-paths are edge-disjoint.

Proof. As the instance has 2m splits of value 1, T has 2m leaves. Each of these leaves is incident to a green or blue split of value 1. As the instance also has 2m splits of each of the values $2, 3, \ldots, 2+3C$, the leaves of T are the starting points of 2m edge-disjoint paths P_1, P_2, \ldots, P_{2m} , each having 2+3C edges in T.

Consider an $x \in A \cup B$ and the splits $2+3C+1, 2+3C+2, \ldots, x$. As x < 4+6C, and as there is no split smaller than 2+3C other than those we have already used to form the paths $P_i, 1 \le i \le 2m$, the splits $2+3C+1, 2+3C+2, \ldots, x$ are assigned to an extension of a path P_i , which, together with P_i , forms a path P_i' with x edges using the splits $1, 2, \ldots, x$. All these paths $P_i', 1 \le i \le 2m$, are edge disjoint and w.l.o.g., green splits are assigned to their edges if they have at most 2+4C edges and blue splits otherwise.

Claim 9 For every $i \in \{1, 2, ..., m\}$, the red split of value $1 + s_i$ is assigned to an edge e_i of T whose vertex u_i is the common extremity of an a-path and a b-path, where u_i is in the subtree of $T - e_i$ that has $s_i + 1$ vertices.

Proof. As no split has value s_i , vertex u_i is incident to another two edges besides e_i . We note that all splits, besides those of the a- and b-paths, have value at least 6+8C. One such split plus the smallest a_j , $1 \le j \le m$, would exceed s_i . So, u_i is the end point of two a/b-paths. These cannot be two a-paths as $a_j + a_k < s_i$, for any $j,k \in \{1,2,\ldots,m\}$ and they cannot be two b-paths as $b_j + b_k > s_i$, for any $j,k \in \{1,2,\ldots,m\}$. Thus, u_i is the common extremity of an a-path and a b-path.

Finally, a solution to the instance (A, B, S) of NMTS is formed by the couples C_1, C_2, \ldots, C_m , where each C_i contains a_{i_a} and b_{i_b} , where i_a and i_b are such that the edge e_i of T, with $b(e_i) = 1 + s_i$, is incident to the a_{i_a} -path and the b_{i_b} -path. This proves the NP-hardness of SR₃.

E Proof of Theorem 9

Theorem 9 (*). CHWSR always admits a solution.

Proof. We show that the answer to CHWSR is always yes: Decompose \mathcal{S} into κ chains $s_1^j < s_2^j < \dots s_{m(j)}^j, \ j=1,\dots,\kappa$, where κ is the maximal multiplicity in \mathcal{S} . Let T be obtained from the star $K_{1,\kappa}$ by subdividing e_j , the j^{th} edge of T, m(j)-1 times (for $j=1,\dots,\kappa$), and root T at the center r of $K_{1,\kappa}$. Map the s_j^i to edges of the subdivided e_j , keeping their order, so that the edge corresponding to s_0^j is incident to a leaf of T. Finally, choose the weight $\omega(r)$ for the root to be equal to the maximum value in \mathcal{S} . For each leaf v of T, set the weight $\omega(v)$ equal to the split assigned to the edge $\{v,u\}$, where u is the parent of v. Any other vertex v is given a weight equal to the difference of splits assigned to the edges incident to v. This choice of T and ω clearly satisfies the requirements. \square

Remark. Due to the construction provided by the proof of Theorem 9, we note that we are not only always able to construct a tree T as required, but the structure of this tree is also rather simple. In particular, the realization of the split sequence is a path if each split in S repeats at most twice.