


Maximizing Phylogenetic Diversity Under Ecological Constraints: A Parameterized Complexity Study

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Abstract

In the NP-hard OPTIMIZING PHYLOGENETIC DIVERSITY WITH DEPENDENCIES (PDD) problem, the input consists of a phylogenetic tree \mathcal{T} over a set of taxa X , a food-web that describes the prey-predator relationships in X , and integers k and D . The task is to find a set S of k species that is viable in the food-web such that the subtree of \mathcal{T} obtained by retaining only the vertices of S has total edge weight at least D . Herein, viable means that for every predator taxon of S , the set S contains at least one prey taxon.

We provide the first systematic analysis of PDD and its special case with star trees, s-PDD, from a parameterized complexity perspective. For solution-size related parameters, we show that PDD is fixed-parameter tractable (FPT) with respect to D and with respect to k plus the height of the phylogenetic tree. Moreover, we consider structural parameterizations of the food-web. For example, we show an FPT-algorithm for the parameter that measures the vertex deletion distance to graphs where every connected component is a complete graph. Finally, we show that s-PDD admits an FPT-algorithm for the treewidth of the food-web. This disproves, unless $P = NP$, a conjecture of Faller et al. [Annals of Combinatorics, 2011] who conjectured that s-PDD is NP-hard even when the food-web is a tree.

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1 Introduction

Human activity has greatly accelerated the rate at which biological species go extinct. The conservation of biological diversity is thus one of mankind's most urgent tasks. The inherently limited amount of resources that one may devote to this task, however, necessitates decisions on which conservation strategies to pursue. To support such decisions, one needs to incorporate quantitative information on the possible impact and the success likelihood of conservation strategies. In this context, one task is to compute an optimal conservation strategy in light of this information.

To find a conservation strategy with the best positive impact, one would ideally aim to maximize the functional diversity of the surviving taxa (species). However, measuring this diversity is hard or impossible in many scenarios [18]. As a result, maximizing phylogenetic diversity has become the standard, albeit imperfect, surrogate for maximizing functional diversity [11, 13, 18]. Informally, phylogenetic diversity measures the evolutionary distance of a set of taxa. In its most simple form, this measurement is based on an edge-weighted



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phylogenetic tree \mathcal{T} of the whole set of taxa X , and the phylogenetic diversity of a subset of taxa S is the sum of the weights of the edges of the subtree of \mathcal{T} obtained by retaining only the taxa of S . Assuming equal protection costs for all taxa, the task is to find a set S of at most k taxa that achieves maximal phylogenetic diversity. This problem, called MAXIMIZE PHYLOGENETIC DIVERSITY [9], can be solved very efficiently by a greedy algorithm [9, 19, 23, 27].

Computing an optimal conservation strategy becomes much more difficult, however, when the success likelihood of a strategy is included in the model. One way to achieve this is to add concrete survival probabilities for protected taxa, leading in its most general form to the NP-hard GENERALIZED NOAH'S ARK PROBLEM [12, 16]. This problem formulation, however, still has a central drawback: It ignores that the survival of some taxa may also depend on the survival of other taxa. This aspect was first considered by Moulton et al. [21] in the OPTIMIZING PD WITH DEPENDENCIES (PDD) problem. Here, the input additionally contains a directed acyclic graph \mathcal{F} with vertex set X where an arc uv is present if the existence of taxa u provides all the necessary foundations for the existence of taxon v . In other words, \mathcal{F} models ecological dependencies between taxa. Now, a taxon v may survive only if (i) it does not depend on other taxa at all, that is, it has no incoming arcs, or (ii) at least one taxon u survives such that \mathcal{F} contains the arc uv . The most-wide spread interpretation of such ecological dependency networks are food-webs where the arc uv means that taxon v feeds on taxon u .¹ A subset of taxa X where every vertex fulfills (i) or (ii) is called *viable*. The task in PDD is to select a *viable* set of k taxa that achieves a maximal phylogenetic diversity. In this work, we study PDD from an algorithmic point of view.

Moulton et al. [21] showed that PDD can be solved by the greedy algorithm if the objective of maximizing phylogenetic diversity agrees with the viability constraint in a precise technical sense. Later, PDD was conjectured to be NP-hard [26]. This conjecture was confirmed by Faller et al. [10], who showed that PDD is NP-hard even if the food-web \mathcal{F} is a tree. Further, Faller et al. [10] considered s-PDD, the special case where the phylogenetic tree is restricted to be a star, and showed that s-PDD is NP-hard even for food-webs which have a bipartite graph as underlying graph. Polynomial-time algorithms were provided for very restricted special cases, for example for PDD when the food-web is a *directed* tree [10]. Finally, for food-webs with constant depth, PDD was shown to admit a constant-factor approximation algorithm [8].

Our Contribution. As PDD is NP-hard even on very restricted instances [10], we turn to parameterized complexity in order to overcome this intractability. In particular, we aim to identify problem-specific parameters κ such that PDD can be solved in $f(\kappa) \cdot |I|^{\mathcal{O}(1)}$ time (these are called FPT-algorithms) or to show that such algorithms are unlikely, by showing W[1]-hardness for the parameter κ . Here, we consider the most natural parameters related to the solution, such as the solution size k and the threshold of diversity D , and parameters that describe the structure of the input food-web \mathcal{F} . We formally consider the decision problem, where we ask for the existence of a viable solution with diversity at least D , but our algorithms actually solve the optimization problem as well.

Our most important results are the following; Table 1 gives an overview. In Theorem 3.4, we prove that PDD is FPT when parameterized with the solution size k plus the height of the phylogenetic tree \mathcal{T} . This also implies that PDD is FPT with respect to D , the diversity threshold. We also consider the dual parameter \overline{D} , that is, the amount of diversity that is lost from \mathcal{T} and show that PDD is W[1]-hard with respect to \overline{D} .

¹ We remark that previous works [21, 10] consider a reversed interpretation of the arcs. We define the order such that a source of the network also corresponds to a source of the ecosystem.

■ **Table 1** Parameterized complexity results for PDD and s-PDD. Here, D.t. τ stands for Distance to τ – the number of vertices that need to be removed to obtain a graph from graph class τ .

Parameter		s-PDD		PDD
Budget k	FPT	Thm. 3.2	XP (FPT is <i>open</i>)	Obs. 3.1
Diversity D	FPT	Thm. 4.1	FPT	Thm. 4.1
Species-loss \bar{k}	W[1]-hard, XP	Prop. 4.2, Obs. 3.1	W[1]-hard, XP	Prop. 4.2, Obs. 3.1
Diversity-loss \bar{D}	W[1]-hard, XP	Prop. 4.2, Obs. 3.1	W[1]-hard, XP	Prop. 4.2, Obs. 3.1
D.t. Cluster	FPT	Thm. 5.1	NP-h for 0	Thm. 5.3
D.t. Co-Cluster	FPT	Thm. 5.5	FPT	Thm. 5.5
Treewidth $tw_{\mathcal{F}}$	FPT	Thm. 5.6	NP-h for $tw_{\mathcal{F}} = 1$	[10]

We then consider the structure of the food-web. In particular, we consider the special case that each connected component of the food-web \mathcal{F} is a complete digraph. As we will show, this case is structurally equivalent to the case that each connected component of \mathcal{F} is a star with one source vertex. Thus, this case describes a particularly simple dependency structure, where taxa are either completely independent or have a common source. We show that PDD is NP-hard in this special case while s-PDD has an FPT-algorithm when parameterized by the vertex deletion distance to this special case. Our results thus yield structured classes of food-webs where the complexity of s-PDD and PDD strongly differ. Finally, we show that s-PDD is FPT with respect to the treewidth of the food-web and therefore can be solved in polynomial time if the food-web is a tree (Theorem 5.6). Our result disproves a conjecture of Faller et al. [10, Conjecture 4.2] that s-PDD is NP-hard even when the food-web is a tree (unless $P = NP$). Again, this result shows that s-PDD can be substantially easier than PDD on some structured classes of food-webs.

Structure of the Paper. In Section 2, we formally define OPTIMIZING PD WITH DEPENDENCIES, give an overview of previous results and our contribution, and prove some simple initial results. In Section 3, we study s-PDD and PDD with respect to k , the solution size. In Section 4, we show that PDD is FPT with respect to the desired diversity but W[1]-hard for the acceptable loss of diversity. In Section 5, we consider parameterization by structural parameters of the food-web. Finally, in Section 6, we discuss future research ideas. The proofs of theorems, lemmas, and observations marked with (\star) are deferred to a full version of this work.

2 Preliminaries

2.1 Definitions

For a positive integer a , by $[a]$ we denote the set $\{1, 2, \dots, a\}$, and by $[a]_0$ the set $\{0\} \cup [a]$. We generalize functions $f : A \rightarrow B$, where B is a family of sets, to handle subsets $A' \subseteq A$ of the domain by defining $f(A') := \bigcup_{a \in A'} f(a)$.

For any graph G , we write $V(G)$ and $E(G)$, respectively, to denote the set of vertices and edges of G . We write $\{u, v\}$ for an undirected edge between u and v . For a directed edge from u to v , we write uv or (u, v) to increase readability. For a vertex set $V' \subseteq V(G)$, we let $G[V'] := (V', \{e \in E(G) \mid \text{both endpoints of } e \text{ are in } V'\})$ denote the subgraph of G induced by V' . Moreover, with $G - V' := G[V \setminus V']$ we denote the graph obtained from G by removing V' and its incident edges.

Phylogenetic Trees and Phylogenetic Diversity. A tree $T = (V, E)$ is a directed graph in which the *root* is the only vertex with an in-degree of zero, each other vertex has an in-degree of one. The root is denoted with ρ . The *leaves* of a tree are the vertices which have an out-degree of zero. We refer to the non-leaf vertices of a tree as *internal vertices*. A tree is a star if the root is the only internal vertex and all other vertices are leaves. For a given set X , a *phylogenetic X -tree* $\mathcal{T} = (V, E, \omega)$ is a tree $T = (V, E)$ with an *edge-weight* function $\omega : E \rightarrow \mathbb{N}_{>0}$ and a bijective labeling of the leaves with elements from X where all non-leaves in \mathcal{T} have out-degree at least two. We write \max_ω to denote the biggest edge weight in \mathcal{T} . The set X is a set of *taxa* (species). Because of the bijective labeling, we interchangeably use the words taxon and leaf. In biological applications, the set X is a set of taxa, the internal vertices of \mathcal{T} correspond to biological ancestors of these taxa and $\omega(e)$ describes the phylogenetic distance between the endpoints of e , as these endpoints correspond to distinct (possibly extinct) taxa, we may assume this distance is greater than zero.

For a directed edge $uv \in E$, we say u is the *parent* of v and v is a *child* of u . If there is a directed path from u to v in \mathcal{T} (including when $u = v$), we say that u is an *ancestor* of v and v is a *descendant* of u . The sets of ancestors and descendants of v are denoted by $\text{anc}(v)$ and $\text{desc}(v)$, respectively. The set of descendants of v which are in X are *offspring* $\text{off}(v)$ of a vertex v . For an edge $e = uv \in E$, we denote $\text{off}(e) = \text{off}(v)$.

For a tree $T = (V, E)$ and a vertex set $V' \subseteq V$, the *spanning tree of V'* is denoted by $T(V')$. The *subtree of T rooted at v* is $T(\{v\} \cup \text{off}(v))$ and denoted by T_v , for some vertex $v \in V$. Given a set of taxa $A \subseteq X$, let $E_{\mathcal{T}}(A)$ denote the set of edges $e \in E$ with $\text{off}(e) \cap A \neq \emptyset$. The *phylogenetic diversity* $PD_{\mathcal{T}}(A)$ of A is defined by

$$PD_{\mathcal{T}}(A) := \sum_{e \in E_{\mathcal{T}}(A)} \omega(e). \quad (1)$$

In other words, the phylogenetic diversity $PD_{\mathcal{T}}(A)$ of a set A of taxa is the sum of the weights of edges which have offspring in A .

Food-Webs. For a set of taxa X , a *food-web* $\mathcal{F} = (X, E)$ on X is a directed acyclic graph. If xy is an edge of E then x is *prey* of y and y is a *predator* of x . The set of prey and predators of x is denoted with $N_{<}(x)$ and $N_{>}(x)$, respectively. A taxon x with an empty set of prey is a *source* and $\text{sources}(\mathcal{F})$ denotes the set of sources in the food-web \mathcal{F} . For a taxon $x \in X$ we define $X_{\leq x}$ to be the set of taxa X which can reach x in \mathcal{F} . Analogously, $X_{\geq x}$ is the set of taxa which x can reach in \mathcal{F} .

For a given food-web \mathcal{F} and a set $Z \subseteq X$ of taxa, a set of taxa $A \subseteq Z$ is *Z -viable* if $\text{sources}(\mathcal{F}[A]) \subseteq \text{sources}(\mathcal{F}[Z])$. A set of taxa $A \subseteq X$ is *viable* if A is X -viable. In other words, a set $A \subseteq Z$ is Z -viable or viable if each source in $\mathcal{F}[A]$ is also a source in $\mathcal{F}[Z]$ or in \mathcal{F} , respectively.

Problem Definitions and Parameterizations. Our main problem is defined as follows.

OPTIMIZING PD WITH DEPENDENCIES (PDD)

Input: A phylogenetic X -tree \mathcal{T} , a food-web \mathcal{F} on X , and integers k and D .

Question: Is there a viable set $S \subseteq X$ such that $|S| \leq k$ and $PD_{\mathcal{T}}(S) \geq D$?

Additionally in OPTIMIZING PD IN VERTEX-WEIGHTED FOOD-WEBS (s-PDD) we consider the special case of PDD in which the phylogenetic X -tree \mathcal{T} is a star. Throughout the paper, we adopt the convention that n is the number of taxa $|X|$ and we let m denote the number of edges in the food-web $|E(\mathcal{F})|$. Observe that \mathcal{T} has $\mathcal{O}(n)$ edges.

For an instance $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ of PDD, we define $\overline{D} := PD_{\mathcal{T}}(X) - D = \sum_{e \in E} \omega(e) - D$. Informally, \overline{D} is the acceptable loss of diversity: If we save a set of taxa $A \subseteq X$ with $PD_{\mathcal{T}}(A) \geq D$, then the total amount of diversity we lose from \mathcal{T} is at most \overline{D} . Similarly, we define $\overline{k} := |X| - k$. That is, \overline{k} is the minimum number of species that need to become extinct.

Parameterized Complexity. Throughout this paper, we consider a number of parameterizations of PDD and s-PDD. For a detailed introduction to parameterized complexity refer to the standard monographs [5, 7]; we only give a brief overview here.

A parameterization of a problem Π associates with each input instance \mathcal{I} of Π the value of a specific *parameter* κ . A parameterized problem Π is *fixed-parameter tractable* (FPT) with respect to some parameter κ if there exists an algorithm solving every instance (\mathcal{I}, κ) of Π in time $f(\kappa) \cdot |\mathcal{I}|^{\mathcal{O}(1)}$. A parameterized problem Π is *slice-wise polynomial* (XP) with respect to some parameter κ if there exists an algorithm solving every instance (\mathcal{I}, κ) of Π in time $|\mathcal{I}|^{f(\kappa)}$. Here, in both cases, f is some computable function only depending on κ . Parameterized problems that are W[1]-hard are believed not to be FPT. We use the \mathcal{O}^* -notation which omits factors polynomial in the input size.

Color Coding. For an in-depth treatment of color coding, we refer the reader to [5, Chapter 5] and [1]. Here, we give some definitions which we use throughout the paper.

For integers n and k , an (n, k) -perfect hash family \mathcal{H} is a family of functions $f : [n] \rightarrow [k]$ such that for every subset Z of $[n]$ of size k , some $f \in \mathcal{H}$ exists which is injective when restricted to Z . For any integers $n, k \geq 1$ an (n, k) -perfect hash family which contains $e^k k^{\mathcal{O}(\log k)} \cdot \log n$ functions can be constructed in time $e^k k^{\mathcal{O}(\log k)} \cdot n \log n$ [22, 5].

2.2 Preliminary Observations

We start with some observations and reduction rules which we use throughout the paper.

► **Observation 2.1.** *Let \mathcal{F} be a food-web. A set $A \subseteq X$ is viable if and only if there are edges $E_A \subseteq E(\mathcal{F})$ such that every connected component in the graph (A, E_A) is a tree with root in $\text{sources}(\mathcal{F})$.*

Proof. If A is viable, then $\text{sources}(\mathcal{F}[A])$ is a subset of $\text{sources}(\mathcal{F})$. It follows that for each taxon $x \in A$, either x is a source in \mathcal{F} or A contains a prey y of x . Conversely, if such a graph (A, E_A) exists then explicitly the sources of $\mathcal{F}[A]$ are a subset of $\text{sources}(\mathcal{F})$. ◀

► **Observation 2.2.** *Let $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ be a yes-instance of PDD. Then $k > |X|$ or a viable set $S \subseteq X$ with $PD_{\mathcal{T}}(S) \geq D$ exists which has size exactly k .*

Proof. Let S be a solution for \mathcal{I} . If S has a size of k , nothing remains to be shown. Otherwise, observe that $S \cup \{x\}$ is viable and $PD_{\mathcal{T}}(S \cup \{x\}) \geq PD_{\mathcal{T}}(S)$ for each taxon $x \in (N_{>}(S) \cup \text{sources}(\mathcal{F})) \setminus S$. Because $(N_{>}(S) \cup \text{sources}(\mathcal{F})) \setminus S$ is non-empty unless $S = X$, we conclude that $S \cup \{x\}$ is a solution and iteratively, there is a solution of size k . ◀

► **Observation 2.3.** *Let $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ be an instance of PDD. In $\mathcal{O}(|\mathcal{I}|^2)$ time one can compute an equivalent instance $\mathcal{I}' := (\mathcal{T}', \mathcal{F}', k', D')$ of PDD with only one source in \mathcal{F}' , $k' := k + 1$ and $D' \in \mathcal{O}(D)$.*

Proof. Let $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ be an instance of PDD. Add a new taxon \star to \mathcal{F} and add edges from \star to each taxon x of $\text{sources}(\mathcal{F})$ to obtain \mathcal{F}' . To obtain \mathcal{T}' , add \star as a child to the root ρ of \mathcal{T} and set $\omega'(\rho\star) = D + 1$ and $\omega'(e) = \omega(e)$ for each $e \in E(\mathcal{T})$. Finally, set $k' := k + 1$ and $D' := 2 \cdot D + 1$ and let $\mathcal{I}' = (\mathcal{T}', \mathcal{F}', k + 1, 2 \cdot D + 1)$. All steps can be performed in $\mathcal{O}(|\mathcal{I}|^2)$ time.

The equivalence of \mathcal{I} and \mathcal{I}' follows from the observation that $S \subseteq X$ is a solution for \mathcal{I} if and only if $S \cup \{\star\}$ is a solution for \mathcal{I}' . ◀

► **Reduction Rule 1.** Let $R \subseteq X$ be the set of taxa which have a distance of at least k to every source. Then, set $\mathcal{F}' := \mathcal{F} - R$ and $\mathcal{T}' := \mathcal{T} - R$.

► **Lemma 2.4.** Reduction Rule 1 is correct and can be applied exhaustively in $\mathcal{O}(n + m)$ time.

Proof. By definition, each viable set of taxa which has a size of k is disjoint from R . Therefore, the set R is disjoint from every solution. The set R can be found in $\mathcal{O}(n + m)$ time by breadth-first search. This is also the total running time for the rule, since one application of the rule is exhaustive. ◀

After Reduction Rule 1 has been applied exhaustively, for any taxon $x \in X$ there is a viable set S_x of size at most k with $x \in S_x$. If some edge e has weight at least D , then for each taxon x which is an offspring of e , the set S_x is viable, has size at most k , and $PD_{\mathcal{T}}(S_x) \geq PD_{\mathcal{T}}(\{x\}) \geq D$. So, S_x is a solution. This implies the correctness of the following rule.

► **Reduction Rule 2.** Apply Reduction Rule 1 exhaustively. If $\max_{\omega} \geq D$ return **yes**.

We can also remove some edges which are not important for guaranteeing viability.

► **Reduction Rule 3.** Given an instance $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ of PDD with $vw \in E(\mathcal{F})$. If v is not a source and $uw \in E(\mathcal{F})$ for each $u \in N_{<}(v)$, then remove vw from $E(\mathcal{F})$.

► **Lemma 2.5.** Reduction Rule 3 is correct and can be applied exhaustively in $\mathcal{O}(n^3)$ time.

Proof. First, observe that if \mathcal{I}' is a **yes**-instance, then so is \mathcal{I} because every set that is viable in \mathcal{I}' is viable in \mathcal{I} . Conversely, let \mathcal{I} be a **yes**-instance of PDD with solution S . If $v \notin S$, then S is also a solution for instance \mathcal{I}' . If $v \in S$ then because S is viable in \mathcal{F} , some vertex u of $N_{<}(v)$ is in S . Consequently, S is also viable in $\mathcal{F} - vw$, as w still could be fed by u (if $w \in S$).

The running time can be seen as follows. For each pair of taxa v and w , we can check $N_{<}(v) \subseteq N_{<}(w)$ in $\mathcal{O}(n)$ time. Consequently, an exhaustive application of Reduction Rule 3 takes $\mathcal{O}(n^3)$ time. ◀

3 Parameterization by the Solution Size

In this section, we consider parameterization by the size of the solution k . First, we observe that PDD is XP when parameterized by k and \bar{k} . In Section 3.1 we show that s-PDD is FPT with respect to k . We generalize this result in Section 3.2 by showing that PDD is FPT when parameterized by $k + \text{height}_{\mathcal{T}}$. Recall that $\bar{k} := n - k$.

► **Observation 3.1.** PDD can be solved in $\mathcal{O}(n^{k+2})$ and $\mathcal{O}(n^{\bar{k}+2})$ time.

Proof. One may use the following brute-force algorithm: Iterate over the sets S of X of size k . Return **yes** if there is a viable set S with $PD_{\mathcal{T}}(S) \geq D$. Return **no** if there is no such set.

The correctness of the algorithm follows from Observation 2.2. Checking whether a set S is viable and has diversity of at least D can be done $\mathcal{O}(n^2)$ time. The running time bound now follows because there are $\binom{n}{k} = \binom{n}{n-k} = \binom{n}{\bar{k}}$ subsets of X of size k . ◀

3.1 s-PDD

We show that s-PDD is FPT when parameterized by the size of the solution k .

► **Theorem 3.2** (\star). *s-PDD can be solved in $\mathcal{O}(2^{3 \cdot 03k + o(k)} \cdot nm \cdot \log n)$ time.*

The idea behind the algorithm is to color the taxa and require that a solution should contain at most one taxon of each color. Formally, we consider the following auxiliary problem. In k -COLORED OPTIMIZING PD IN VERTEX-WEIGHTED FOOD-WEBS (k -C-S-PDD), alongside the usual input $(\mathcal{T}, \mathcal{F}, k, D)$ of s-PDD, we are given a coloring $c : X \rightarrow [k]$ which assigns each taxon a *color* $c(x) \in [k]$. We ask whether there is a viable set $S \subseteq X$ of taxa such that $PD_{\mathcal{T}}(S) \geq D$, and $c(S)$ is *colorful*. A set $c(S)$ is colorful if c is injective on S . Observe that each colorful set S satisfies $|S| \leq k$. We first show how to solve k -C-S-PDD via dynamic programming. Then, applying the color-coding toolbox allows us to extend this result to the uncolored version.

► **Lemma 3.3.** *k -C-S-PDD can be solved in $\mathcal{O}(3^k \cdot n \cdot m)$ time.*

Proof.

Table definition. Let $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D, c)$ be an instance of k -C-S-PDD and by Observation 2.3 we assume that $\star \in X$ is the only source in \mathcal{F} .

Given $x \in X$, a set of colors $C \subseteq [k]$, and a set of taxa $X' \subseteq X$, we say that a set $S \subseteq X' \subseteq X$ is (C, X') -feasible if (i) $c(S) = C$, (ii) $c(S)$ is colorful, and (iii) S is X' -viable. We define a dynamic programming algorithm with tables DP and DP'. For $x \in X$, $C \subseteq [k]$ we want entry DP[x, C] to store the maximum $PD_{\mathcal{T}}(S)$ of $(C, X_{\geq x})$ -feasible sets S . Recall $X_{\geq x}$ is the set of taxa which x can reach in \mathcal{F} . If no $(C, X_{\geq x})$ -feasible set $S \subseteq X'$ exists, we want DP[x, C] to store $-\infty$. In other words, in DP[x, C] we store the biggest phylogenetic diversity of a set S which is $X_{\geq x}$ -viable and c bijectively maps S to C .

For any taxon x , let y_1, \dots, y_q be an arbitrary but fixed order of $N_{>}(x)$. In the auxiliary table DP', we want entry DP'[x, p, C] for $p \in [q]$, and $C \subseteq [k]$ to store the maximum $PD_{\mathcal{T}}(S)$ of (C, X') -feasible sets $S \subseteq X'$, where $X' = \{x\} \cup X_{\geq y_1} \cup \dots \cup X_{\geq y_p}$. If no (C, X') -feasible set $S \subseteq X'$ exists, we want DP'[x, p, C] to store $-\infty$.

Algorithm. As a base case for each $x \in X$ and $p \in [|N_{>}(x)|]$ let DP[x, \emptyset] and DP[x, p, \emptyset] store 0 and let DP[x, C] store $-\infty$ if C is non-empty and $c(x) \notin C$. For each $x \in X$ with $N_{>}(x) = \emptyset$, we store $\omega(\rho x)$ in DP[$x, \{c(x)\}$]. Recall that ρx is an edge because \mathcal{T} is a star.

Fix a taxon $x \in X$. For every $Z \subseteq C \setminus \{c(x)\}$, we set DP'[$x, 1, \{c(x)\} \cup Z$] := DP[y_1, Z]. To compute further values, once DP'[x, q, Z] for each $q \in [p]$, and every $Z \subseteq C$ is computed, for $Z \subseteq C \setminus \{c(x)\}$ we use the recurrence

$$DP'[x, p+1, \{c(x)\} \cup Z] := \max_{Z' \subseteq Z} DP'[x, p, \{c(x)\} \cup Z \setminus Z'] + DP[y_{p+1}, Z']. \quad (2)$$

Finally, we set DP[x, C] := DP'[x, q, C] for every $C \subseteq [k]$.

We return **yes** if DP[\star, C] stores at least d for some $C \subseteq [k]$. Otherwise, we return **no**.

Correctness. The base cases are correct. The tables are computed first for taxa further away from the source and with increasing size of C . Assume that for a fixed taxon x with predators y_1, \dots, y_q and a fixed $p \in [q]$, the entries DP[x', Z] and DP'[x, p', Z] for each $x' \in N_{>}(x)$, for each $p' \in [p]$, and every $Z \subseteq [k]$ store the desired value. Fix a set $C \subseteq [k]$ with $c(x) \in C$. We show that if DP'[$x, p+1, C$] stores d then there is a (C, X') -feasible set

$S \subseteq X' \cup X_{\geq y_{p+1}}$ for $X' := \{x\} \cup X_{\geq y_1} \cup \dots \cup X_{\geq y_p}$ with $PD_{\mathcal{T}}(S) = d$. Afterward, we show that if $S \subseteq X' \cup X_{\geq y_{p+1}}$ with $PD_{\mathcal{T}}(S) = d$ is a (C, X') -feasible set then $DP'[x, p+1, C]$ stores at least d .

If $DP'[x, p+1, C] = d > 0$ then by Recurrence (2), there is a set $Z \subseteq C \setminus \{c(x)\}$ such that $DP'[x, p, C \setminus Z] = d_x$ and $DP[y_{p+1}, Z] = d_y$ with $d = d_x + d_y$. Therefore, there is a $(C \setminus Z, X')$ -feasible set $S_x \subseteq X'$ with $PD_{\mathcal{T}}(S_x) = d_x$ and a $(Z, X_{\geq y_{p+1}})$ -feasible set $S_y \subseteq X_{\geq y_{p+1}}$ with $PD_{\mathcal{T}}(S_y) = d_y$. Define $S := S_x \cup S_y$ and observe that $PD_{\mathcal{T}}(S) = d$. It remains to show that S is a $(C, X' \cup X_{\geq y_{p+1}})$ -feasible set. First, observe that because $C \setminus Z$ and Z are disjoint, we conclude that $c(S)$ is colorful. Then, $c(S) = c(S_x) \cup c(S_y) = C \setminus Z \cup Z = C$ where the first equation holds because $c(S)$ is colorful. The taxa x and y_{p+1} are the only sources in $\mathcal{F}[X_{\geq x}]$ and $\mathcal{F}[X_{\geq y_{p+1}}]$, respectively. Therefore, x is in S_x and y_{p+1} is in S_y unless S_y is empty. If $S_y = \emptyset$ then $S = S_x$ and S is $X' \cup X_{\geq y_{p+1}}$ -viable because S is X' -viable. Otherwise, if S_y is non-empty then because S_y is $X_{\geq y_{p+1}}$ -viable, we conclude $\text{sources}(\mathcal{F}[S_y]) = \{y_{p+1}\}$. As $x \in S$ and $y_{p+1} \in N_{>}(x)$ we conclude $\text{sources}(\mathcal{F}[S]) = \{x\}$ and so S is $X' \cup X_{\geq y_{p+1}}$ -viable. Therefore, S is a $(C, X' \cup X_{\geq y_{p+1}})$ -feasible set.

Conversely, let $S \subseteq X' \cup X_{\geq y_{p+1}}$ be a non-empty $(C, X' \cup X_{\geq y_{p+1}})$ -feasible set with $PD_{\mathcal{T}}(S) = d$. Observe that X' and $X_{\geq y_{p+1}}$ are not necessarily disjoint. We define S_y to be the set of taxa of $X_{\geq y_{p+1}}$ which are connected to y_{p+1} in $\mathcal{F}[X_{\geq y_{p+1}}]$. Further, define $Z := c(S_y)$ and define $S_x := S \setminus S_y$. As $c(S)$ is colorful especially $c(S_x)$ and $c(S_y)$ are colorful. Thus, S_y is a $(Z, X_{\geq y_{p+1}})$ -feasible time. Further, $c(S_x) = C \setminus c(S_y) = C \setminus Z$. As $\text{sources}(\mathcal{F}[S]) = \text{sources}(\mathcal{F}[X' \cup X_{\geq y_{p+1}}]) = \{x\}$, we conclude $x \in S$. Because \mathcal{F} is a DAG, x is not in $X_{\geq y_{p+1}}$ and so x is in S_x . Each vertex of S which can reach y_{p+1} in $\mathcal{F}[S]$ is in $F_{\geq y_{p+1}}$ and subsequently in S_y . Consequently, because S is $X' \cup X_{\geq y_{p+1}}$ -viable we conclude $\text{sources}(\mathcal{F}[S_x]) = \{x\}$. Thus, S_x is $(C \setminus Z, X')$ -feasible. So, $DP[y_{p+1}, Z] = PD_{\mathcal{T}}(S_x)$ and $DP'[x, p, C \setminus Z] = PD_{\mathcal{T}}(S_y)$. Hence, $DP'[x, p+1, C]$ stores at least $PD_{\mathcal{T}}(S)$.

Running time. The base cases can be checked in $\mathcal{O}(k)$ time. As each $c \in [k]$ in Recurrence (2) can either be in Z' , in $\{c(x)\} \cup Z \setminus Z'$ or in $[k] \setminus (\{c(x)\} \cup Z)$, all entries of the tables can be computed in $\mathcal{O}(3^k \cdot n \cdot m)$ time. \blacktriangleleft

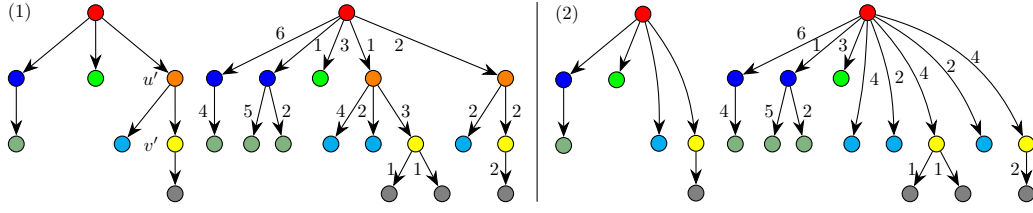
We defer the details of the proof of Theorem 3.2 to the long version since this is essentially standard application of color coding using a perfect hash family as defined in Section 2.1.

3.2 PDD on Trees with Bounded Height

Next, we generalize the result of the previous subsection and we show that PDD is FPT when parameterized with the size of the solution k plus $\text{height}_{\mathcal{T}}$, the height of the phylogenetic tree. The algorithm uses color-coding, data reduction rules, and the enumeration of trees.

► **Theorem 3.4.** PDD can be solved in $\mathcal{O}^*(K^K \cdot 2^{3.028K + o(K)})$ time where $K := k \cdot \text{height}_{\mathcal{T}}$.

To show Theorem 3.4, we use a subroutine for solving the following problem. We define a *pattern-tree* $\mathcal{T}_P = (V_P, E_P, c_P)$ to be a tree (V_P, E_P) with a vertex-coloring $c_P : V_P \rightarrow [k \cdot \text{height}_{\mathcal{T}}]$. Recall that $\mathcal{T}(Y)$ is the spanning tree of the vertices in Y . In OPTIMIZING PD WITH PATTERN-DEPENDENCIES (PDD-PATTERN), we are given alongside the usual input $(\mathcal{T}, \mathcal{F}, k, D)$ of PDD a pattern-tree $\mathcal{T}_P = (V_P, E_P, c_P)$, and a vertex-coloring $c : V(\mathcal{T}) \rightarrow [k \cdot \text{height}_{\mathcal{T}}]$. We ask whether there is a viable set $S \subseteq X$ of taxa such that S has a size of at most k , $c(\mathcal{T}\langle S \cup \{\rho\} \rangle)$ is colorful, and $\mathcal{T}\langle S \cup \{\rho\} \rangle$ and \mathcal{T}_P are *color-equal*. That is, there is an edge uv of $\mathcal{T}\langle S \cup \{\rho\} \rangle$ with $c(u) = c_u$ and $c(v) = c_v$ if and only if there is an edge $u'v'$ of \mathcal{T}_P with $c(u') = c_u$ and $c(v') = c_v$. Informally, given a pattern-tree we want that it matches the colors of the spanning tree induced by the root and the solution.



■ **Figure 1** An example for Reduction Rule 6. (1) An instance of PDD-PATTERN (2) The instance after an application of Reduction Rule 6 to the marked vertices. In both instances, the pattern-tree is on the left and the phylogenetic tree is on the right.

Next we present reduction rules with which we can reduce the phylogenetic tree in an instance of PDD-PATTERN to be a star which subsequently can be solved with Theorem 3.2. Afterward, we show how to apply this knowledge to compute a solution for PDD.

► **Reduction Rule 4.** *Let uv be an edge of \mathcal{T} . If there is no edge $u'v' \in E_P$ with $c_P(u') = c(u)$ and $c_P(v') = c(v)$, then set $\mathcal{T}' := \mathcal{T} - \text{desc}(v)$ and $\mathcal{F}' := \mathcal{F} - \text{off}(v)$.*

► **Lemma 3.5.** *Reduction Rule 4 is correct and can be applied exhaustively in $\mathcal{O}(n^3)$ time.*

Proof. Assume $S \subseteq X$ is a solution of the instance of PDD-PATTERN. As there is no edge $u'v' \in E_P$ with $c_P(u') = c(u)$ and $c_P(v') = c(v)$ we conclude that $S \cap \text{desc}(v) = \emptyset$ and so the reduction rule is safe.

The running time can be seen as follows. To check whether Reduction Rule 4 can be applied, we need to iterate over both $E(\mathcal{T})$ and E_P . Therefore, a single application can be executed in $\mathcal{O}(n^2)$ time. In each application of Reduction Rule 4 we remove at least one vertex so that an exhaustive application can be computed in $\mathcal{O}(n^3)$ time. ◀

► **Reduction Rule 5.** *Let $u'v'$ be an edge of \mathcal{T}_P . For each vertex $u \in V(\mathcal{T})$ with $c(u) = c_P(u')$ such that u has no child v with $c(v) = c_P(v')$, set $\mathcal{T}' := \mathcal{T} - \text{desc}(u)$ and $\mathcal{F}' := \mathcal{F} - \text{off}(u)$.*

► **Lemma 3.6.** *Reduction Rule 5 is correct and can be applied exhaustively in $\mathcal{O}(n^3)$ time.*

Proof. Let S be a solution for the instance of PDD-PATTERN. The spanning tree $\mathcal{T}\langle S \cup \{\rho\} \rangle$ contains exactly one vertex w with color $c(u)$. As $c(w) = c_P(u')$ we conclude that w has a child w' and $c(w') = c_P(v')$. Consequently, $w \neq u$ and $S \cap \text{desc}(u) = \emptyset$.

As in Reduction Rule 4, we may apply the rule by iterating over the edges of \mathcal{T} and \mathcal{T}_P . Each application either removes at least one vertex or concludes that the reduction rule is applied exhaustively. ◀

► **Reduction Rule 6.** *Apply Reduction Rules 4 and 5 exhaustively. Let ρ be the root of \mathcal{T} and let ρ_P be the root of \mathcal{T}_P . Let v' be a grand-child of ρ_P and let u' be the parent of v' . Then, do the following.*

1. For each vertex u of \mathcal{T} with $c(u) = c_P(u')$ add edges ρv to \mathcal{T} for every child v of u .
2. Set the weight of ρv to be $\omega(uv)$ if $c(v) \neq c_P(v')$ or $\omega(uv) + \omega(\rho u)$ if $c(v) = c_P(v')$.
3. Add edges $\rho_P w'$ to \mathcal{T}_P for every child w' of u' .
4. Set $\mathcal{T}'_P := \mathcal{T}_P - u'$ and $\mathcal{T}' := \mathcal{T} - u$.

Figure 1 depicts an application of Reduction Rule 6.

► **Lemma 3.7.** *Reduction Rule 6 is correct and can be applied exhaustively in $\mathcal{O}(n^3 m)$ time.*

Proof. Assume that \mathcal{I} is a **yes**-instance of PDD-PATTERN with solution S . Because $\mathcal{T}\langle S \cup \{\rho\} \rangle$ and \mathcal{T}_P are color-equal also $\mathcal{T}'\langle S \cup \{\rho\} \rangle$ and \mathcal{T}'_P are color-equal. Let u^* and w_1 be the unique vertices in $\mathcal{T}\langle S \cup \{\rho\} \rangle$ with $c(u^*) = c_P(u')$ and $c(w_1) = c_P(v')$. Let w_2, \dots, w_ℓ be the other children of u^* . As $PD_{\mathcal{T}'}(S)$ is the sum of the weights of the edges of $\mathcal{T}'\langle S \cup \{\rho\} \rangle$ we conclude $PD_{\mathcal{T}'}(S) = PD_{\mathcal{T}}(S) - (\omega(\rho u^*) + \sum_{i=1}^{\ell} \omega(u^* w_i)) + \sum_{i=1}^{\ell} \omega'(\rho w_i)$. Since $\omega'(\rho w_1) = \omega(\rho u^*) + \omega(u^* w_1)$ and $\omega'(\rho w_i) = \omega(u^* w_i)$ for $i \in [\ell] \setminus \{1\}$, we conclude that $PD_{\mathcal{T}'}(S) = PD_{\mathcal{T}}(S) \geq D$. Therefore, S is a solution for \mathcal{I}' . The converse direction of the equivalence can be shown analogously.

It remains to bound the running time. For a given grand-child v' of ρ_P , one performs $\mathcal{O}(n)$ color-checks and adds $\mathcal{O}(n)$ edges. As the reduction rule can be applied at most $|\mathcal{T}_P| \in \mathcal{O}(n)$ times, an exhaustive application takes $\mathcal{O}(n^2)$ time. So, the predominant factor in the running time is the exhaustive application of the other reduction rules. \blacktriangleleft

With these reduction rules, we can reduce the phylogenetic tree of a given instance of PDD-PATTERN to only be a star and then solve PDD-PATTERN by applying Theorem 3.2.

► **Lemma 3.8.** PDD-PATTERN can be solved in $\mathcal{O}(3^k \cdot n \cdot m + n^3)$ time.

Proof. Let $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D, \mathcal{T}_P = (V_P, E_P, c_P), c)$ be a given instance of PDD-PATTERN. We use the following algorithm. If there is a vertex $v \in V_P$ and $c_P(v) \notin c(V(\mathcal{T}))$ then return **no**. If $c(\rho) \neq c_P(\rho_P)$ where ρ and ρ_P are the roots of \mathcal{T} and \mathcal{T}_P respectively, return **no**. Otherwise, apply Reduction Rule 6 exhaustively. Then, both \mathcal{T}_P and \mathcal{T} are stars. Return **yes** if and only if $(\mathcal{T}', \mathcal{F}', k, D, c)$ is a **yes**-instance of k -C-S-PDD.

For the correctness, first observe that if \mathcal{T}_P contains a vertex v with $c_P(v) \notin c(V(\mathcal{T}))$, or if $c(\rho) \neq c_P(\rho_P)$, then \mathcal{I} is a **no**-instance. For the remaining cases, the correctness follows from Lemma 3.7 and Lemma 3.3.

The running time can be seen as follows. By Reduction Rule 6 can be applied exhaustively in $\mathcal{O}(n^2 \cdot (n+m))$ time. By Lemma 3.3, the overall running time thus is $\mathcal{O}(3^k \cdot n \cdot m + n^3)$. \blacktriangleleft

To prove Theorem 3.4 we reduce from PDD to PDD-PATTERN and apply Lemma 3.8. For this, we use the fact that there are n^{n-2} labeled directed trees with n vertices [25] which can be enumerated in $\mathcal{O}(n^{n-2})$ time [2]. To solve instance \mathcal{I} of PDD, we will check each of these trees as a pattern-tree for a given coloring of the phylogenetic tree. These colorings will be defined with a perfect hash family as defined in Section 2.1. Recall that $K = k \cdot \text{height}_{\mathcal{T}}$.

Proof of Theorem 3.4.

Algorithm. Let $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ be an instance of PDD. Let the vertices of \mathcal{T} be $v_1, \dots, v_{|V(\mathcal{T})|}$. Iterate over $i \in [\min\{K, |V(\mathcal{T})|\}]$. Compute a $(|V(\mathcal{T})|, i)$ -perfect hash family \mathcal{H}_i . Compute the set \mathcal{P}_i of labeled directed trees with i vertices.

For every $\mathcal{T}_P = (V_P, E_P, c_P) \in \mathcal{P}_i$, proceed as follows. Assume that the labels of \mathcal{T}_P are in $[i]$. For every $f \in \mathcal{H}_i$, first construct the coloring c_f such that $c_f(v_j) = f(j)$ for each $v_j \in V(\mathcal{T})$. Then, solve instance $\mathcal{I}_{\mathcal{T}_P, f} := (\mathcal{T}, \mathcal{F}, k, D, \mathcal{T}_P, c_f)$ of PDD-PATTERN using Lemma 3.8. Return **yes** if and only if $\mathcal{I}_{\mathcal{T}_P, f}$ is a **yes**-instance for some $f \in \mathcal{H}_i$ and some $\mathcal{T}_P \in \mathcal{P}_i$.

Correctness. Any solution of an instance $\mathcal{I}_{\mathcal{T}_P, f}$ of PDD-PATTERN clearly is a solution for \mathcal{I} .

Conversely, we show that if S is a solution for \mathcal{I} , then there are \mathcal{T}_P and f such that $\mathcal{I}_{\mathcal{T}_P, f}$ is a **yes**-instance of PDD-PATTERN. So let S be a viable set of taxa with $|S| \leq k$ and $PD_{\mathcal{T}}(S) \geq D$. Let $V^* \subseteq V(\mathcal{T})$ be the set of vertices v that have offspring in S . It follows $|V^*| \leq \text{height}_{\mathcal{T}} \cdot |S| \leq K$. Then, there is a hash function $f \in \mathcal{H}_{V^*}$ mapping V^* bijectively to $[|V^*|]$. Consequently, $\mathcal{P}_{|V^*|}$ contains a tree \mathcal{T}_P which is isomorphic to $\mathcal{T}[V^*]$ with labels c_f . Hence, $\mathcal{I}_{\mathcal{T}_P, f}$ is a **yes**-instance of PDD-PATTERN.

Running Time. For a fixed $i \in [K]$, the set \mathcal{H}_i contains $e^{i \cdot \mathcal{O}(\log i)} \cdot \log n$ hash functions and the set \mathcal{P}_i contains $\mathcal{O}(i^{i-2})$ labeled trees. Both sets can be computed in $\mathcal{O}(i^{i-2} \cdot n \log n)$ time.

Each instance $\mathcal{I}_{\mathcal{T}_P, f}$ of PDD-PATTERN is constructed in $\mathcal{O}(n)$ time and can be solved in $\mathcal{O}(3^k \cdot n^3)$ time. Thus, the overall running time is $\mathcal{O}(K \cdot e^K K^{K-2+\mathcal{O}(\log K)} \cdot 3^k \cdot n^3 \log n)$, which summarizes to $\mathcal{O}(K^K \cdot 2^{1.443K+1.585k+o(K)} \cdot n^3 \log n)$. ◀

4 Parameterization by Desired Diversity and Accepted Diversity Loss

In this section, we first consider parameterization with the diversity threshold D . For this parameter, we present an FPT algorithm for PDD. Afterward, we show that s-PDD is intractable with respect to \bar{D} , the acceptable loss of phylogenetic diversity. As the edge-weights are integers, we conclude that we can return **yes** if $k \geq D$ or if the height of the phylogenetic tree \mathcal{T} is at least D , after Reduction Rule 1 has been applied exhaustively. Otherwise, $k + \text{height}_{\mathcal{T}} \in \mathcal{O}(D)$ and thus the FPT algorithm for $k + \text{height}_{\mathcal{T}}$ (Theorem 3.4) directly gives an FPT algorithm for PDD in that case.

Here, we present another algorithm with a faster running time. To obtain this algorithm, we subdivide edges of the phylogenetic tree according to their edge weights. We then use color coding on the vertices of the subdivided tree. Let us remark that this technique is closely related to an algorithm of Jones and Schestag [15] for another hard problem related to diversity maximization.

► **Theorem 4.1** (\star). PDD can be solved in $\mathcal{O}(2^{3.03(2D+k)+o(D)} \cdot nm + n^2)$ time.

In some instances, the diversity threshold D may be very large. Then, however, the acceptable loss of diversity $\bar{D} = PD_{\mathcal{T}}(X) - D$ could be small. Encouraged by this observation, recently, several problems in maximizing phylogenetic diversity have been studied with respect to the acceptable diversity loss [14, 15]. In this section, we show that, unfortunately, s-PDD is already $W[1]$ -hard with respect to \bar{D} even if the edge weights are at most two.

To show this, we reduce from RED-BLUE NON-BLOCKER. Here, the input is an undirected bipartite graph G with vertex bipartition $V = V_r \cup V_b$ and an integer k . The question is whether there is a set $S \subseteq V_r$ of size at least k such that the neighborhood of $V_r \setminus S$ is V_b . RED-BLUE NON-BLOCKER is $W[1]$ -hard when parameterized by the solution size k [6].

► **Proposition 4.2.** s-PDD is $W[1]$ -hard with respect to \bar{D} , even if $\max_{\omega} = 2$.

Proof.

Reduction. Let $\mathcal{I} := (G = (V = V_r \cup V_b, E), k)$ be an instance of RED-BLUE NON-BLOCKER. We construct an instance $\mathcal{I}' = (\mathcal{T}, \mathcal{F}, k', D)$ of s-PDD as follows. Let \mathcal{T} be a star with root $\rho \notin V$ and leaves V . In \mathcal{T} , an edge $e = \rho u$ has weight 1 if $u \in V_r$ and otherwise $\omega(e) = 2$, if $u \in V_b$. Define a food-web \mathcal{F} with vertices V and for each edge $\{u, v\} \in E$, and every tuple of vertices $u \in V_b, v \in V_r$, add an edge uv to \mathcal{F} . Finally, set $k' := |V| - k$ and $D := 2 \cdot |V_b| + |V_r| - k$, or equivalently $\bar{k} = \bar{D} = k$.

Correctness. The reduction can be computed in polynomial time. We show that if \mathcal{I} is a **yes**-instance of RED-BLUE NON-BLOCKER then \mathcal{I}' is a **yes**-instance of PDD. Afterward, we show the converse.

Assume that \mathcal{I} is a **yes**-instance of RED-BLUE NON-BLOCKER. Therefore, there is a set $S \subseteq V_r$ of size at least k such that $N_G(V_r \setminus S) = V_b$. (We assume $|S| = k$ as $N_G(V_r \setminus S) = V_b$ still holds if we shrink S .) We define $S' := V \setminus S$ and show that S' is a solution for \mathcal{I}' . The size

of S' is $|V \setminus S| = |V| - |S| = k'$. Further, $PD_{\mathcal{T}}(S) = 2 \cdot |V_b| + |V_r \setminus S| = 2 \cdot |V_b| + |V_r| - k = D$. By definition, the vertices in V_r are sources. Further, because S is a solution for \mathcal{I} , each vertex of V_b has a neighbor in $V_r \setminus S$. So, S' is viable and \mathcal{I}' is a **yes**-instance of s-PDD.

Conversely, let $S' \subseteq V$ be a solution for instance \mathcal{I}' of s-PDD. Without loss of generality, S' contains r vertices from V_r and b vertices of V_b . Consequently, $|V| - k \geq |S'| = b + r$ and $2 \cdot |V_b| + |V_r| - k = D \leq PD_{\mathcal{T}}(S') = 2b + r$. We conclude $r \leq |V| - k - b$ and so $2b \geq 2 \cdot |V_b| + |V_r| - k - r \geq 2 \cdot |V_b| + |V_r| - k - (|V| - k - b) = |V_b| + b$. Therefore, $b = |V_b|$ and $V_b \subseteq S'$. Further, $r = |V_r| - k$. We define $S := V_r \setminus S'$ and conclude $|S| = |V_r| - r = k$. Because S' is viable, each vertex in V_b has a neighbor in $S' \setminus V_b$. Therefore, S is a solution for the **yes**-instance \mathcal{I} of RED-BLUE NON-BLOCKER. \blacktriangleleft

5 Structural Parameters of the Food-Web

Next, we study how the structure of the food-web affects the complexity of s-PDD and PDD. First, we consider parameterization with respect to the distance of the food-web to a cluster graph, denoted cvd . We show that PDD is NP-hard even if the food-web is a cluster graph but s-PDD is FPT when parameterized by cvd . Afterward, we show that PDD is FPT with respect to the distance to co-cluster and s-PDD is FPT with respect to the treewidth of the food-web, denoted by $\text{tw}_{\mathcal{F}}$.

5.1 Distance to Cluster Graphs

In this subsection, we consider the special case that given an instance of PDD or s-PDD, we need to remove few vertices from the undirected underlying graph of the food-web \mathcal{F} to obtain a cluster graph. Here, a graph is a cluster graph if every connected component is a clique. We show that s-PDD is easy on graphs that are close to being a cluster graph. More precisely, in Theorem 5.1, we show that s-PDD is FPT with respect to the distance to cluster. Herein, for a graph $G = (V, E)$ the *distance to cluster* $\text{cvd}(G)$ is the smallest number d such that there exists a set $Y \subseteq V$ of size at most d such that $G - Y$ is a cluster graph. The FPT-algorithm shows in particular that s-PDD is tractable even on some very dense classes of food-webs. Afterward, we show that PDD is NP-hard on cluster graphs.

The FPT-algorithm exploits the following fact: If \mathcal{F} is acyclic and its underlying graph is a cluster graph, then every clique in \mathcal{F} has exactly one vertex $v_0 \in V(C)$ such that $v_0 \in N_{<}(v)$ for each $v \in V(C) \setminus \{v_0\}$. After applying Reduction Rule 3 exhaustively to a cluster graph, each connected component of the food-web is thus an out-star.

► **Theorem 5.1** (\star). *s-PDD can be solved in $\mathcal{O}(6^d \cdot n^2 \cdot m \cdot k^2)$ time, when we are given a set $Y \subseteq X$ of size d such that $\mathcal{F} - Y$ is a cluster graph.*

To prove Theorem 5.1, we first show how to solve the case where we want to save all taxa in Y .

► **Lemma 5.2.** *Given an instance $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ of s-PDD and a set $Y \subseteq X$ of size d such that $\mathcal{F} - Y$ is a cluster graph, we can compute whether there is a viable set $S \cup Y$ with $|S \cup Y| \leq k$ and $PD_{\mathcal{T}}(S \cup Y) \geq D$ in $\mathcal{O}(3^d \cdot n \cdot k^2)$ time.*

Proof. We provide a dynamic programming algorithm. Let C_1, \dots, C_c be the connected components of $\mathcal{F} - Y$ and let $x_1^{(i)}, \dots, x_{|C_i|}^{(i)}$ be an order of C_i such that $(x_{j_1}^{(i)}, x_{j_2}^{(i)}) \in E(\mathcal{F})$ for $j_1 < j_2$.

Table definition. A set $S \subseteq X \setminus Y$ of taxa is (ℓ, Z) -feasible, if $|S| \leq \ell$ and $S \cup Z$ is viable. The dynamic programming algorithm has tables DP and DP_i for each $i \in [c]$. The entry $DP[i, \ell, Z]$ for $i \in [c]$, $\ell \in [k]_0$, and $Z \subseteq Y$ stores the largest phylogenetic diversity $PD_{\mathcal{T}}(S)$ of an (ℓ, Z) -feasible set $S \subseteq C_1 \cup \dots \cup C_i$ and $-\infty$ if no such set S exists.

The table entries $DP_i[j, b, \ell, Z]$ additionally have a dimension b with $b \in \{0, 1\}$. For $b = 0$, an entry $DP_i[j, b, \ell, Z]$ with $b \in \{0, 1\}$ stores the largest phylogenetic diversity $PD_{\mathcal{T}}(S)$ of an (ℓ, Z) -feasible set $S \subseteq \{x_1^{(i)}, \dots, x_j^{(i)}\}$. For $b = 1$, additionally some vertex $v_{j'}^{(i)}$ with $j' < j$ needs to be contained in S .

Algorithm. Iterate over the edges of \mathcal{F} . For each edge $uv \in E(\mathcal{F})$ with $u, v \in Y$, remove all edges incoming at v , including uv , from $E(\mathcal{F})$. After this removal, v is a new source.

We initialize the base cases of DP_i by setting $DP_i[j, 0, 0, Z] := 0$ for each $i \in [c]$, each $j \in [|C_i|]$, and every $Z \subseteq \text{sources}(\mathcal{F})$. Moreover, $DP_i[1, b, \ell, Z] := \omega(\rho v_1^{(i)})$ if $\ell \geq 1$ and $Z \subseteq N_{>}(v_1^{(i)}) \cup \text{sources}(\mathcal{F})$; and $DP_i[1, b, \ell, Z] := -\infty$, otherwise.

To compute further values for $j \in [|C_i| - 1]$, $b \in \{0, 1\}$, and $\ell \in [k]$ we use the recurrences

$$DP_i[j + 1, b, \ell, Z] = \max\{DP_i[j, b, \ell, Z], DP_i[j, b', \ell - 1, Z \setminus N_{>}(v_{j+1}^{(i)})] + \omega(\rho v_{j+1}^{(i)})\}, \quad (3)$$

where $b' = 0$ if there is an edge from a vertex in Y to $x_{j+1}^{(i)}$ and otherwise $b' = 1$.

Finally, we set $DP[1, \ell, Z] := DP_1[|C_1|, 0, \ell, Z]$ and compute further values with

$$DP[i + 1, \ell, Z] = \max_{Z' \subseteq Z, \ell' \in [\ell]_0} DP[i, \ell', Z'] + DP_{i+1}[|C_{i+1}|, 0, \ell - \ell', Z \setminus Z']. \quad (4)$$

There is a viable set $S \cup Y$ with $|S \cup Y| \leq k$ and $PD_{\mathcal{T}}(S \cup Y) \geq D$ if and only if $DP[c, k - |Y|, Z] \geq D - PD_{\mathcal{T}}(Y)$.

Correctness. Assume that DP stores the intended values. Then, if $DP[c, k - |Y|, Z] \geq D - PD_{\mathcal{T}}(Y)$, there is an (ℓ, Z) -feasible set $S \subseteq X \setminus Y$. First, this implies that $S \cup Y$ is viable. Moreover, since S has size at most $k - |Y|$, we obtain $|S \cup Y| \leq k$. Finally, because \mathcal{T} is a star and S and Y are disjoint, $PD_{\mathcal{T}}(S) \geq D - PD_{\mathcal{T}}(Y)$ implies $PD_{\mathcal{T}}(S \cup Y) \geq D$. The converse direction can be shown analogously.

It remains to show that DP and DP_i store the right values. The base cases are correct. Towards the correctness of Recurrence (3), as an induction hypothesis, assume that $DP_i[j, b, \ell, Z]$ stores the desired value for a fixed $j \in [|C_i| - 1]$, each $i \in [c]$, $b \in \{0, 1\}$, $\ell \in [k]_0$ and every $Z \subseteq Y$. Let $DP_i[j + 1, b, \ell, Z]$ store d . We show that there is an (ℓ, Z) -feasible set $S \subseteq \{x_1^{(i)}, \dots, x_{j+1}^{(i)}\}$. By Recurrence (3), $DP_i[j, b, \ell, Z]$ stores d or $DP_i[j, 1, \ell - 1, Z \setminus N_{>}(v_{j+1}^{(i)})]$ stores $d - \omega(\rho v_{j+1}^{(i)})$. If $DP_i[j, b, \ell, Z]$ stores d then there is an (ℓ, Z) -feasible set $S \subseteq \{x_1^{(i)}, \dots, x_j^{(i)}\} \subseteq \{x_1^{(i)}, \dots, x_{j+1}^{(i)}\}$. If $DP_i[j, 1, \ell - 1, Z \setminus N_{>}(v_{j+1}^{(i)})]$ stores $d - \omega(\rho v_{j+1}^{(i)})$ then there is an $(\ell - 1, Z \setminus N_{>}(v_{j+1}^{(i)}))$ -feasible set $S \subseteq \{x_1^{(i)}, \dots, x_j^{(i)}\}$ containing $x_1^{(i)}$ or $x_{j'}^{(i)} \in N_{>}(Y)$. Consequently, also $S \cup \{x_{j+1}^{(i)}\}$ is (ℓ, Z) -feasible.

Now, let $S \subseteq \{x_1^{(i)}, \dots, x_{j+1}^{(i)}\}$ be an (ℓ, Z) -feasible set. We show that $DP_i[j + 1, b, \ell, Z]$ stores at least $PD_{\mathcal{T}}(S)$. If $S \subseteq \{x_1^{(i)}, \dots, x_j^{(i)}\}$ then we know from the induction hypothesis that $DP_i[j, b, \ell, Z]$ stores $PD_{\mathcal{T}}(S)$ and then also $DP_i[j + 1, b, \ell, Z]$ stores $PD_{\mathcal{T}}(S)$. If $x_{j+1}^{(i)} \in S$, then S contains $x_1^{(i)}$ or some $x_{j'}^{(i)} \in N_{>}(Y)$. Define $S' := S \setminus \{x_{j+1}^{(i)}\}$. Then, $|S'| = \ell - 1$ and $S' \cup (Z \setminus N_{>}(x_{j+1}^{(i)}))$ is viable because S is (ℓ, Z) -feasible. Consequently, $DP_i[j, 1, \ell - 1, Z \setminus N_{>}(x_{j+1}^{(i)})] \geq PD_{\mathcal{T}}(S') = PD_{\mathcal{T}}(S) - \omega(\rho x_{j+1}^{(i)})$. Therefore, $DP_i[j + 1, b, \ell, Z] \geq PD_{\mathcal{T}}(S)$.

Now, we focus on the correctness of Recurrence (4). Let $\text{DP}[i+1, \ell, Z]$ store d . We show that there is an (ℓ, Z) -feasible set $S \subseteq C_1 \cup \dots \cup C_{i+1}$ with $PD_{\mathcal{T}}(S) = d$. Because $\text{DP}[i+1, \ell, Z]$ stores d , by Recurrence (4), there are $Z' \subseteq Z$ and $\ell' \in [\ell]_0$ such that $\text{DP}[i, \ell', Z'] = d_1$, $\text{DP}_{i+1}[|C_{i+1}|, 0, \ell - \ell', Z \setminus Z'] = d_2$ and $d_1 + d_2 = d$. By the induction hypothesis, there is an (ℓ', Z') -feasible set $S_1 \subseteq C_1 \cup \dots \cup C_i$ and an $(\ell - \ell', Z \setminus Z')$ -feasible set $S_2 \subseteq C_{i+1}$ such that $PD_{\mathcal{T}}(S_1) = d_1$ and $PD_{\mathcal{T}}(S_2) = d_2$. Then, $S := S_1 \cup S_2$ holds $|S| \leq |S_1| + |S_2| \leq \ell' + (\ell - \ell') = \ell$. Further, because Y has no outgoing edges $Z' \subseteq N_{>}(S_1) \cup \text{sources}(\mathcal{F})$ and $Z \setminus Z' \subseteq N_{>}(S_2) \cup \text{sources}(\mathcal{F})$. Therefore, $Z \subseteq N_{>}(S) \cup \text{sources}(\mathcal{F})$ and $S \cup Z$ is viable. We conclude that S is the desired set.

Let there be an (ℓ, Z) -feasible set $S \subseteq C_1 \cup \dots \cup C_{i+1}$ with $PD_{\mathcal{T}}(S) = d$. We show that $\text{DP}[i+1, \ell, Z]$ stores at least d . Define $S_1 := S \cap (C_1 \cup \dots \cup C_i)$ and $Z' := N_{>}(S_1) \cap Z$. We conclude that $S_1 \cap Z'$ is viable. Then, S_1 is (ℓ', Z') -feasible, where $\ell' := |S_1|$. Define $S_2 := S \cap C_{i+1} = S \setminus S_1$. Because $S \cup Z$ is viable and Z does not have outgoing edges, we know that $Z \subseteq N_{>}(S) \cup \text{sources}(\mathcal{F})$. So, $Z \setminus Z' \subseteq N_{>}(S_2) \cup \text{sources}(\mathcal{F})$ and because $|S_2| = |S| - |S_1| = \ell - \ell'$ we conclude that S_2 is $(\ell - \ell', Z \setminus Z')$ -feasible. Consequently, $\text{DP}[i, \ell', Z'] \geq PD_{\mathcal{T}}(S_1)$ and $\text{DP}_{i+1}[|C_{i+1}|, \ell - \ell', Z \setminus Z'] \geq PD_{\mathcal{T}}(S_2)$. Hence, $\text{DP}[i+1, \ell, Z] \geq PD_{\mathcal{T}}(S_1) + PD_{\mathcal{T}}(S_2) = PD_{\mathcal{T}}(S)$ because \mathcal{T} is a star. \blacktriangleleft

Running time. The tables DP and DP_i for $i \in [c]$ have $\mathcal{O}(2^d \cdot n \cdot k)$ entries in total. Whether one of the base cases applies can be checked in linear time. We can compute the set $Z \setminus N_{>}(x)$ for any given $Z \subseteq Y$ and $x \in X$ in $\mathcal{O}(d^2)$ time. Therefore, the $\mathcal{O}(2^d \cdot n \cdot k)$ times we need to apply Recurrence (3) consume $\mathcal{O}(2^d d^2 \cdot n \cdot k)$ time in total. In Recurrence (4), each $x \in Y$ can be in Z' , in $Z \setminus Z'$ or in $Y \setminus Z$ so that we can compute all the table entries of DP in $\mathcal{O}(3^d \cdot n \cdot k^2)$ which is also the overall running time. \blacktriangleleft

Now Theorem 5.1 can be shown by reducing the general case to the special case of Lemma 5.2 as follows: Iterate over the $\mathcal{O}(2^d)$ subsets of Y . For each subset $Z \subseteq Y$, compute whether there is a solution S for \mathcal{I} with $S \cap Y = Z$; we defer the details of this branching to the long version.

Next, we show that, in contrast to s-PDD, PDD is NP-hard even when the food-web is restricted to be a cluster graph. We obtain this hardness by a reduction from VERTEX COVER on cubic graphs. Here, we are given an undirected graph $G = (V, E)$ in which every vertex has degree *exactly* three and an integer k and ask whether a set $C \subseteq V$ of size at most k exists such that $u \in C$ or $v \in C$ for each $\{u, v\} \in E$. The set C is called a *vertex cover*. VERTEX COVER remains NP-hard on cubic graphs [20].

► **Theorem 5.3.** *PDD is NP-hard even if the food-web is a cluster graph.*

Proof.

Reduction. Let (G, k) be an instance of VERTEX COVER, where $G = (V, E)$ is cubic. We define an instance $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k', D)$ of PDD as follows. Let \mathcal{T} have a root ρ . For each vertex $v \in V$, we add a child v of ρ . For each edge $e = \{u, v\} \in E$, we add a child e of ρ and two children $[u, e]$ and $[v, e]$ of e . Let N be a big integer. We set the weight of ρe to $N - 1$ for each edge e in E . All other edges of \mathcal{T} have a weight of 1. Additionally, for each edge $e = \{u, v\} \in E$ we add edges $(u, [u, e])$ and $(v, [v, e])$ to \mathcal{F} . Finally, we set $k' := |E| + k$ and $D := N \cdot |E| + k$.

Correctness. The instance \mathcal{I} of PDD is constructed in polynomial time. The sources of \mathcal{F} are V . Let e_1, e_2 , and e_3 be the edges incident with $v \in V(G)$. Each connected component in \mathcal{F} contains four vertices, v , and $[v, e_i]$ for $i \in \{1, 2, 3\}$.

We show that (G, k) is a **yes**-instance of VERTEX COVER if and only if \mathcal{I} is a **yes**-instance of PDD. Let $C \subseteq V$ be a vertex cover of G of size at most k . If necessary, add vertices to C until $|C| = k$. For each edge $e \in E$, let v_e be an endpoint of e that is contained in C . Note that v_e exists since C is a vertex cover. We show that $S := C \cup \{[v_e, e] \mid e \in E\}$ is a solution for \mathcal{I} : The size of S is $|C| + |E| = k + |E|$. By definition, for each taxon $[v_e, e]$ we have $v_e \in C \subseteq S$, so S is viable. Further, as S contains a taxon $[v_e, e]$ for each edge $e \in E$, we conclude that $PD_{\mathcal{T}}(S) \geq N \cdot |E| + PD_{\mathcal{T}}(C) = N \cdot |E| + k = D$. Therefore, S is a solution.

Let S be a solution of instance \mathcal{I} of PDD. Define $C := S \cap V(G)$ and define $S' := S \setminus C$. Because $PD_{\mathcal{T}}(S) \geq D$, we conclude that for each $e \in E$ at least one taxon $[u, e]$ with $u \in e$ is contained in S' . Thus, $|S'| \geq |E|$ and $|C| \leq k$. Because S is viable we conclude that $u \in C$ for each $[u, e] \in S'$. Hence, C is a vertex cover of size at most k of G . ◀

5.2 Distance to Co-cluster Graphs

In this section, we show that PDD is FPT with respect to the distance to co-cluster of the food-web. A graph is a co-cluster graph if its complement graph is a cluster graph. Herein, the complement graph is the graph obtained by replacing edges with non-edges and vice versa. In other words, a graph is a co-cluster graph if its vertex set can be partitioned into independent sets such that each pair of vertices from different independent sets is adjacent.

We define an auxiliary problem HITTING SET WITH TREE-PROFITS in which we are given a universe \mathcal{U} , a family of sets \mathcal{W} over \mathcal{U} , a \mathcal{U} -tree \mathcal{T} , and integers k and D . We ask whether there is a set $S \subseteq \mathcal{U}$ of size at most k such that $PD_{\mathcal{T}}(S) \geq D$ and $S \cap W \neq \emptyset$ for each $W \in \mathcal{W}$. Solutions to this problem can be found with a dynamic programming algorithm over the tree, similar to the idea in [24]. The proof is therefore deferred to the long version.

► **Lemma 5.4** (\star). HITTING SET WITH TREE-PROFITS can be solved in $\mathcal{O}(3^{|\mathcal{W}|} \cdot n)$ time.

In the following we reduce from PDD to HITTING SET WITH TREE-PROFITS. Herein, we select a subset of the modulator Y to survive. Additionally, we select the first taxon x_i which survives in $X \setminus Y$. Because $\mathcal{F} - Y$ is a co-cluster graph, x_i is in a specific independent set $I \subseteq X$ and any taxon $X \setminus (I \cup Y)$ feed on x_i . Then, by selecting taxon $x_j \in X \setminus (I \cup Y)$, any other taxon in $X \setminus Y$ has some prey. Subsequently, a solution is found by Lemma 5.4.

► **Theorem 5.5**. PDD can be solved in $\mathcal{O}(6^d \cdot n^3)$ time, when we are given a set $Y \subseteq X$ of size d such that $\mathcal{F} - Y$ is a co-cluster graph.

Proof.

Algorithm. Given an instance $\mathcal{I} = (\mathcal{T}, \mathcal{F}, k, D)$ of PDD. Let x_1, \dots, x_n be a topological ordering of X which is induced by \mathcal{F} . Iterate over the subsets Z of Y . Let P_Z be the sources of \mathcal{F} in $X \setminus Y$ and let Q_Z be $N_{>}(Z) \setminus Y$, the taxa in $X \setminus Y$ which are being fed by Z . Further, define $R_Z := P_Z \cup Q_Z \subseteq X \setminus Y$. Iterate over the vertices $x_i \in R_Z$. Let x_i be from the independent set I of the co-cluster graph $\mathcal{F} - Y$. Iterate over the vertices $x_j \in X \setminus (Y \cup I)$.

For each set Z , and taxa x_i, x_j , with Lemma 5.4 we compute the optimal solution for the case that Z is the set of taxa of Y that survive while all taxa of $Y \setminus Z$ go extinct, x_i is the first taxon in $X \setminus Y$, and x_j the first taxon in $X \setminus (Y \cup I)$ to survive. (The special cases that only taxa from $I \cup Y$ or only from Y survive are omitted here.)

We define an instance $\mathcal{I}_{Z,i,j}$ of HITTING SET WITH TREE-PROFITS as follows. Let the universe $\mathcal{U}_{i,j}$ be the union of $\{x_{i+1}, \dots, x_{j-1}\} \cap I$ and $\{x_{j+1}, \dots, x_n\} \setminus Y$. For each taxon $x \in Z$ compute $N_{<}(x)$. If $x \notin \text{sources}(\mathcal{F})$ and $N_{<}(x) \cap (Z \cup \{x_i, x_j\}) = \emptyset$, then add $N_{<}(x) \setminus Y$ to the family of sets $\mathcal{W}_{Z,i,j}$. Contract edges $e \in E(\mathcal{T})$ with $\text{off}(e) \cap (Z \cup \{x_i, x_j\}) \neq \emptyset$ to obtain $\mathcal{T}_{Z,i,j}$. Finally, we define $k' := k - |Z| - 2$ and $D' := D - PD_{\mathcal{T}}(Z \cup \{x_i, x_j\})$.

Solve $\mathcal{I}_{Z,i,j}$. If $\mathcal{I}_{Z,i,j}$ is a **yes**-instance then return **yes**. Otherwise, continue with the iteration. If $\mathcal{I}_{Z,i,j}$ is a **no**-instance for every $Z \subseteq Y$, and each $i, j \in [n]$, then return **no**.

Correctness. We show that the algorithm returns **yes** if and only if \mathcal{I} is a **yes**-instance.

First, assume the algorithm returns **yes**. Then, there is a set $Z \subseteq Y$, and there are taxa $x_i \in X \setminus Y$ and $x_j \in X \setminus (Y \cup V(I))$ such that $\mathcal{I}_{Z,i,j}$ is a **yes**-instance of HITTING SET WITH TREE-PROFITS. Here, I is the independent set such that $x_i \in V(I)$. Consequently, there is a set $S \subseteq \mathcal{U}_{i,j}$ of size at most $k - |Z| - 2$ such that $PD_{\mathcal{T}_{Z,i,j}}(S) \geq D' = D - PD_{\mathcal{T}}(Z \cup \{x_i, x_j\})$ and $S \cap W \neq \emptyset$ for each $W \in \mathcal{W}_{Z,i,j}$. We show that $S^* := S \cup Z \cup \{x_i, x_j\}$ is a solution for instance \mathcal{I} of PDD. Clearly, $|S^*| = |S| + |Z| + 2 \leq k$ and $PD_{\mathcal{T}}(S^*) = PD_{\mathcal{T}_{Z,i,j}}(S) + PD_{\mathcal{T}}(Z \cup \{x_i, x_j\}) \geq D$ as $\mathcal{T}_{Z,i,j}$ is the $Z \cup \{x_i, x_j\}$ -contraction of \mathcal{T} . Further, by definition $x_i \in (\text{sources}(\mathcal{F}) \cup N_{>}(Z)) \setminus Y$. Because $\mathcal{F} - Y$ is a co-cluster graph and x_j is not in I , the independent set in which x_i is, we conclude that $x_j \in N_{>}(x_i)$. As $S \cap W \neq \emptyset$ for each $W \in \mathcal{W}_{Z,i,j}$, each taxon $x \in Z$ has a prey in $Z \cup \{x_i, x_j\}$ or in S so that $N_{<}(x) \cap S^* \neq \emptyset$. Therefore, S^* is viable and indeed a solution for \mathcal{I} .

Assume now that S is a solution for instance \mathcal{I} of PDD. We define $Z := S \cap Y$ and let x_i and x_j be the taxa in $S \setminus Y$, respectively $S \setminus (Y \cup I)$, with the smallest index. As before, I is the independent set of x_i . We show that instance $\mathcal{I}_{Z,i,j}$ of HITTING SET WITH TREE-PROFITS has solution $S^* := S \setminus (Z \cup \{x_i, x_j\})$. Clearly, $|S^*| = |S| - |Z| - 2 \leq k'$ and by the definition of $\mathcal{T}_{Z,i,j}$ we also conclude $PD_{\mathcal{T}_{Z,i,j}}(S^*) \geq D'$. Let $M \in \mathcal{W}_{Z,i,j}$. By definition, there is a taxon $z \in Z$ with $M = N_{<}(z) \setminus Y$, and $z \notin \text{sources}(\mathcal{F})$, and $N_{<}(z) \cap (Z \cup \{x_i, x_j\}) = \emptyset$. Consequently, as S is viable, there is a taxon $x \in S \cap N_{<}(z)$ so that $S \cap M \neq \emptyset$. Hence, S^* is a solution of instance $\mathcal{I}_{Z,i,j}$ of HITTING SET WITH TREE-PROFITS.

Running time. For a given $Z \subseteq Y$, we can compute the topological order x_1, \dots, x_n and the set R_Y in $\mathcal{O}(n^2)$ time. The iterations over x_i and x_j take $\mathcal{O}(n^2)$ time. Observe, $|\mathcal{W}_{Z,i,j}| \leq |Z|$. By Lemma 5.4 checking whether $\mathcal{I}_{Z,i,j}$ is a **yes**-instance takes $\mathcal{O}(3^d n)$ time each. The overall running time is $\mathcal{O}(6^d \cdot n^3)$ time. ◀

5.3 Treewidth

Faller et al. [10] conjectured that s-PDD remains NP-hard even when the underlying graph of the food-web is a tree. We disprove this conjecture by showing that s-PDD can be solved in polynomial time on food-webs which are trees (assuming $P \neq NP$). We even show a stronger result: s-PDD is FPT with respect to the treewidth of the food-web.

► **Theorem 5.6** (*). s-PDD can be solved in $\mathcal{O}(9^{\text{tw}_{\mathcal{F}}} \cdot nk)$ time.

To show Theorem 5.6, we define a dynamic programming algorithm over a tree-decomposition of \mathcal{F} . In each bag, we divide the taxa into three sets indicating that they a) are supposed to go extinct, b) will be saved but still need prey, c) or will be saved without restrictions. The algorithm is similar to the standard treewidth algorithm for DOMINATING SET [5].

6 Discussion

Several interesting questions remain open after our examination of PDD and s-PDD. Arguably the most relevant one is whether PDD is FPT with respect to k , the size of the solution. Also, it remains open whether PDD can be solved in polynomial time if each connected component in the food-web contains at most two vertices.

Clearly, further structural parameterizations can be considered. We only considered structural parameters which consider the underlying graph. But parameters which also consider the orientation of edges, such as the largest anti-chain, could give a better view on the structure of the food-web than parameters which only consider the underlying graph.

Liebermann et al. [17] introduced and analyzed weighted food-webs. Such a weighted model may provide a more realistic view of a species' effect on and interaction with other species [4]. Maximizing phylogenetic diversity with respect to a weighted food-web in which one potentially needs to save several prey per predator would be an interesting generalization for our work and has the special case in which one needs to save all prey for each predator.

Recent works consider the maximization of phylogenetic diversity in phylogenetic networks [29, 3, 14, 28] which may provide a more realistic evolutionary model of the considered species. It would be interesting to study these problems also under ecological constraints. Do the resulting problems become much harder than PDD? Finally, it has been reported that maximizing phylogenetic diversity is only marginally better than selecting a random set of species when it comes to maximizing the functional diversity of the surviving species [18]. The situation could be different, however, when ecological constraints are incorporated. Here, investigating the following two questions seems fruitful: First, do randomly selected viable species sets have a higher functional diversity than randomly selected species? Second, do viable sets with maximal phylogenetic diversity have a higher functional diversity than randomly selected viable sets?

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