Superdominance Order and Distance of Trees

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Introduction

The concept of distance ranks among the particularly simple and yet frequently used ideas in graph theory. Apart from pure mathematical interest, its importance is also underlined by the wide applicability of distance-related topics in many different scientific fields. Examples range from the design of a communication network having minimum routing costs to the classification of organic molecules and the evaluation of floor plans in architecture.

As a result of this close interplay between a branch of graph theory and its applications, a vast amount of papers dealing with distance-related problems can be found both in and outside the mathematical literature. The main topic of this thesis, the *distance of trees*, has apparently been studied first in chemistry. Consider a finite connected graph $G = (V, E)$ and let $d_G(u, v)$ denote the distance of the vertices u, v in G, i.e., $d_G(u, v)$ is the length of a shortest path between u and v in G. Then

$$\sigma(G) = \sum_{\{u,v\} \subseteq V} d_G(u, v)$$

is called the *distance* of G. This graph invariant has been investigated by several authors (see e.g. Buckley and Harary [6], Doyle and Graver [11], Entringer [12], Entringer, Jackson and Snyder [13], Plesník [24], Šoltés [26]) using a variety of other names like *transmission*, *total status*, *distance sum* and *sum of all distances*. In the special case of trees, also the terms *path number*, *Wiener index* and *Wiener number* can be found, the latter two notions being particularly popular in the chemical literature. They are used in honor of the chemist Wiener who seems to be the first to study the correlation between the distance of certain trees related to paraffin hydrocarbons and some physico-chemical properties of these molecules, see Wiener [29, 30].

Let $\mathcal{T}(n)$ denote the class of all trees of a fixed order n. This thesis deals with the problem of determining the trees having minimum and maximum distance within certain subclasses of $\mathcal{T}(n)$. The problem is easily solved in the class $\mathcal{T}(n)$, the star $K_{1,n-1}$ and the path P_n being the unique optimal trees. Since the maximum degree of the stars is unbounded and applications in chemistry are obviously restricted to the case of atoms of bounded valency, one may ask for those trees of fixed order and bounded maximum degree that have minimum distance. Further natural generalizations deal with the class of all trees with a given degree sequence and with weighted versions of the distance of a tree.

In order to solve these optimization problems, a new approach based on an idea of Triesch is applied in this thesis. The distance of a tree T can be related to a multiset of non-negative integers that can be derived from the tree by considering a barycenter of T and by assigning certain heights to the edges of T. These multisets can be partially ordered by a weaker variant of the well-known dominance order on partitions, called *superdominance order*, and the original problem on distances of trees is transformed into the task of determining the minimal and maximal multisets in this partial order.

The thesis is organized as follows. The first chapter contains a brief survey of basic definitions and notations concerning partial orders, graphs and trees. In the second chapter the relevant tools involving the superdominance order, barycenters of trees and edge heights are introduced, and the new approach is presented in detail. In the next two chapters the trees having minimum and maximum distance within several subclasses of $\mathcal{T}(n)$ are characterized. We obtain a complete solution, consisting of a unique tree, except for the case of the maximum distance problem in the class of all trees with a given degree sequence. As may have been intuitively expected the optimal trees are, roughly speaking, as close to the star and the path as is possible, given the restrictions opposed by the class of trees under consideration. Finally, two weighted distance problems that can be reduced to the unweighted case are treated in the fifth chapter.

Using different techniques, some of the optimization problems of this thesis have already been considered by other authors. For instance, Fischermann, Hoffmann, Rautenbach, Székely and Volkmann [14] have also determined the trees of bounded maximum degree that have minimum distance. In fact, an earlier version of their paper, in which the result was stated as a conjecture, was the starting point for our studies.

Comparing the method used in [14] to the one introduced here, both are necessarily concerned with performing certain exchanging operations in trees. In view of these exchanges, we think that our approach has the advantage that the task of 'bookkeeping' is facilitated. Moreover, the trees having minimum distance within the class of all trees with a given degree sequence can be characterized and several weighted distance problems can be solved. Both results seem to be quite cumbersome to obtain by using the known techniques and have, as far as we know, not been given before. Our approach has the additional advantage that the main idea of most proofs can easily be visualized. Therefore, we will frequently use figures and examples to illustrate and elucidate the steps taken.

As already noted above, there is an extensive literature concerned with the distance of trees. In this thesis we confine ourselves to characterize the trees having an extremal distance so that numerous related topics will not be treated here. These topics include other formulae and computational aspects of the distance of trees, the connection between the distance and other graph invariants and the characterization of branching in trees, to mention but a few. For further information and a comprehensive survey of both the theory and the applications of the distance of trees, the reader is referred to the recent article of Dobrynin, Entringer and Gutman [10] and the references cited therein.

Chapter 1

Basic Definitions and Notation

The terminology used throughout this thesis is mostly standard and can also be found in many textbooks, see e.g. Marshall and Olkin [23] for terms concerning partial orders on number partitions and Bollobás [5] for an introduction to graph theory. For easy reference and in order to clarify the notation, we give a brief survey of the basic items in this chapter.

1.1 Sets and Multisets

The set of all integers, positive integers and real numbers is denoted by $\mathbb{Z}$, $\mathbb{N}$ and $\mathbb{R}$ respectively. The cardinality of a set S is denoted by $|S|$.

Roughly speaking, a *multiset* M is a set in which some elements may occur more than once. More precisely, M is an ordered pair (S, m) consisting of a finite set S and a mapping $m : S \to \mathbb{N}$, with $m(s)$ indicating the *multiplicity* of $s \in S$ in M. If $S = \{s_1, s_2, \ldots, s_p\}$, we often write

$$M = (S, m) = (s_1^{m(s_1)}, s_2^{m(s_2)}, \ldots, s_p^{m(s_p)}),$$

with multiplicities equal to one not explicitly indicated. The *cardinality* $|M|$ of M is the number of elements in S counted with their multiplicities. A multiset M with $|M| = p$ is simply called a *p-multiset*. For instance, $(5, 5, 4, 3, 3, 3, 1) = (5^2, 4, 3^3, 1)$ is a 7-multiset. Two multisets $M = (S, m)$ and $M' = (S', m')$ are *equal*, denoted by $M = M'$, if $S = S'$ and $m = m'$. The simple notation (M, M') is used to denote the multiset $(S \cup S', m^+)$ with

$$m^+(s) = \begin{cases} m(s), & \text{if } s \in S \setminus S'; \\ m'(s), & \text{if } s \in S' \setminus S; \\ m(s) + m'(s), & \text{if } s \in S \cap S'. \end{cases}$$

1.2 Partitions and Partial Orders

Given a p-multiset $x = (x_1, x_2, \ldots, x_p)$ of non-negative integers let $\Sigma(x)$ denote the sum of all components of x. If $\Sigma(x) = a$, then x is called a *(number) partition* of a of *length* p. For a partition $x = (x_1, x_2, \ldots, x_p)$ let

$$x_{[1]} \geq x_{[2]} \geq \ldots \geq x_{[p]} \quad \text{and} \quad x_{(1)} \leq x_{(2)} \leq \ldots \leq x_{(p)}$$

denote the components of x in decreasing and increasing order respectively, and let

$$x_{\downarrow} = (x_{[1]}, x_{[2]}, \ldots, x_{[p]}) \quad \text{and} \quad x_{\uparrow} = (x_{(1)}, x_{(2)}, \ldots, x_{(p)})$$

denote the *decreasing* and *increasing rearrangement* of x respectively.

The well-known *elementwise vector ordering* $\leq$ can easily be carried over to p-multisets x and y by defining $x \leq y$ if and only if $x_{\uparrow} \leq y_{\uparrow}$.

A partition $y = (y_1, y_2, \ldots, y_p)$ is *dominated* (also called *majorized*) by $x = (x_1, x_2, \ldots, x_p)$, denoted by $y \preceq x$ or $x \succeq y$, if and only if

$$\sum_{i=1}^{k} x_{[i]} \geq \sum_{i=1}^{k} y_{[i]} \quad \text{for } k = 1, \ldots, p \quad \text{and} \quad \Sigma(x) = \Sigma(y),$$

or, equivalently,

$$\sum_{i=1}^{k} x_{(i)} \leq \sum_{i=1}^{k} y_{(i)} \quad \text{for } k = 1, \ldots, p \quad \text{and} \quad \Sigma(x) = \Sigma(y). \tag{1.1}$$

The set of all partitions of a given integer is partially ordered by this *dominance order* and forms a lattice.

If the condition $\Sigma(x) = \Sigma(y)$ in definition (1.1) of the dominance order is dropped, a weaker partial order is obtained. Marshall and Olkin [23] denote this order by $\prec^w$ and call it *weak supermajorization*, the prefix 'super-' arising from characterizations involving doubly superstochastic matrices, see [23] for details. We prefer to use both the simpler term *superdominance order* and the symbol $\preceq^w$. Thus, for partitions x and y as above,

$$y \preceq^w x \quad \text{if and only if} \quad \sum_{i=1}^{k} x_{(i)} \leq \sum_{i=1}^{k} y_{(i)} \quad \text{for } k = 1, \ldots, p.$$

We use the notation $y \prec^w x$ if and only if $y \preceq^w x$ and $y \neq x$.

For any partial order $\preccurlyeq$ on multisets, the expression $y \preccurlyeq\cdot\, x$ indicates that x *covers* y in $\preccurlyeq$, i.e., $x \neq y$ and $y \preccurlyeq \tilde{y} \preccurlyeq x$ implies $\tilde{y} = x$ or $\tilde{y} = y$. If a set S is partially ordered by $\preccurlyeq$, we simply write $(S, \preccurlyeq)$ for the resulting poset.

Using the same definitions as above, the partial orders $\leq$, $\preceq$ and $\preceq^w$ can also be defined for multisets of real numbers. This generalization is only used in few passages of this thesis.

1.3 Graph Theory

A *finite undirected simple graph* $G = (V(G), E(G))$ consists of a finite set $V(G)$, the *vertex set*, and a set $E(G) \subseteq \{X : X \subseteq V(G), |X| = 2\}$, called the *edge set*. The elements of $V(G)$ are the *vertices*, the elements of $E(G)$ the *edges* of G. The *order* of G, denoted by $|G|$, is the number of vertices in G. In this thesis the term *graph* is used instead of 'finite undirected simple graph', and an edge $e = \{u, v\} \in E(G)$ is simply denoted by $e = uv$. Furthermore we write $G = (V, E)$ instead of $G = (V(G), E(G))$ whenever there are no ambiguities.

Two vertices u, v of a graph G are called *adjacent* if $e = uv \in E$. In this case u is called a *neighbor* of v (and vice versa), u and v are the *endvertices* of e, and the edge e is *incident* with u and v. The *degree* $\deg_G(v)$ of a vertex v is the number of neighbors of v in G. A vertex of degree 0 is called *isolated* and the maximum degree of G is denoted by $\Delta(G)$. The multiset formed by the degrees of the vertices of G is called the *degree sequence* $\pi(G)$ of G. Obviously, $\Sigma(\pi(G)) = 2|E|$, commonly known as the *handshaking lemma*.

Two graphs $G = (V, E)$ and $G' = (V', E')$ are called *isomorphic*, denoted by $G \simeq G'$, if there exists a bijection $\phi : V \to V'$ such that $uv \in E$ if and only if $\phi(u)\phi(v) \in E'$. Usually we do not distinguish between isomorphic graphs, unless we consider graphs with a distinguished vertex like rooted trees, see below. A graph $H = (X, F)$ is a *subgraph* of the graph $G = (V, E)$, denoted by $H \subseteq G$, if $X \subseteq V$ and $F \subseteq E$. If F consists of all the edges of E that have both endvertices in X, then H is the subgraph *induced by* X, denoted by $H = G[X]$. If $X = V \setminus \{v\}$ for some $v \in V$, we simply write $G - v$ instead of $G[V \setminus \{v\}]$. Analogously, for any $F \subseteq E$, $G - F$ denotes the graph with vertex set V and edge set $E \setminus F$. For $e \in E$ we write $G - e$ instead of $G - \{e\}$.

The *complete graphs* K_n and the *complete bipartite graphs* $K_{m,n}$ are two important types of graphs. K_n consists of n vertices with any two vertices being adjacent. $K_{m,n}$ is the graph whose vertex set is the union of two disjoint sets A and B of cardinality m and n respectively, the edge set consisting of all edges ab with $a \in A$ and $b \in B$. A *bipartite* graph is any subgraph of a complete bipartite graph. The graph $K_{1,n-1}$ is called the *star* of order n.

A *walk* W of *length* $\ell = \ell(W) \geq 0$ in a graph $G = (V, E)$ is an alternating sequence $v_0 e_1 v_1 e_2 \ldots e_\ell v_\ell$ with $v_i \in V$ and $e_i = v_{i-1} v_i \in E$. A walk is *closed* if $v_0 = v_\ell$. A *path* is a walk in which all vertices are distinct, and a *cycle* is a closed walk of length $\ell \geq 3$ in which $v_1, \ldots, v_\ell$ are distinct. Usually a path is simply denoted by $v_0 v_1 \ldots v_\ell$ and v_0 and v_ℓ are called the *endvertices* of the path. The subgraph $(\{v_0, \ldots, v_\ell\}, \{e_1, \ldots, e_\ell\})$ of G is often also called a path. The generic path of order n and length $n - 1$ is denoted by P_n. We write $u \sim v$ if there exists a path with endvertices u and v in G. Obviously, $\sim$

is an equivalence relation on V, each equivalence class inducing a *connected component* or simply a *component* of G. The graph is called *connected* if there is only one component, or, equivalently, if there exists a path between any two of its vertices. The minimum length of a path between two vertices u, v in a connected graph G is called the *distance* of u and v and is denoted by $d_G(u, v)$. The *distance* $\sigma(G)$ of a connected graph G is the sum of all distances $d_G(u, v)$ for $\{u, v\} \subseteq V$.

A *forest* is a graph that does not contain a cycle and a *tree* T is a connected forest. Clearly, there is exactly one path connecting two vertices u, v in a tree T and this path is denoted by $P_T(u, v)$ or simply $P(u, v)$. A vertex of degree one in T is called a *leaf*. A *branch* of T *at the vertex* v is a maximal subtree that contains v as a leaf.

We call a tree $T = (V, E)$ *rooted at the vertex* r simply by distinguishing $r \in V$ from the remaining vertices. In this case $\ell(v) = \ell(P(v, r))$ is called the *depth* of the vertex v. The *depth* of T, denoted by $\ell(T)$, is the maximum depth of a vertex of T. Given any tree T rooted at r and two vertices u, v we say that u is a *successor* of v in T if $\ell(u) > \ell(v)$ and $P(v, r) \subseteq P(u, r)$. If u is both a successor and a neighbor of v, then u is called a *child* of v and v is the *parent* of u. For any vertex u of a rooted tree T, let $T(u)$ denote the subtree that is induced by u and all its successors and that is rooted at u. Given two rooted trees $T = (V, E)$ and $T' = (V', E')$ with roots r and r', we write $T \simeq_r T'$ if there exists a bijection $\phi : V \to V'$ with $\phi(r) = r'$ such that T and T' are isomorphic relative to ϕ.

When depicting a rooted tree, the children of any vertex v will be drawn on the first level below v, starting with the root on top of the picture. This drawing convention will be applied throughout this thesis except for the case of path-like trees in Chapters 4 and 5 where a horizontal representation of the tree is chosen and the root is marked by an encircled vertex.

Chapter 2

Tools and Preliminaries

This chapter is intended to give a detailed exposition of the main tools used in subsequent parts. In the first two sections several characterizations and results concerning the superdominance order and barycenters of trees are derived. Then the edge height multiset of a rooted tree is introduced and it is shown how these concepts can be combined to yield a new approach for studying the distance of trees. Finally, the general framework for a natural weighted distance problem in trees is outlined and a basic theorem on rearrangements of multisets is recalled.

2.1 Superdominance Order

Numerous characterizations of both the dominance and the superdominance order are contained in the book of Marshall and Olkin [23]. While most of the results are stated there in a general form for multisets of real numbers, we are mainly concerned with partial orders defined on multisets of non-negative integers. Focussing on this special kind of multiset, we first extend the characterization of the dominance order by means of elementary steps to an analogous result for the superdominance order.

Let us recall the well-known characterization of the dominance order $\preceq$ by *steps* (sometimes also called *transformations*) and *elementary steps* and consider a partition $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ of non-negative integers, given in decreasing order. Let $x_{p+1} = 0$ and assume that there are indices $1 \leq i < j \leq p+1$ with $x_i \geq x_j + 2$, where $i = \max\{\ell : x_\ell = x_i\}$ and $j = \min\{\ell : x_\ell = x_j\}$. Then x' arises from x by an (i,j)-*step* if x_i is decreased by one and x_j is increased by one. The step is *elementary* if additionally $j = \min\{\ell : x_\ell \leq x_i - 2\}$. Obviously, $x' \preceq x$ and x' is still arranged in decreasing order. Moreover, $y \preceq\cdot\, x$ if and only if y arises from

x by an elementary step. Proofs of these results can be found in Aigner [1] and Gutman and Ruch [15].

In view of the superdominance order, $y \preceq^w x$ is also possible if x and y are not partitions of the same integer, i.e., if $\Sigma(x) < \Sigma(y)$. In order to cover this case, we introduce another simple transformation. Consider once again a partition $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ of non-negative integers and let j be an index with $1 \leq j \leq p$ and $j = \min\{\ell : x_\ell = x_j\}$. Then x' arises from x by a *j-step* if x_j is increased by one. Clearly, $x' \preceq^w x$ and x' is again arranged decreasingly.

In the following considerations a multiset of non-negative integers is tacitly assumed to be in decreasing order whenever one of the two types of steps is applied to it. Furthermore, if y is derived from x by an elementary (i,j)-step or a j-step, we write $y = (x)_{i,j}$ and $y = (x)_j$ respectively.

Theorem 2.1. *Let x, y be p-multisets of non-negative integers. Then $y \preceq^w\!\cdot\, x$ if and only if $y = (x)_{i,j}$ for some $1 \leq i < j \leq p$ or $y = (x)_1$.*

Proof. Assume first that $y \preceq^w\!\cdot\, x$. If $\Sigma(x) = \Sigma(y)$, we infer that $y \preceq\!\cdot\, x$ and thus $y = (x)_{i,j}$ for some $1 \leq i < j \leq p$ by the characterization of the dominance order. Otherwise $\Sigma(x) < \Sigma(y)$, and it is now easy to see that $y \preceq^w (x)_1 \prec^w x$, which is only possible if $y = (x)_1$.

Conversely, if $y = (x)_{i,j}$ for some $1 \leq i < j \leq p$, then $y \preceq\!\cdot\, x$ and this implies $y \preceq^w\!\cdot\, x$. Finally, let $y = (x)_1$ and assume that $y \preceq^w \tilde{y} \prec^w x$ for some multiset $\tilde{y}$ of integers. Since $\Sigma(\tilde{y}) = \Sigma(x)$ is impossible, we have $\Sigma(\tilde{y}) = \Sigma(y)$ and this implies $\tilde{y} = y$ and $y \preceq^w\!\cdot\, x$. □

Corollary 2.2. *Let x, y be p-multisets of non-negative integers. Then $y \preceq^w x$ if and only if y can be derived from x by a successive application of a finite number of elementary (i,j)-steps and 1-steps.*

With Theorem 2.1 and Corollary 2.2 at hand, several tools involving the superdominance order can now be proven fairly easily. First of all consider the classical characterization of the dominance order by means of convex functions, given by Hardy, Littlewood and Pólya [16, 17] and independently by Karamata [20]. This result was extended to the superdominance order by Tomić [28], see also Marshall and Olkin [23] for further references and some historical remarks.

Theorem 2.3. *Let x, y be p-multisets of non-negative integers. Then $y \preceq^w x$ if and only if*

$$\sum_{k=1}^{p} g(x_k) \leq \sum_{k=1}^{p} g(y_k) \tag{2.1}$$

for all increasing concave functions $g : \mathbb{R} \to \mathbb{R}$.

Proof. Assume first that $y \preceq^w x$ and let g be any increasing concave function. Obviously it suffices to consider the case $y \preceq^{w\cdot} x$, which is characterized in Theorem 2.1. Let $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ be given in decreasing order. If $y = (x)_{i,j}$ for some $1 \leq i < j \leq p$, then

$$\sum_{k=1}^{p} g(y_k) = g(x_j + 1) + g(x_i - 1) - g(x_j) - g(x_i) + \sum_{k=1}^{p} g(x_k),$$

and the concavity of g implies

$$2g(x_j + \nu + 1) \geq g(x_j + \nu) + g(x_j + \nu + 2) \tag{2.2}$$

for $\nu = 0, 1, \ldots, x_i - x_j - 2$. Adding up these inequalities yields

$$g(x_j + 1) + g(x_i - 1) \geq g(x_j) + g(x_i),$$

and thus (2.1) holds. If $y = (x)_1$, we immediately obtain

$$\sum_{k=1}^{p} g(y_k) = g(x_1 + 1) - g(x_1) + \sum_{k=1}^{p} g(x_k) \geq \sum_{k=1}^{p} g(x_k), \tag{2.3}$$

since g is increasing.

Conversely, assume that (2.1) holds for all increasing concave functions g. If $y \not\preceq^w x$, let j denote the minimum index in $\{1, \ldots, p\}$ such that

$$\sum_{k=1}^{j} x_{(k)} > \sum_{k=1}^{j} y_{(k)}. \tag{2.4}$$

Clearly, $x_{(j)} > y_{(j)}$. Consider the function g defined by $g(t) = \min(0, t - x_{(j)})$. Then (2.1) implies

$$\sum_{k=1}^{j} x_{(k)} = jx_{(j)} + \sum_{k=1}^{p} g(x_{(k)}) \leq jx_{(j)} + \sum_{k=1}^{p} g(y_{(k)}) \leq \sum_{k=1}^{j} y_{(k)},$$

in contradiction to (2.4). Hence $y \preceq^w x$. □

Corollary 2.4. *Let x, y be p-multisets of non-negative integers. Then $y \preceq^w x$ if and only if*

$$\sum_{k=1}^{p} \min(0, x_k - a) \leq \sum_{k=1}^{p} \min(0, y_k - a)$$

for all $a \in \mathbb{Z}$.

Corollary 2.5. *Let x, y be p-multisets of non-negative integers. If $y \prec^w x$ and g is a strictly increasing and strictly concave function, then*

$$\sum_{k=1}^{p} g(x_k) < \sum_{k=1}^{p} g(y_k).$$

Proof. In the proof of Theorem 2.3 we now have a strict inequality in (2.2) and (2.3). $\square$

Using the extended definition of the superdominance order for multisets of real numbers, the next result provides a slight refinement of the necessary condition of Theorem 2.3. If $x = (x_1, \ldots, x_p)$ is a multiset and $g : \mathbb{R} \to \mathbb{R}$ is any function, let $g[x]$ denote the multiset $(g(x_1), \ldots, g(x_p))$.

Theorem 2.6. *Let x, y be p-multisets of non-negative integers and let g be an increasing concave function. Then $y \preceq^w x$ implies $g[y] \preceq^w g[x]$.*

Proof. Since $y \preceq^w x$,

$$(y_{(1)}, y_{(2)}, \ldots, y_{(k)}) \preceq^w (x_{(1)}, x_{(2)}, \ldots, x_{(k)}) \quad \text{for } k = 1, \ldots, p, \tag{2.5}$$

implying

$$\sum_{i=1}^{k} g(x_{(i)}) \leq \sum_{i=1}^{k} g(y_{(i)}) \quad \text{for } k = 1, \ldots, p \tag{2.6}$$

by Theorem 2.3. Furthermore, since g is increasing,

$$g(x_{(1)}) \leq g(x_{(2)}) \leq \ldots \leq g(x_{(p)}) \quad \text{and} \quad g(y_{(1)}) \leq g(y_{(2)}) \leq \ldots \leq g(y_{(p)}),$$

and thus (2.6) is equivalent to $g[y] \preceq^w g[x]$. $\square$

Corollary 2.7. *Let x, y be p-multisets of non-negative integers and let g be a strictly increasing and strictly concave function. Then $y \prec^w x$ implies $g[y] \prec^w g[x]$.*

Proof. Since $y \prec^w x$, there is at least one index $k \in \{1, \ldots, p\}$ for which we have $\prec^w$ instead of $\preceq^w$ in (2.5). Therefore, by Corollary 2.5, we have at least one strict inequality in (2.6). $\square$

A further immediate consequence of Theorem 2.3, which in case of the dominance order seems to have been given first by Rado (see Hardy, Littlewood and Pólya [17, p. 63]), is the following result. It is frequently applied in subsequent parts and will be referred to as the *merging lemma*.

Lemma 2.8. *Let x, y, x', y' be multisets of non-negative integers and assume that $|x| = |y|$ and $|x'| = |y'|$. If $y \preceq^w x$ and $y' \preceq^w x'$, then $(y, y') \preceq^w (x, x')$. In particular, $x \leq y$ implies $y \preceq^w x$.*

Let $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ be a multiset of non-negative integers, given in decreasing order, let $\delta \in \mathbb{N}$ with $\delta < x_p$ and let $x^{+\delta} = (x_i^{+\delta})_{i=1,\ldots,p}$ and $x^{-\delta} = (x_i^{-\delta})_{i=1,\ldots,p}$ denote the multisets defined by $x_i^{+\delta} = x_i + \delta$ and $x_i^{-\delta} = x_i - \delta$ for $1 \leq i \leq p$, respectively. Obviously, $x^{+\delta}$ and $x^{-\delta}$ are still arranged decreasingly. The following technical lemma is an easy consequence of the merging lemma.

Lemma 2.9. *Let $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ and $y = (y_1 \geq y_2 \geq \ldots \geq y_{p+1})$ be p- and $(p+1)$-multisets of non-negative integers, each given in decreasing order. Let $\delta \in \mathbb{N}$ and assume further that*

$$\min(x_i, y_i) \geq \max(x_{i+1}, y_{i+1}) \quad \textit{for } 1 \leq i \leq p-1$$

and

$$\min(x_p, y_p) \geq y_{p+1} > \delta\,.$$

Then $(x, y) \prec^w (x^{+\delta}, y^{-\delta})$.

Proof. Since $x_i \geq y_{i+1}$, we have $(x_i, y_{i+1}) \prec^w (x_i + \delta, y_{i+1} - \delta) = (x_i^{+\delta}, y_{i+1}^{-\delta})$ for all $i = 1, \ldots, p$. Furthermore, $(y_1) \prec^w (y_1^{-\delta})$. Now the assertion follows directly from the merging lemma. □

For the final tool concerning the superdominance order, consider a fixed vector $c = (c_1, \ldots, c_p) \in \mathbb{R}^p$ and the linear function $\psi_c : \mathbb{R}^p \to \mathbb{R}$ defined by $\psi_c(z) = c \cdot z = \sum_{k=1}^{p} c_k z_k$ for $z = (z_1, \ldots, z_p) \in \mathbb{R}^p$.

Theorem 2.10. *Let $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ and $y = (y_1 \geq y_2 \geq \ldots \geq y_p)$ be p-multisets of non-negative integers, given in decreasing order. If $y \preceq^w x$ and $c = (c_1 \leq c_2 \leq \ldots \leq c_p)$ with $c_1 \geq 0$, then*

$$\psi_c(x) = \sum_{k=1}^{p} c_k x_k \leq \sum_{k=1}^{p} c_k y_k = \psi_c(y)\,. \tag{2.7}$$

Proof. It suffices to consider the case $y \preceq^{w\cdot} x$, characterized in Theorem 2.1. If $y = (x)_{i,j}$ for some $1 \leq i < j \leq p$, we have $y_i = x_i - 1$, $y_j = x_j + 1$ and $x_k = y_k$ for $k \neq i, j$, and thus

$$\psi_c(x) = \sum_{k=1}^{p} c_k x_k = c_i - c_j + \sum_{k=1}^{p} c_k y_k \leq \psi_c(y)\,,$$

since $c_i \leq c_j$. If $y = (x)_1$, then $y_1 = x_1 + 1$ and $x_k = y_k$ for $k = 2, \ldots, p$. Therefore

$$\psi_c(x) = c_1 x_1 + \sum_{k=2}^{p} c_k x_k = c_1 y_1 - c_1 + \sum_{k=2}^{p} c_k y_k \leq \psi_c(y), \tag{2.8}$$

since $c_1 \geq 0$. $\square$

The simple example $c = (1^2)$, $x = (3, 1)$ and $y = (2^2)$ shows that strict inequality in (2.7) is not assured if the assumptions in Theorem 2.10 are strengthened to $y \prec^w x$ and $c = (c_1 \leq c_2 \leq \ldots \leq c_p)$ with $c_1 > 0$. Strict inequality can be deduced if additionally $\Sigma(x) < \Sigma(y)$ is assumed.

Corollary 2.11. *Let x, y be p-multisets of non-negative integers, given in decreasing order. If $y \prec^w x$ with $\Sigma(x) < \Sigma(y)$ and $c = (c_1 \leq c_2 \leq \ldots \leq c_p)$ with $c_1 > 0$, then $\psi_c(x) < \psi_c(y)$.*

Proof. Since $\Sigma(x) < \Sigma(y)$, the assertion follows immediately from the case $y = (x)_1$ in the proof of Theorem 2.10, with $c_1 > 0$ now yielding a strict inequality in (2.8). $\square$

Note that another set of conditions ensuring strict inequality in (2.7) is given by $y \prec^w x$ and $c = (c_1 < c_2 < \ldots < c_p)$ with $c_1 > 0$. It will become apparent in Section 5.1, however, that Corollary 2.11 is the relevant result for our purposes.

If the components of the non-negative vector c are not arranged increasingly or if some or all components of c are negative, there is no result analogous to Theorem 2.10. This is easily seen by inspecting the proof given above. In particular, the arrangement $c = (c_1 \geq c_2 \geq \ldots \geq c_p)$ with $c_p \geq 0$ is not covered. Rather surprisingly, the following simple result will be sufficient in this case. It is convenient to state it here, although only the elementwise vector ordering and not the superdominance order is involved.

Lemma 2.12. *Let $x = (x_1 \geq x_2 \geq \ldots \geq x_p)$ and $y = (y_1 \geq y_2 \geq \ldots \geq y_p)$ be p-multisets of non-negative integers, given in decreasing order. If $x \leq y$ and $c = (c_1 \geq c_2 \geq \ldots \geq c_p)$ with $c_p \geq 0$, then $\psi_c(x) \leq \psi_c(y)$. If additionally $x \neq y$ and $c_p > 0$, then $\psi_c(x) < \psi_c(y)$.*

Proof. We have $c_k x_k \leq c_k y_k$ for $1 \leq k \leq p$ and there is at least one strict inequality if $x \neq y$ and $c_p > 0$. $\square$

2.2 Barycenters of Trees

In recent years several concepts of graphical centrality have been introduced and extensively studied, see e.g. Buckley and Harary [6] for a detailed overview. In our approach barycenters of trees play an important role.

For any vertex v of a tree $T = (V, E)$ let

$$\sigma_T(v) = \sum_{u \in V} d_T(v, u)$$

denote the *distance of the vertex* v. We omit the index T and simply write $\sigma(v)$ whenever there are no ambiguities. Clearly, the distance of T and the distances of the vertices of T are connected by the equation

$$\sigma(T) = \sum_{\{u,v\} \subseteq V} d_T(u, v) = \tfrac{1}{2} \sum_{v \in V} \sigma(v). \tag{2.9}$$

A vertex v is called a *barycenter* of T (also known as a *centroid vertex* or *mass center*) if $\sigma(v) = \min\{\sigma(u) : u \in V\}$. This definition should not be confused with the notion of a *center* (or *central vertex*) of T, the latter being a vertex v whose *eccentricity* $\mathrm{ecc}(v) = \max\{d_T(u, v) : u \in V\}$ is equal to the *radius* of T, i.e., $\mathrm{ecc}(v) = \mathrm{rad}(T) = \min\{\mathrm{ecc}(u) : u \in V\}$.

There is an alternative characterization of the barycenters of a tree T in terms of branches. Recall that any maximal subtree containing the vertex v as a leaf is called a *branch* of T at v. The *weight* of a branch of T at v is the number of edges in it and the *branch weight* $\mathrm{bw}(v)$ of a vertex v is the maximum weight of the branches at v. Now the barycenters are exactly those vertices that have minimum branch weight, see Theorem 2.17 below.

Barycenters and the distances of the vertices of a tree have been studied by several authors, see e.g. Barefoot, Entringer and Székely [3], Entringer, Jackson and Snyder [13] and Zelinka [31]. Following the solution to exercise 6.22 in Lovász [22], some basic properties of the function σ can easily be derived. For any edge $e = uv$ of a tree T, let T_u and T_v denote the component of $T - e$ containing u and v respectively.

Lemma 2.13. *Let uv be an edge of a tree T. Then $\sigma(u) - \sigma(v) = |T_v| - |T_u|$.*

Proof. We have $d_T(u, v') = d_T(v, v') + 1$ for any v' in T_v and similarly $d_T(v, u') = d_T(u, u') + 1$ for any u' in T_u. Hence $\sigma(u) - \sigma(v) = |T_v| - |T_u|$. □

Lemma 2.14. *For any tree T the function σ is strictly convex in the following sense: If $v_1 u v_2$ is a path in T, then $2\sigma(u) < \sigma(v_1) + \sigma(v_2)$.*

Proof. Let $n(v_1)$ and $n(v_2)$ denote the order of the component of $T - u$ containing v_1 and v_2 respectively. By Lemma 2.13,

$$\sigma(u) = \sigma(v_1) + n(v_1) - (|T| - n(v_1)) = \sigma(v_1) + 2n(v_1) - |T|$$

and similarly,

$$\sigma(u) = \sigma(v_2) + 2n(v_2) - |T|.$$

Adding up, we obtain

$$2\sigma(u) = \sigma(v_1) + \sigma(v_2) + 2(n(v_1) + n(v_2) - |T|) < \sigma(v_1) + \sigma(v_2),$$

completing the proof. □

A successive application of Lemma 2.14 yields the following two results.

Corollary 2.15. *Let $v_0 v_1 \dots v_\ell$ be a path of length $\ell \geq 2$ in a tree T. If $\sigma(v_0) \leq \sigma(v_1)$, then $\sigma(v_i) < \sigma(v_{i+1})$ for $i = 1, \dots, \ell - 1$.*

Corollary 2.16. *There are at most two barycenters in a tree. If there are two, then they are adjacent.*

The last result has already been obtained by Jordan [19] in 1869. He also gave the following characterization of barycenters in terms of branch weights.

Theorem 2.17. *Let B denote the set of barycenters of a tree $T = (V, E)$ of order n. If there are two barycenters b_1, b_2, then $\mathrm{bw}(b_1) = \mathrm{bw}(b_2) = \frac{n}{2}$. Otherwise, $\mathrm{bw}(b) < \frac{n}{2}$ for the barycenter b of T. In both cases, $\mathrm{bw}(v) > \frac{n}{2}$ for $v \in V \setminus B$.*

Proof. Let $b \in B$ and let $v \in V \setminus B$ be adjacent to b. Then $|T_v| < |T_b|$ by Lemma 2.13, and this implies $\mathrm{bw}(v) = |T_b| > \frac{n}{2}$, since $|T_v| + |T_b| = n$. If b is the only barycenter of T, also $\mathrm{bw}(b) < \frac{n}{2}$ is immediately deduced. In case of two barycenters b_1 and b_2, the same reasoning as above yields $|T_{b_1}| = |T_{b_2}| = \frac{n}{2}$ and $\mathrm{bw}(b_1) = \mathrm{bw}(b_2) = \frac{n}{2}$. Finally, for vertices $v \in V \setminus B$ that are not adjacent to a barycenter, the assertion is an easy consequence of the previous results and the definition of the branch weight. □

A deeper discussion of Jordan's results along with some historical remarks can be found in the books of Biggs, Lloyd and Wilson [4] and König [21].

2.3 Edge Height and Distance

We now take a slightly different view on the distance of a vertex and the distance of a tree. Consider a tree $T = (V, E)$, a vertex $r \in V$ and an edge $e \in E$ and let $h_T(r, e)$ be defined by

$$h_T(r, e) = |\{u \in V : e \in P_T(r, u)\}|.$$

We call $h_T(r, e)$ the *height* of e *relative to* r and $h(r, T) = (h_T(r, e))_{e \in E}$ the *edge height multiset relative to* r. If T is rooted at r and $e = uv$ is an edge with $\ell(v) < \ell(u)$, then $h_T(r, e) = |T(u)|$. Since edge heights of rooted trees are a fundamental tool in this thesis, we also use the shorter notation $h(e) = h(r, e) = h_T(r, e)$ and $h(T) = h(r, T)$, omitting both the index T and the root r whenever there are no ambiguities. Furthermore we simply speak of the *height* $h(e)$ of e and the *edge height multiset* $h(T)$ in this case.

The distance of a vertex and the function h are connected as follows.

Lemma 2.18. *Let v be a vertex of the tree $T = (V, E)$. Then*

$$\sigma(v) = \sum_{e \in E} h(v, e).$$

Proof. Let $d = \deg_T(v)$ and let $T_1, \ldots, T_d$ denote the branches of T at v. Then

$$\sigma(v) = \sum_{i=1}^{d} \sum_{u \in V(T_i)} d(v, u) = \sum_{i=1}^{d} \sum_{e \in E(T_i)} h(v, e) = \sum_{e \in E} h(v, e)$$

by simply counting in two ways the number of times that an edge $e \in E(T_i)$ is considered in the sum. $\square$

It is not difficult to derive a relation between the edge height multisets $h(u, T)$ and $h(v, T)$ for arbitrary vertices u, v of T. The following special case is important for our purposes.

Lemma 2.19. *Let T be a tree and let uv be an edge with $\sigma(u) \le \sigma(v)$. Then $h(v, T) \preceq^w h(u, T)$ with equality if and only if both u and v are barycenters of T. In particular, the edge height multisets $h(v, T)$ that are maximal in the superdominance order are derived by choosing v to be a barycenter of T.*

Proof. We have $h(u, uv) = |T_v| \le |T_u| = h(v, uv)$ by Lemma 2.13 and $h(u, e) = h(v, e)$ for all other edges $e \ne uv$. Thus, by the merging lemma, $h(v, T) \preceq^w h(u, T)$ with equality if and only if $|T_v| = |T_u|$, i.e., if both u and v are barycenters of T. This proves the first assertion. The second one is easily deduced from this by Corollary 2.15. $\square$

According to Lemma 2.18 and equation (2.9), a relation between the distance $\sigma(T)$ of a tree $T = (V, E)$ and the sum of the heights $h_T(v, e)$ of all edges $e \in E$ relative to all vertices $v \in V$ is immediately established. We will now deduce a formula for the distance of T in which only edge heights relative to *one* vertex of T are involved.

To this end let us first derive another formula for $\sigma(T)$, which is already contained in the work of Wiener [29]. Consider a tree $T = (V, E)$ and an edge $e = uv \in E$. As above, let T_u and T_v denote the component of $T - e$ containing u and v respectively. Let $f(e)$ be defined by

$$f(e) = f_T(e) = \min(|T_u|, |T_v|),$$

and let g_n denote the parabola defined by $g_n(t) = t(n-t)$ for $n \in \mathbb{N}$ and $t \in \mathbb{R}$. Then the distance of a tree T of order n is given by

$$\sigma(T) = \sum_{\{u,v\}\subseteq V} d(u, v) = \sum_{e\in E} g_n(f(e)), \tag{2.10}$$

since $g_n(f(e))$ counts the number of those paths in T that contain the edge e. Consequently, $g_n(f(e))$ is sometimes called the *path number* of e. Note that $f(e) \le \frac{n}{2}$ for any edge e and that g_n is a strictly concave and strictly increasing function on the interval $[0, \frac{n}{2}]$.

Consider now a class $\mathcal{T}$ of trees of a fixed order and let $\mathcal{F}$ denote the set of all multisets $f(T) = (f_T(e))_{e\in E(T)}$ for $T \in \mathcal{T}$. Then, in view of (2.10), Theorem 2.3 and Corollary 2.5, the problem of minimizing (maximizing) the distance within the class $\mathcal{T}$ can be transformed into the problem of determining the maximal (minimal) elements in the poset $(\mathcal{F}, \preceq^w)$. Choosing a barycenter as the root of the trees, the problem can be further reduced to edge height multisets. Before we state this result, recall that trees T having two barycenters r and $\tilde{r}$ do not cause any problems in view of their edge height multisets. Indeed, since $h(r, T) = h(\tilde{r}, T)$ by Lemma 2.19, it does not matter which barycenter is chosen as the root of T.

Lemma 2.20. *Let r be both the root and a barycenter of a tree T and let $e = uv$ be an edge of T. Then $f(e) = h(r, e) = h(e)$.*

Proof. We may assume that $e \in P_T(r, u)$. Then $\sigma(u) \ge \sigma(v)$, implying $|T_u| \le |T_v|$ by Lemma 2.13. Hence $f(e) = |T_u| = |T(u)| = h(e)$. □

Thus, if a tree T of order n is rooted at a barycenter, its distance is given by

$$\sigma(T) = \sum_{e\in E} g_n(h(e)). \tag{2.11}$$

Combining all the tools, the heart of our approach for studying distance problems in trees can now be stated as follows.

Theorem 2.21. *Let $\mathcal{T}$ be a class of trees of a fixed order and assume that each tree $T \in \mathcal{T}$ is rooted at a barycenter r of T. Let $\mathcal{H}$ denote the set of all multisets $h(T) = h(r, T)$ for $T \in \mathcal{T}$.*

(i) If a tree T has minimum (maximum) distance within the class $\mathcal{T}$, then the multiset $h(T)$ is a maximal (minimal) element in the poset $(\mathcal{H}, \preceq^w)$.

(ii) If $(\mathcal{H}, \preceq^w)$ has a maximum (minimum) element h^*, then all trees $T \in \mathcal{T}$ with $h(T) = h^*$ have minimum (maximum) distance within the class $\mathcal{T}$. In particular, if there exists only one tree T^* with $h(T^*) = h^*$, then T^* is the unique tree that has minimum (maximum) distance in $\mathcal{T}$.

Proof. This follows directly from (2.11), Theorem 2.3, Corollary 2.5 and the remarks preceding Lemma 2.20. □

Note that the poset $(\mathcal{H}, \preceq^w)$ might contain several minimal or maximal elements. Furthermore, even if a minimum or maximum element exists in $(\mathcal{H}, \preceq^w)$, it is a priori not ensured that this multiset is only realizable as the edge height multiset of exactly one tree in $\mathcal{T}$. Indeed, both phenomena will occur in certain instances of the maximum distance problem in trees. In all our minimization problems, however, there will be a uniquely realizable maximum element in $(\mathcal{H}, \preceq^w)$ and hence a unique optimal tree.

2.4 Weighted Distance and Rearrangements

A natural generalization of the concept of distance in a tree is obtained if the distance between two vertices is defined relative to certain weights that have been assigned to the edges of the tree.

Consider the following situation. We are given a class $\mathcal{T}$ of trees of a fixed order n and an $(n-1)$-multiset $c = (c_1, c_2, \ldots, c_{n-1})$ of real numbers. For $T = (V, E) \in \mathcal{T}$, any function $\gamma : E \to \mathbb{R}$ with $(\gamma(e))_{e \in E} = c$ (understood as an equality between multisets) is called a *c-valuation* of T. It is convenient to think of the c_i as given weights that have to be assigned to the edges of T. Therefore, c is also called a *multiset of edge weights*.

Given a c-valuation γ and two vertices u, v of T, the *weighted distance* $d_\gamma(u, v)$ of u and v *relative to* γ is defined by

$$d_\gamma(u, v) = \sum_{e \in P_T(u,v)} \gamma(e),$$

and the *weighted distance* $\sigma_\gamma(T)$ of T *relative to* γ is given by

$$\sigma_\gamma(T) = \sum_{\{u,v\}\subseteq V} d_\gamma(u,v).$$

Clearly, the usual distance $d(u,v)$ between two vertices of T and the distance $\sigma(T)$ are obtained in the special case $c = (1^{n-1})$.

As for $\sigma(T)$, we may ask for a tree $T \in \mathcal{T}$ and a c-valuation γ of T such that $\sigma_\gamma(T)$ is minimum or maximum. In these optimization problems, which will generally be referred to as the *minimum (maximum) c-weighted distance problem*, the two tasks of determining a tree and of choosing a suitable valuation can be solved separately. This is easily seen if we first derive an alternative formula for computing $\sigma_\gamma(T)$, analogous to the equations (2.10) and (2.11) for $\sigma(T)$. Indeed,

$$\sigma_\gamma(T) = \sum_{\{u,v\}\subseteq V} d_\gamma(u,v) = \sum_{\{u,v\}\subseteq V} \sum_{e\in P_T(u,v)} \gamma(e) = \sum_{e\in E} \gamma(e)\, g_n(f(e)),$$

where the parabola g_n and the path number $g_n(f(e))$ of the edge e are defined as in the previous section. If T is once again rooted at a barycenter, then, by Lemma 2.20,

$$\sigma_\gamma(T) = \sum_{e\in E} \gamma(e)\, g_n(h(e)). \tag{2.12}$$

Note that the structure of the tree T is completely encoded in the multiset $g_n[h(T)] = (g_n(h(e)))_{e\in E}$, while the c-valuation γ of T is represented by the multiset $(\gamma(e))_{e\in E} = c$.

For simplicity, let us introduce a further notation. Given two p-multisets $x = (x_1, x_2, \ldots, x_p)$ and $y = (y_1, y_2, \ldots, y_p)$, let

$$x \cdot y = \sum_{i=1}^{p} x_i y_i$$

denote the *inner (or scalar) product* of x and y. Dealing with multisets, the value of $x \cdot y$ naturally depends on the chosen order of the components in x and y, see also Theorem 2.22 below.

Inspecting equation (2.12) again, the sum is now immediately identified as an inner product of the multisets $c = (\gamma(e))_{e\in E}$ and $g_n[h(T)] = (g_n(h(e)))_{e\in E}$. Thus, the minimum and maximum c-weighted distance problems ask for a tree $T \in \mathcal{T}$ and a c-valuation γ of T such that this inner product is minimal and maximal respectively.

For the remainder of this section consider a fixed tree $T \in \mathcal{T}$ that is rooted at a barycenter. Let us denote the extremal values of $\sigma_\gamma(T)$ by

$$\sigma_{\min}(T,c) = \min\{\sigma_\gamma(T) : \gamma \text{ is a } c\text{-valuation of } T\}$$

and

$$\sigma_{\max}(T,c) = \max\{\sigma_\gamma(T) : \gamma \text{ is a } c\text{-valuation of } T\}.$$

Since both c and $g_n[h(T)]$ are fixed multisets, determining $\sigma_{\min}(T,c)$ and $\sigma_{\max}(T,c)$ is just a basic *rearrangement problem* for two $(n-1)$-multisets of real numbers. This problem has a classical solution due to Hardy, Littlewood and Pólya [17].

Theorem 2.22. *Let $x = (x_1, \ldots, x_p)$ and $y = (y_1, \ldots, y_p)$ be p-multisets of real numbers. Then*

$$\sum_{i=1}^{p} x_{(i)} y_{(p-i+1)} \le \sum_{i=1}^{p} x_i y_i \le \sum_{i=1}^{p} x_{(i)} y_{(i)}, \tag{2.13}$$

or, equivalently in short notation, $x_\uparrow \cdot y_\downarrow \le x \cdot y \le x_\uparrow \cdot y_\uparrow$.

Obviously, $x_\uparrow \cdot y_\uparrow = x_\downarrow \cdot y_\downarrow$ and $x_\uparrow \cdot y_\downarrow = x_\downarrow \cdot y_\uparrow$. Apart from these trivial identities, equality in (2.13) is also possible for other arrangements of x and y, namely if some components of x or y are equal. For instance,

$$(3,3,2,1) \cdot (3,2,1,1) = (3,3,1,2) \cdot (2,3,1,1) = 18,$$

and

$$(3,2,1,1) \cdot (1,1,2,3) = (2,3,1,1) \cdot (1,1,3,2) = 10.$$

Following Hardy, Littlewood and Pólya, we say that the maximum and minimum value in Theorem 2.22 correspond to multisets x and y that are *similarly ordered* and *oppositely ordered* respectively. In view of c-weighted distance problems, we deduce the following result.

Corollary 2.23. *Let T be a tree of order n, rooted at a barycenter, and let c be an $(n-1)$-multiset of edge weights. Then the extremal values $\sigma_{\min}(T,c)$ and $\sigma_{\max}(T,c)$ of $\sigma_\gamma(T)$ are obtained if the c-valuation γ is chosen such that $c = (\gamma(e))_{e\in E}$ and $g_n[h(T)]$ are oppositely and similarly ordered respectively.*

Chapter 3

Minimum Distance of Trees

Having introduced the fundamental tools, we now turn our attention to distance problems in trees, starting with trees having minimum distance in this chapter. We confine ourselves to study four classes of trees, namely the class of all trees of a fixed order and its three subclasses consisting of q-ary trees, trees with bounded maximum degree and trees with a given degree sequence. Although the first two of these subclasses are closely connected it is convenient to treat them in separate sections, following the presentation used in Jelen and Triesch [18]. Using the approach stated in Theorem 2.21, the minimum distance problem is solved completely in each of these four classes of trees. Moreover, the optimal trees turn out to be unique and can easily be constructed.

3.1 The Class $\mathcal{T}(n)$

Let $\mathcal{T}(n)$ denote the class of all trees of order n for $n \in \mathbb{N}$. Minimizing the distance in this class of trees is fairly easy.

Theorem 3.1. *Let $T \in \mathcal{T}(n)$ have minimum distance. Then $T \simeq K_{1,n-1}$.*

Proof. The cases $n \leq 2$ are trivial. Thus assume that $n \geq 3$ and let T be rooted at a barycenter r. Since $h_T(r, e) \geq 1$ for any edge e of T, we deduce that $h(r, T) \preceq^w (1^{n-1})$. Clearly, (1^{n-1}) is only realizable as an edge height multiset of a tree in $\mathcal{T}(n)$ by taking the star $K_{1,n-1}$ rooted at its barycenter. Hence, $T \simeq K_{1,n-1}$ by Theorem 2.21. □

Further easy proofs that do not rely on the superdominance order can be found in Entringer, Jackson and Snyder [13] and Lovász [22, exercise 6.23].

3.2 Rooted q-Ary Trees

The first subclass of $\mathcal{T}(n)$ that will be considered consists of all q-ary trees in $\mathcal{T}(n)$. Recall that, for $n, q \in \mathbb{N}$ with $q \geq 2$, a tree $T = (V, E)$ rooted at r is called an *(n,q)-tree* if $|V| = n$ and any vertex of T has at most q children. In general, without specifying the order n, we simply speak of a *q-ary tree*. For $\ell \geq 0$, a rooted tree T is called a *complete q-ary tree of depth* ℓ if $\ell(T) = \ell$ and any vertex v with $\ell(v) < \ell$ has exactly q children. In this case we also say that T is *complete*. The class of all (n,q)-trees is denoted by $\mathcal{T}(n,q)$. Analogously, the set of all edge height multisets $h(T) = h(r,T)$ for $T \in \mathcal{T}(n,q)$ is denoted by $\mathcal{H}(n,q)$.

For fixed $q \geq 2$, let the family $T^*(n,q) = (V^*(n,q), E^*(n,q))$ of q-ary trees be recursively defined as follows. The vertex set of $T^*(n,q)$ is

$$V^*(n,q) = \{v_1, v_2, \ldots, v_n\}$$

with n pairwise distinct vertices v_i, the root being v_1. The first edge sets are given by $E^*(1,q) = \emptyset$ and $E^*(n,q) = \{v_1v_2, v_1v_3, \ldots, v_1v_n\}$ for $2 \leq n \leq q+1$, such that $T^*(n,q) \simeq K_{1,n-1}$ for $2 \leq n \leq q+1$. For $n \geq q+2$, let j denote the minimum index in $\{2, 3, \ldots, n-1\}$ such that v_j has at most $q-1$ children in $T^*(n-1,q)$. Then the edge set of $T^*(n,q)$ is given by

$$E^*(n,q) = E^*(n-1,q) \cup \{v_jv_n\}.$$

To avoid any confusion, note that the root v_1 is not necessarily a barycenter of $T^*(n,q)$. For instance, the vertex v_2 is the only barycenter of the tree $T^*(21,3)$ depicted in Figure 3.1. In fact, using the construction of $T^*(n,q)$ and Theorem 2.17, it is easily seen that only v_1 and v_2 can possibly occur as a barycenter in $T^*(n,q)$. Note, however, that v_2 has degree $q+1$ in $T^*(n,q)$ for $n \geq 2q+1$. Thus, in most cases, choosing v_2 as the root of $T^*(n,q)$ does not yield a q-ary tree any more.

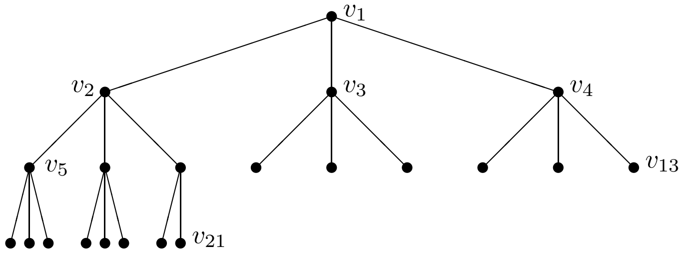

Figure 3.1: The tree $T^*(21,3)$

The next result shows that $T^*(n,q)$ is the (n,q)-tree whose edge height multiset $h(T^*(n,q)) = h(v_1, T^*(n,q))$ is the maximum element in the poset $(\mathcal{H}(n,q), \preceq^w)$.

Theorem 3.2. *Let $T \in \mathcal{T}(n,q)$ be rooted at r. Then $h(r,T) \preceq^w h(T^*(n,q))$ with equality if and only if $T \simeq_r T^*(n,q)$.*

Proof. Fix $q \geq 2$. We apply induction on n, the cases $n \leq q+1$ being trivial, since $T^*(n,q) \simeq K_{1,n-1}$ is already known to be the unique optimal tree by Theorem 3.1. Thus let $n > q+1$ and assume that the assertion is true for any q-ary tree of order less than n. Assume further that $T \not\simeq_r T^*(n,q)$ is an (n,q)-tree rooted at r such that $h(T) = h(r,T)$ is a maximal element in $(\mathcal{H}(n,q), \preceq^w)$. For simplicity, let $d = \deg_T(r)$, let $e_i = rr_i$ denote the edges incident to r for $1 \leq i \leq d$ and let $n_i = |T(r_i)|$ and $\ell_i = \ell(T(r_i))$ denote the order and the depth of $T(r_i)$ respectively. We may assume that $n_1 \geq n_2 \geq \ldots \geq n_d$. Then $n_1 \geq 2$ and hence $\ell_1 \geq 1$, since $n > q+1$.

Assume first that $d < q$. Consider any leaf u of $T(r_1)$ with $\ell(u) = \ell_1$ and let v be the parent of u (note that $v = r_1$ if $\ell_1 = 1$). Let T' denote the tree that is rooted at r and that is obtained from T by deleting the edge vu and by adding ru instead, see Figure 3.2. Obviously, $h_T(vu) = h_{T'}(ru) = 1$, $h_T(e) > h_{T'}(e)$ for all edges e of the path $P(r,v)$ (containing at least the edge e_1) and $h_T(e) = h_{T'}(e)$ for all other edges e. This implies $h(T) \prec^w h(T')$ by the merging lemma, a contradiction.

Thus $d = q$. Applying the induction hypothesis to each q-ary tree $T(r_i)$ and using the merging lemma yields $T(r_i) \simeq_r T^*(n_i,q)$ for $1 \leq i \leq q$ and hence $\ell_1 \geq \ell_2 \geq \ldots \geq \ell_q$. We distinguish three cases.

Case 1. $\ell_1 \geq \ell_q + 2$

Let u be a vertex in $T(r_1)$ such that $T(u)$ has depth $\ell_q + 1$ and let v denote the parent of u. Then $u \neq r_1$, $v = r_1$ if $\ell_1 = \ell_q + 2$, and $h_T(vu) > h_T(rr_q)$.

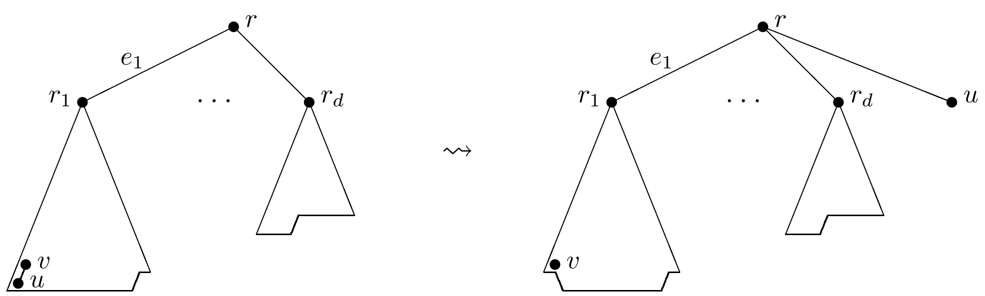

Figure 3.2: The trees T and T' in case $d < q$

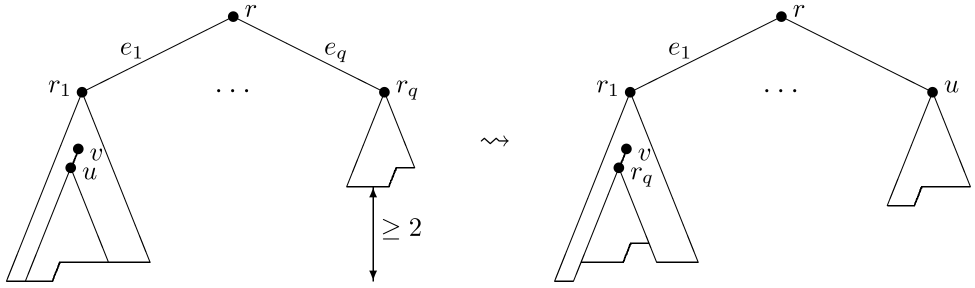

Figure 3.3: The trees T and T' in Case 1

We exchange the subtrees $T(r_q)$ and $T(u)$ in T and obtain a tree T', see Figure 3.3. Let $F = E(T) \setminus \{e_q, vu\} = E(T') \setminus \{ru, vr_q\}$. Then

$$h(T) = (h_T(e_q), h_T(vu), (h_T(e))_{e \in F})$$

and

$$h(T') = (h_{T'}(vr_q), h_{T'}(ru), (h_{T'}(e))_{e \in F}).$$

Clearly, $h_T(e_q) = h_{T'}(vr_q)$, $h_T(vu) = h_{T'}(ru)$ and $h_T(e) > h_{T'}(e)$ for all edges e of the path $P(r, v)$. Since $h_T(e) = h_{T'}(e)$ for $e \in F \setminus E(P(r, v))$, the merging lemma yields $h(T) \prec^w h(T')$, a contradiction.

Case 2. $\ell_1 = \ell_q + 1$ *and* $T(r_q)$ *is not complete*

Note that $\ell_q \geq 1$, since $T(r_q)$ is not complete. Let u be a child of r_1 such that $T(u)$ has depth ℓ_q. If $h_T(r_1u) > h_T(rr_q)$, we proceed as in Case 1, exchange the subtrees $T(r_q)$ and $T(u)$ in T and obtain the same contradiction as above.

Thus, $h_T(r_1u) \leq h_T(rr_q)$. Consider an auxiliary tree $\widetilde{T}$ consisting of a root $\tilde{r}$ of degree q having $T(r_q)$ (via the edge $\tilde{r}r_q$) and $T(u)$ (via the edge $\tilde{r}u$) as two of its q subtrees, the other $q-2$ subtrees being complete q-ary trees of depth $\ell_q - 1$. See the left part of Figure 3.4 for an example with $q = 3$.

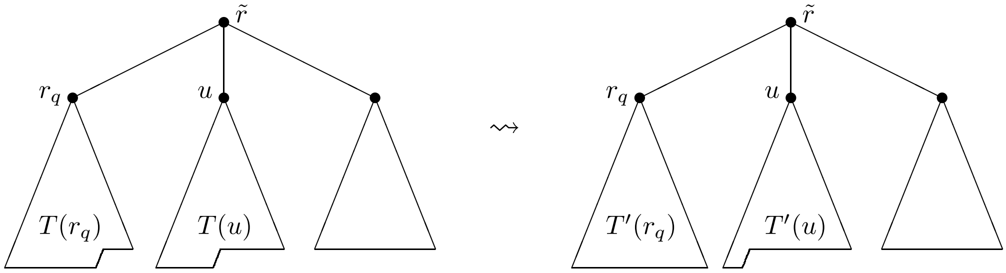

Figure 3.4: The auxiliary trees $\widetilde{T}$ and $\widetilde{T}'$ in Case 2 with $q = 3$

Let $\tilde{n}$ denote the order of $\widetilde{T}$. Obviously, $\tilde{n} < n$ and $\widetilde{T} \not\simeq_r T^*(\tilde{n}, q)$. By induction, $h(\tilde{r}, \widetilde{T})$ can be improved (in view of $\preceq^w$) by deleting some or all leaves of depth ℓ_q in $T(u)$ and by adding them as leaves in $T(r_q)$ instead. Let us denote the resulting trees by $T'(u)$, $T'(r_q)$ and $\widetilde{T}'$ respectively, see again Figure 3.4. Then $h(\tilde{r}, \widetilde{T}) \prec^w h(\tilde{r}, \widetilde{T}')$, due to the alterations in the heights of $\tilde{r}r_q$ and $\tilde{r}u$ and the change from $T(r_q)$ and $T(u)$ to $T'(r_q)$ and $T'(u)$.

If we perform this exchange of leaves in T instead of $\widetilde{T}$, the vertices r and r_1 take the role of $\tilde{r}$ and the height of e_1 decreases. Since all edge heights not mentioned so far remain unchanged during this operation, we arrive at a tree T' with $h(T) \prec^w h(T')$, a contradiction.

Case 3. *$\ell_1 = \ell_q$ or ($\ell_1 = \ell_q + 1$ and $T(r_q)$ is complete)*

Since $T \not\simeq_r T^*(n, q)$ and both $n_1 \geq n_2 \geq \ldots \geq n_q$ and $\ell_1 \geq \ell_2 \geq \ldots \geq \ell_q$, there exists an index $1 \leq i \leq q-1$ such that the subtrees $T(r_i)$ and $T(r_{i+1})$ are not complete and have the same depth $\ell = \ell_i = \ell_{i+1} = \ell_1 \geq 1$. Note that the degree of r_i in $T(r_i)$ is greater or equal to the degree of r_{i+1} in $T(r_{i+1})$ and recall that $T(r_i) \simeq_r T^*(n_i, q)$ and $T(r_{i+1}) \simeq_r T^*(n_{i+1}, q)$. Let us denote the children of r_i by $u_1, u_2, \ldots, u_\alpha$ and the children of r_{i+1} by $v_1, v_2, \ldots, v_\beta$ for some $1 \leq \beta \leq \alpha \leq q$. We may assume that $|T(u_1)| \geq \ldots \geq |T(u_\alpha)|$ and $|T(v_1)| \geq \ldots \geq |T(v_\beta)|$.

If $\ell = 1$, then $\alpha < q$ and deleting the edge $r_{i+1}v_\beta$ and adding $r_i v_\beta$ instead yields a tree T' with

$$(h_T(r_{i+1}v_\beta), h_T(e_i), h_T(e_{i+1})) \prec^w (h_{T'}(r_i v_\beta), h_{T'}(e_i), h_{T'}(e_{i+1})).$$

Since no other edge height has changed, $h(T) \prec^w h(T')$, a contradiction.

Hence $\ell \geq 2$ and $\alpha = \beta = q$. Let j denote the minimum index in $\{1, \ldots, q\}$ such that $T(u_j)$ is not a complete q-ary tree of depth $\ell - 1$, see Figure 3.5 for an example with $q = 3$ and $j = 3$.

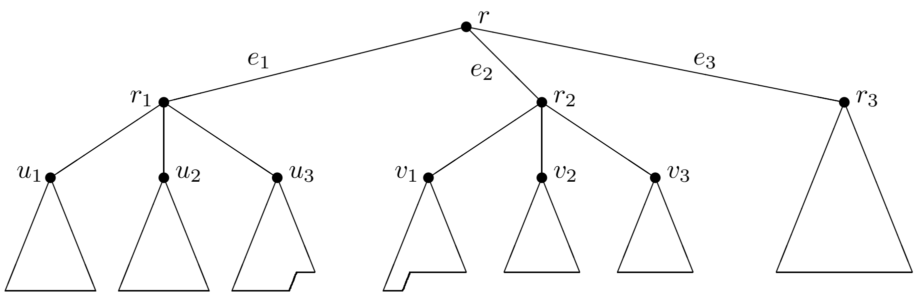

Figure 3.5: An example to Case 3 with $q = 3$, $\ell \geq 2$, $i = 1$ and $j = 3$

If $|T(u_j)| < |T(v_1)|$, exchanging the subtrees $T(u_j)$ and $T(v_1)$ in T yields a tree T' with

$$(h_T(e_i), h_T(e_{i+1})) \prec^w (h_{T'}(e_i), h_{T'}(e_{i+1})),$$

again a contradiction to the optimality of T.

Thus we are left with the case $|T(u_j)| \geq |T(v_1)|$. Note that both $T(u_j)$ and $T(v_1)$ have depth $\ell - 1$ and are not complete. Consider once more an auxiliary tree $\widetilde{T}$ consisting of a root $\tilde{r}$ of degree q having $T(u_j)$ (via the edge $\tilde{r}u_j$) and $T(v_1)$ (via the edge $\tilde{r}v_1$) as two of its q subtrees, the other $q-2$ subtrees being complete q-ary trees of depth $\ell - 2$. Completely analogous to the reasoning in Case 2, $h(\tilde{r}, \widetilde{T})$ can be improved (in view of $\preceq^w$) by deleting certain leaves in $T(v_1)$ and by adding them as leaves in $T(u_j)$ instead. Performing this exchange in T instead of $\widetilde{T}$ yields a tree T'. As before

$$(h_T(e_i), h_T(e_{i+1})) \prec^w (h_{T'}(e_i), h_{T'}(e_{i+1})),$$

implying $h(T) \prec^w h(T')$. This final contradiction completes the proof. $\square$

Although $h(T^*(n, q))$ is the maximum element in $(\mathcal{H}(n, q), \preceq^w)$, the tree $T^*(n, q)$ need not have minimum distance within the class $\mathcal{T}(n, q)$. A simple counterexample is depicted in Figure 3.6. The left tree $T^*(6, 3)$ is rooted at its barycenter v_1, while the right tree $T^{\pitchfork}$ is rooted at r and has the barycenter $b \neq r$. Obviously, $T^{\pitchfork}$ rooted at r belongs to the class $\mathcal{T}(6, 3)$. Since

$$h(v_1, T^*(6, 3)) = (1^4, 3) \prec^w (1^4, 2) = h(b, T^{\pitchfork}),$$

the considerations leading to Theorem 2.21 yield $\sigma(T^{\pitchfork}) < \sigma(T^*(6, 3))$. Note that

$$h(r, T^{\pitchfork}) = (1^4, 4) \prec^w (1^4, 3) = h(v_1, T^*(6, 3)),$$

in accordance with the previous theorem.

In fact, except for some trivial cases in which the order n is small relative to q, none of the trees $T^*(n, q)$ has minimum distance within the class $\mathcal{T}(n, q)$. We will return to this question at the end of the next section.

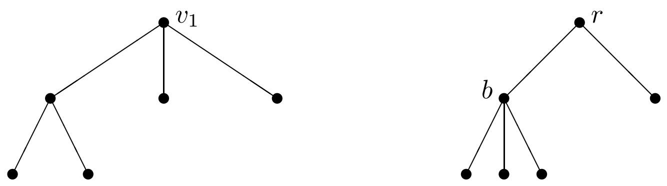

Figure 3.6: The trees $T^*(6, 3)$ and $T^{\pitchfork}$ in the class $\mathcal{T}(6, 3)$

3.3 Trees with Bounded Maximum Degree

As long as the star $K_{1,n-1}$ belongs to a subclass $\mathcal{T}$ of $\mathcal{T}(n)$, the minimum distance problem in $\mathcal{T}$ is immediately solved by Theorem 3.1. In order to exclude such highly branched trees as stars, a natural restriction is to bound the maximum degree of the trees. Thus, for $\Delta \geq 2$ and $n \in \mathbb{N}$, let $\mathcal{T}_\Delta(n)$ denote the class of all trees T of order n with $\Delta(T) \leq \Delta$. Let $\mathcal{H}_\Delta(n)$ denote the set of all edge height multisets $h(T) = h(r, T)$ that can be derived from trees $T \in \mathcal{T}_\Delta(n)$ that are rooted at a barycenter r.

Fix $\Delta \geq 2$. Similar to the definition of $T^*(n, q)$ in the previous section, we now recursively define a family $T^*_\Delta(n) = (V^*_\Delta(n), E^*_\Delta(n))$ of trees in $\mathcal{T}_\Delta(n)$. The vertex set is given by

$$V^*_\Delta(n) = \{v_1, v_2, \ldots, v_n\}$$

with n pairwise distinct vertices v_i. The root of $T^*_\Delta(n)$ is v_1 and $E^*_\Delta(1) = \emptyset$. For $n \geq 2$, let j denote the minimum index in $\{1, 2, \ldots, n-1\}$ such that the degree of v_j in $T^*_\Delta(n-1)$ is less than Δ. Then $T^*_\Delta(n)$ has the edge set

$$E^*_\Delta(n) = E^*_\Delta(n-1) \cup \{v_j v_n\}.$$

The tree $T^*_3(17)$ is depicted in Figure 3.7.

Note that the root v_1 is always a barycenter of $T^*_\Delta(n)$. Although this fact is not used in the following considerations and is indeed an easy consequence of the next theorem and Lemma 2.19, we give a short direct proof. The result is trivially true for $n \leq \Delta + 1$, since v_1 is a barycenter of the star $K_{1,n-1}$. If $n > \Delta + 1$, we have $\mathrm{bw}(v_1) = |T(v_2)|$ and, by construction,

$$|T(v_2)| = 1 + \sum_{u\,:\,u \text{ is a child of } v_2} |T(u)| \leq 1 + \sum_{i=3}^{\Delta+1} |T(v_i)| = n - |T(v_2)|.$$

Hence $\mathrm{bw}(v_1) = |T(v_2)| \leq \frac{n}{2}$ and v_1 is a barycenter of $T^*_\Delta(n)$ by Theorem 2.17.

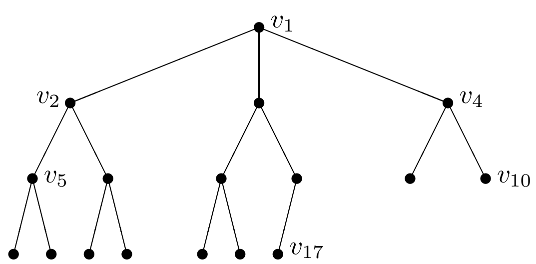

Figure 3.7: The tree $T^*_3(17)$

Applying the result on q-ary trees from the previous section, we can now solve the minimum distance problem in $\mathcal{T}_\Delta(n)$ and $\mathcal{T}(n,q)$.

Theorem 3.3. *Let $T \in \mathcal{T}_\Delta(n)$ have minimum distance. Then $T \simeq T^*_\Delta(n)$.*

Proof. Fix $\Delta \geq 3$, the case $\Delta = 2$ being trivial. We may assume that $n > \Delta + 1$, since otherwise $T^*_\Delta(n) \simeq K_{1,n-1}$ is already known to be the unique optimal tree by Theorem 3.1.

Let $T = (V, E)$ be rooted at a barycenter r. Then, by Theorem 2.21 and the remarks preceding it, $f(T) = h(T) = h(r, T)$ is a maximal element in the poset $(\mathcal{H}_\Delta(n), \preceq^w)$. Let $d = \deg_T(r)$, let $e_i = rr_i$ denote the edges incident to r for $1 \leq i \leq d$ and let T_i denote the subtree of T that is rooted at r and that is induced by $V \setminus V(T(r_i))$. Note that $d \leq \Delta$ and that $d \geq 2$, since otherwise $1 = f(e_1) = h(r, e_1) = n - 1 > \Delta$, a contradiction.

Let n_i denote the order of T_i. Since each T_i is a $(\Delta-1)$-ary tree and $h(T)$ is a maximal element in $(\mathcal{H}_\Delta(n), \preceq^w)$, Theorem 3.2 and Lemma 2.19 yield $T_i \simeq_r T^*(n_i, \Delta - 1)$ for $1 \leq i \leq d$. This immediately implies $d = \Delta$ and $T \simeq T^*_\Delta(n)$, completing the proof. □

A different proof of this result has been given by Fischermann, Hoffmann, Rautenbach, Székely and Volkmann [14]. Note further that the trees $T^*_\Delta(n)$ belong to a broader class of trees called *dendrimers*, see Chen, Gutman, Lee and Yeh [7] and Diudea [8].

Theorem 3.4. *Let $T \in \mathcal{T}(n,q)$ have minimum distance. Then $T \simeq T^*_{q+1}(n)$.*

Proof. Obviously, each tree in $\mathcal{T}(n,q)$ belongs to the class $\mathcal{T}_{q+1}(n)$ as well. Conversely, each tree in $\mathcal{T}_{q+1}(n)$ is an (n,q)-tree if it is rooted at any of its leaves. □

A simple case study shows that $T^*(n,q) \not\simeq T^*_{q+1}(n)$ except for the trivial cases $n \leq q+1$ and the case $n = 2q+1$. For instance, consider the subpath $v_2v_1v_3$ of $T^*(n,q)$ for $n \geq 3q+1$. Since v_2 and v_3 have degree $q+1$ in $T^*(n,q)$, while v_1 has degree q, this path has no isomorphic image in $T^*_{q+1}(n)$. Thus, as already remarked above, almost none of the trees $T^*(n,q)$ has minimum distance in $\mathcal{T}(n,q)$.

3.4 Trees with Given Degree Sequence

Apart from bounding the maximum degree, a further natural restriction is to consider only trees with a given degree sequence. Recall that a partition $\pi = (d_1 \geq \ldots \geq d_n)$ of n non-negative integers is the degree sequence of a tree if and only if $d_n \geq 1$ and $\Sigma(\pi) = 2n - 2$, see Lovász [22, exercise 7.47]. For simplicity, the partitions of this type will be called *tree-graphical*. Given any tree-graphical partition π, let $\mathcal{T}(\pi)$ denote the class of all trees T with degree sequence $\pi(T) = \pi$ and let $\mathcal{H}(\pi)$ denote the set of all edge height multisets $h(r, T)$ that can be derived from trees $T \in \mathcal{T}(\pi)$ that are rooted at a barycenter r.

As before, we will show that there is a unique tree $T^*(\pi)$ having minimum distance within the class $\mathcal{T}(\pi)$. This tree is the rooted tree in $\mathcal{T}(\pi)$ that is completely characterized by the following three conditions:

(C1) For $i \geq 0$ the degree of any vertex of depth i is greater or equal to the degree of any vertex of depth $i+1$.

(C2) For distinct vertices u, v of the same depth with $\deg(u) > \deg(v) \geq 2$ the minimum degree of the children of u is greater or equal to the maximum degree of the children of v.

(C3) For distinct vertices u, v of the same depth with $\deg(u) = \deg(v) \geq 2$ either the minimum degree of the children of u is greater or equal to the maximum degree of the children of v or the same statement holds with the roles of u and v reversed.

More formally, $T^*(\pi)$ can be constructed as follows. If $\pi = (1^2)$, then $T^*(\pi) = K_2$. For a tree-graphical partition $\pi = (d_1 \geq d_2 \geq \ldots \geq d_n)$ of length $n = |\pi| \geq 3$, the vertex set of $T^*(\pi)$ is given by

$$V^*(\pi) = \{v_1, v_2, \ldots, v_n\}$$

with n pairwise distinct vertices v_i, the root being v_1. Let

$$s(\pi) = \max\{j : 1 \leq j \leq n,\, d_j > 1\}.$$

$T^*(\pi)$ is derived as the final tree $F_{s(\pi)}$ in a sequence of auxiliary forests $F_i = (V^*(\pi), E_i)$ for $1 \leq i \leq s(\pi)$. Initially,

$$E_1 = \{v_1 v_j : 2 \leq j \leq d_1 + 1\}.$$

If F_i has already been constructed for some $1 \leq i \leq s(\pi) - 1$, let $s(i)$ denote the minimum index $j \in \{1, \ldots, n\}$ such that v_j is an isolated vertex in F_i. Then the edge set of F_{i+1} is given by

$$E_{i+1} = E_i \cup \{v_{i+1} v_j : s(i) \leq j \leq s(i) + d_{i+1} - 2\}.$$

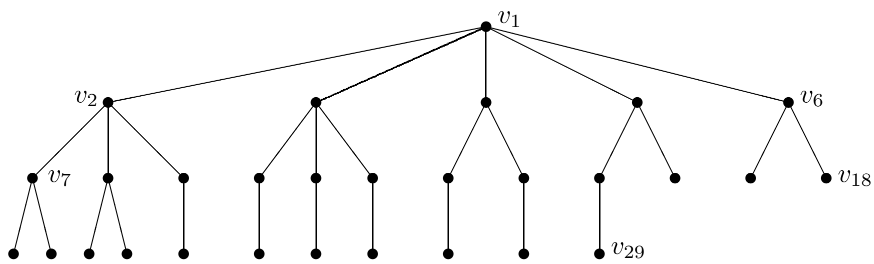

Figure 3.8: The tree $T^*(\pi)$ with $\pi = (5, 4^2, 3^5, 2^7, 1^{14})$

In other words, the leaf v_{i+1} of F_i is given degree d_{i+1} in F_{i+1} by adding edges between v_{i+1} and the $d_{i+1} - 1$ isolated vertices with the smallest indices in F_i. The tree $T^*(\pi)$ with $\pi = (5, 4^2, 3^5, 2^7, 1^{14})$ is depicted in Figure 3.8.

Note that the root v_1 is always a barycenter of $T^*(\pi)$. A direct proof of this fact can be obtained by applying some minor changes to the proof given for $T^*_\Delta(n)$ in the previous section. Moreover, the result is also implicitly contained in the next theorem.

Before we continue, some remarks seem convenient. The main idea in subsequent proofs is the one already known from the proof of Theorem 3.2. It can be summarized as follows. If a tree T does not have a desired property, we construct another tree T' by exchanging certain subtrees of T. Usually, most of the heights of the edges in $E(T) \cap E(T')$ are not touched by this exchange and the heights of the edges deleted in T are equal to the heights of the edges added to T. Thus, the two edge height multisets $h(T)$ and $h(T')$ differ only in a few components. In order to avoid permanent repetitions, we will focus on those edge heights that actually change when moving from T to T', leaving it to the reader to verify that the heights of edges not explicitly mentioned belong to one of the two categories stated above. Finally, if the merging lemma or some other tool developed in Chapter 2 is applied to prove $h(T) \prec^w h(T')$, the phrase 'improving $h(T)$' will be frequently used.

Theorem 3.5. *Let T be a tree rooted at r with degree sequence π. Then $h(r, T) \preceq^w h(v_1, T^*(\pi))$ with equality if and only if $T \simeq_r T^*(\pi)$.*

Proof. We may assume that T and r are chosen such that $h(T) = h(r, T)$ is a maximal element of the poset $(\mathcal{H}(\pi), \preceq^w)$. It clearly suffices to show that the conditions (C1), (C2) and (C3) characterizing $T^*(\pi)$ are also met by T. This will be done by a sequence of claims. For a vertex v of T, any subtree of T that is induced by a child of v and by all of the child's successors is called a *v-subtree*.

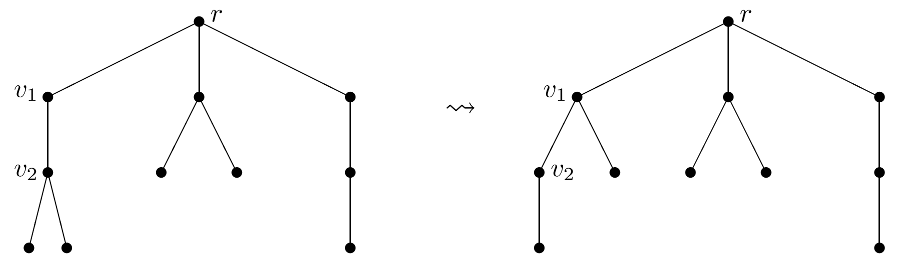

Figure 3.9: An example to Claim 1 with $\pi = (3^3, 2^3, 1^5)$

Claim 1. *Let $rv_1 \dots v_\ell$ be a path of length ℓ in T for some $\ell \geq 1$. Then $\deg_T(r) \geq \deg_T(v_1)$ and $\deg_T(v_{i-1}) \geq \deg_T(v_i)$ for $2 \leq i \leq \ell$.*

Proof. Let $v_0 = r$ and assume that there is an index $i \in \{1, \dots, \ell\}$ with $\delta = \deg_T(v_i) - \deg_T(v_{i-1}) > 0$. By deleting any δ v_i-subtrees and by adding them as subtrees of v_{i-1} instead, the degrees of v_{i-1} and v_i are exchanged and the resulting tree rooted at r still belongs to $\mathcal{T}(\pi)$, see Figure 3.9 for an example. Since the height of $v_{i-1}v_i$ has been decreased, $h(T)$ has been improved, a contradiction. □

Thus, in particular, the root r has maximum degree d_1.

Claim 2. *Let $v_1, \tilde{u}$ be distinct children of the vertex u in T and let $\tilde{v}$ be a child of v_1. Then $|T(\tilde{u})| \geq |T(\tilde{v})|$ and $\deg_T(\tilde{u}) \geq \deg_T(\tilde{v})$.*

Proof. Assume first that $|T(\tilde{u})| < |T(\tilde{v})|$. By exchanging the subtrees $T(\tilde{u})$ and $T(\tilde{v})$ in T, the height of uv_1 is decreased and thus $h(T)$ is improved, a contradiction. This proves the first assertion.

Assume now that $\delta = \deg_T(\tilde{v}) - \deg_T(\tilde{u}) > 0$. By deleting δ $\tilde{v}$-subtrees and by adding them as subtrees of $\tilde{u}$ instead, the degrees of $\tilde{u}$ and $\tilde{v}$ are exchanged and another tree $T' \in \mathcal{T}(\pi)$ is obtained. An example with $\pi = (3^3, 2^3, 1^5)$ is depicted in Figure 3.10.

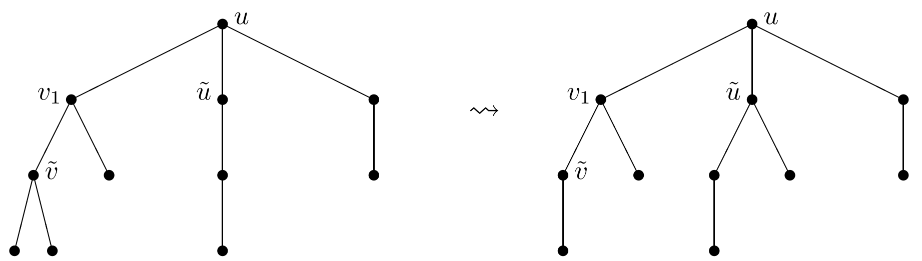

Figure 3.10: An example to Claim 2 with $\pi = (3^3, 2^3, 1^5)$

Let $\tilde{n}$ denote the sum of the orders of the δ subtrees that have been exchanged. Then $h_T(u\tilde{u}) = |T(\tilde{u})| \geq |T(\tilde{v})| = h_T(v_1\tilde{v})$ implies

$$(h_T(u\tilde{u}), h_T(v_1\tilde{v})) \prec^w (h_T(u\tilde{u}) + \tilde{n}, h_T(v_1\tilde{v}) - \tilde{n}) = (h_{T'}(u\tilde{u}), h_{T'}(v_1\tilde{v})).$$

Since the height of uv_1 has also been decreased by $\tilde{n}$, $h(T)$ has been improved, a contradiction. □

Claim 2 can be considered to be the case '$\ell = 0$' of the next claim.

Claim 3. *Let u_1, v_1 be distinct children of the vertex $u_0 = v_0$ in T and let $u_0u_1 \ldots u_\ell\tilde{u}$ and $v_0v_1 \ldots v_{\ell+1}\tilde{v}$ be two paths in T for some $\ell \geq 1$. Then $|T(\tilde{u})| \geq |T(\tilde{v})|$ and $\deg_T(\tilde{u}) \geq \deg_T(\tilde{v})$.*

Proof. Assume that the first assertion is false and consider a counterexample with minimal $\ell \geq 1$. Let $x_i = h_T(u_{i-1}u_i)$ for $1 \leq i \leq \ell$ and $y_j = h_T(v_{j-1}v_j)$ for $1 \leq j \leq \ell + 1$. Then $x_1 > x_2 > \ldots > x_\ell$, $y_1 > y_2 > \ldots > y_{\ell+1}$ and, as we have chosen a minimal counterexample,

$$\min(x_i, y_i) \geq \max(x_{i+1}, y_{i+1}) \quad \text{for } i = 1, \ldots, \ell - 1$$

and

$$\min(x_\ell, y_\ell) \geq y_{\ell+1}.$$

Finally, let $\delta = |T(\tilde{v})| - |T(\tilde{u})| > 0$. By exchanging the subtrees $T(\tilde{u})$ and $T(\tilde{v})$ in T, all x_i are increased by δ, while all y_j are decreased by δ. Since $\delta < |T(\tilde{v})| < |T(v_{\ell+1})| = y_{\ell+1}$, Lemma 2.9 can be applied and we infer that $h(T)$ has been improved by this operation, a contradiction. An example is given in Figure 3.11, where, as in subsequent figures, the decisive edge heights are shown as well.

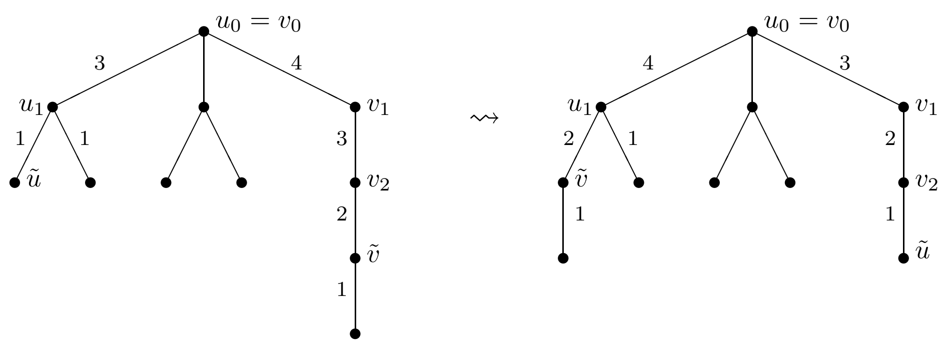

Figure 3.11: First example to Claim 3 with $\pi = (3^3, 2^3, 1^5)$ and $\ell = 1$

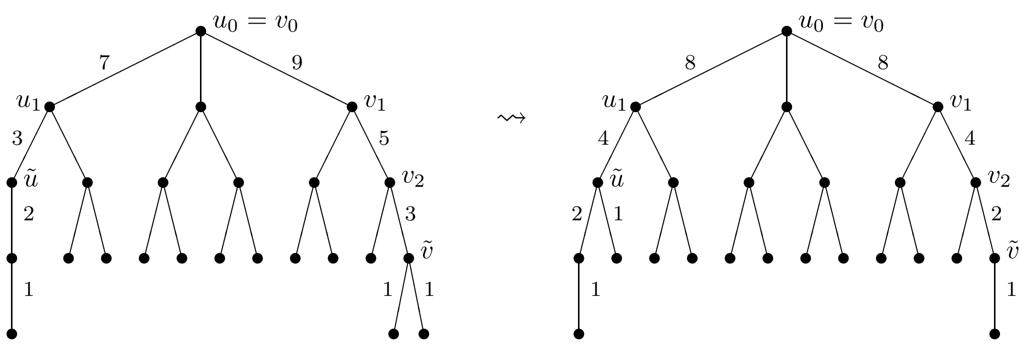

Figure 3.12: Second example to Claim 3 with $\pi = (3^{10}, 2^2, 1^{12})$ and $\ell = 1$

For the proof of the second assertion, we can proceed as in Claim 2. If $\delta = \deg_T(\tilde{v}) - \deg_T(\tilde{u}) > 0$, we delete any δ $\tilde{v}$-subtrees and add them as subtrees of $\tilde{u}$ instead, see Figure 3.12 for an example. Since

$$y_\ell = |T(v_\ell)| \geq h_T(u_\ell \tilde{u}) = |T(\tilde{u})| \geq |T(\tilde{v})| = h_T(v_{\ell+1}\tilde{v}),$$

it is easily seen that Lemma 2.9 can be applied once more, this time to the multisets $(x_1 > \ldots > x_\ell > h_T(u_\ell \tilde{u}))$ and $(y_1 > \ldots > y_{\ell+1} > h_T(v_{\ell+1}\tilde{v}))$. As before, we conclude that $h(T)$ has been improved, a contradiction. $\square$

Thus, so far we have established condition (C1).

Claim 4. *Let u_1, v_1 be distinct children of the vertex $u_0 = v_0$ in T and let $u_0u_1 \ldots u_\ell$ and $v_0v_1 \ldots v_\ell$ be paths of length $\ell \geq 2$ in T. Assume further that $|T(u_i)| \geq |T(v_i)|$ for $1 \leq i \leq \ell - 1$. Then $|T(u_\ell)| \geq |T(v_\ell)|$.*

Proof. As in the previous proof, let us write $x_i = h_T(u_{i-1}u_i) = |T(u_i)|$ and $y_i = h_T(v_{i-1}v_i) = |T(v_i)|$ for $1 \leq i \leq \ell$. If $\delta = y_\ell - x_\ell > 0$, we exchange the subtrees $T(u_\ell)$ and $T(v_\ell)$, see Figure 3.13. Since $(x_i, y_i) \prec^w (x_i + \delta, y_i - \delta)$ for $1 \leq i \leq \ell - 1$, this operation improves $h(T)$, again a contradiction. $\square$

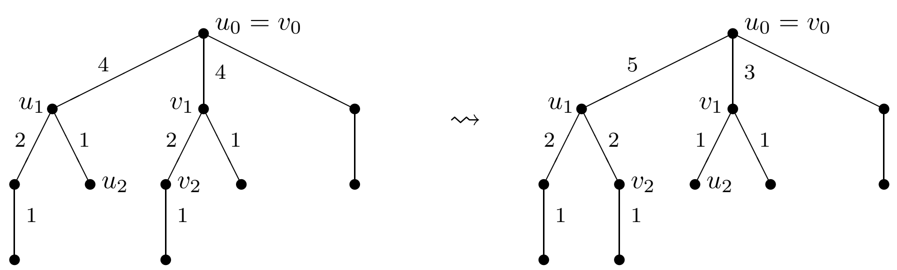

Figure 3.13: An example to Claim 4 with $\pi = (3^3, 2^3, 1^5)$ and $\ell = 2$

Claim 5. *Let u_1, v_1 be distinct children of the vertex $u_0 = v_0$ in T and let $u_0u_1 \dots u_\ell$ and $v_0v_1 \dots v_\ell$ be paths of length $\ell \geq 1$ in T. Assume further that $|T(u_\ell)| \geq |T(v_\ell)|$. Then $\deg_T(u_\ell) \geq \deg_T(v_\ell)$.*

Proof. We may assume that $|T(u_i)| \geq |T(v_i)|$ for $1 \leq i \leq \ell - 1$ by Claim 4. If $\delta = \deg_T(v_\ell) - \deg_T(u_\ell) > 0$, we delete δ v_ℓ-subtrees and add them as subtrees at u_ℓ instead. Now the same reasoning as in Claim 4 yields that $h(T)$ has been improved, a contradiction. $\square$

In order to complete the proof of the theorem, consider a situation as described in conditions (C2) and (C3). Let u, v be distinct vertices of the same depth in T with $\deg_T(u) \geq \deg_T(v) \geq 2$ and let $\tilde{u}$ and $\tilde{v}$ denote a child of u and v respectively. Let $u_0 = v_0$ denote the vertex that has the greatest depth among all vertices common to the paths $P(r, u)$ and $P(r, v)$. By Claim 5, we may assume that $|T(u)| \geq |T(v)|$. Then, by applying Claims 4 and 5 again, we deduce that $\deg_T(\tilde{u}) \geq \deg_T(\tilde{v})$, in accordance with (C2) and (C3). Thus $T \simeq_r T^*(\pi)$. $\square$

The minimum distance problem in $\mathcal{T}(\pi)$ is now immediately solved.

Theorem 3.6. *Let π be a tree-graphical partition and let $T \in \mathcal{T}(\pi)$ have minimum distance. Then $T \simeq T^*(\pi)$.*

Proof. Let T be rooted at a barycenter r. Then, by Theorem 2.21, $h(r, T)$ is a maximal element in $(\mathcal{H}(\pi), \preceq^w)$ and thus $T \simeq T^*(\pi)$ by the preceding theorem. $\square$

To close this section, note that a special case of Theorem 3.6 has been treated before. A tree of order n is called *starlike*, if its degree sequence has the type $(d, 2^{n-(d+1)}, 1^d)$ for some $3 \leq d \leq n - 1$. Using a different formula for $\sigma(T)$ and the dominance order, the starlike trees having minimum and maximum distance have been determined by Araujo, Gutman and Rada [2].

Chapter 4

Maximum Distance of Trees

At first sight, determining the trees having maximum distance seems to be quite similar to the corresponding minimization problem. While this is essentially true in case of the classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$ and $\mathcal{T}_\Delta(n)$, the situation changes considerably in the class $\mathcal{T}(\pi)$. Here we encounter some new difficulties which eventually prevent us from obtaining a complete solution.

Applying the approach stated in Theorem 2.21, we ask now for the trees whose edge height multisets relative to a barycenter are minimal in the superdominance order. In contrast to the minimum distance problem, we are no longer automatically led to barycenters as roots of the trees (see Lemma 2.19) and thus we have to ensure that all trees are rooted at barycenters. Apart from this additional consideration, we apply the same exchanging operations in trees as in the previous chapter. Our presentation will once more be focussed on those edge heights that actually change, see the remarks preceding Theorem 3.5.

4.1 The Classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$ and $\mathcal{T}_\Delta(n)$

Let us start with the class $\mathcal{T}(n)$ and let $\mathcal{H}(n)$ denote the set of all edge height multisets $h(r,T)$ that can be derived from trees $T \in \mathcal{T}(n)$ that are rooted at a barycenter r. As may have been expected, the path P_n is the unique tree having maximum distance in $\mathcal{T}(n)$.

Theorem 4.1. *Let $T \in \mathcal{T}(n)$ have maximum distance. Then $T \simeq P_n$.*

Proof. The cases $n \leq 3$ being trivial, assume that $n \geq 4$ and let T be rooted at a barycenter r of T. Then, by Theorem 2.21, $h(T) = h(r,T)$ is a minimal element of the poset $(\mathcal{H}(n), \preceq^w)$.

Assume first that there is a vertex $v \neq r$ in T with $\deg_T(v) \geq 3$ and let $u, \tilde{u}$ be two children of v. By deleting the edge $v\tilde{u}$ and by adding $u\tilde{u}$

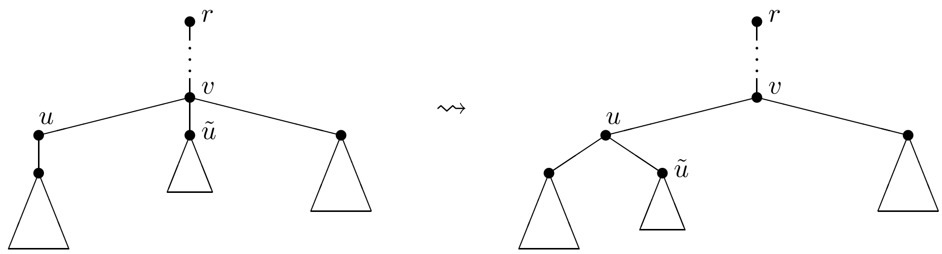

Figure 4.1: Improvement in case $\deg_T(v) \geq 3$ with $v \neq r$

instead, we obtain a tree T' in which the height of vu has been increased, see Figure 4.1. Since the branch weight at r has not changed, r is still a barycenter of T' and we deduce that $h(r,T') \prec^w h(r,T)$, in contradiction to the optimality of T. Thus, all vertices of T except for the root r are either leaves of T or have degree 2.

Assume now that $d = \deg_T(r) \geq 3$ and denote the children of r by $u_1, \tilde{u}_1, v_1, \ldots, v_{d-2}$. We may assume that

$$|T(u_1)| \leq |T(\tilde{u}_1)| \leq |T(v_1)| \leq \ldots \leq |T(v_{d-2})|.$$

Note that all these subtrees are paths by our previous consideration and that $|T(\tilde{u}_1)| \leq \frac{n}{2} - 1$, since otherwise $|T(u_1)| + |T(\tilde{u}_1)| + |T(v_1)| \geq 1 + 2\,\frac{n-1}{2} = n$, a contradiction. Let the two paths $T(u_1)$ and $T(\tilde{u}_1)$ be given by $u_1u_2\ldots u_k$ and $\tilde{u}_1\tilde{u}_2\ldots\tilde{u}_\ell$ for some $1 \leq k \leq \ell$.

If $k = 1$, we delete ru_1 and add $\tilde{u}_1u_1$ instead. By Theorem 2.17, r is still a barycenter of the resulting tree T', since

$$|T'(\tilde{u}_1)| = |T(\tilde{u}_1)| + 1 \leq \tfrac{n}{2} - 1 + 1 = \tfrac{n}{2}.$$

Furthermore

$$(h_{T'}(\tilde{u}_1u_1), h_{T'}(r\tilde{u}_1)) = (1, \ell+1) \prec^w (1,\ell) = (h_T(ru_1), h_T(r\tilde{u}_1)),$$

implying $h(T') \prec^w h(T)$, a contradiction.

If $k \geq 2$, we delete $u_{k-1}u_k$ and add $\tilde{u}_\ell u_k$ instead, see Figure 4.2. Again, r is still a barycenter of the resulting tree T' (by the same reasoning as above) and

$$\begin{aligned}(h_{T'}(P_{T'}(r,u_{k-1})), h_{T'}(P_{T'}(r,u_k))) &= (1^2, \ldots, (k-1)^2, k, k+1, \ldots, \ell+1)\\ &\prec^w (1^2, \ldots, (k-1)^2, k^2, k+1, \ldots, \ell)\\ &= (h_T(P_T(r,u_k)), h_T(P_T(r,\tilde{u}_\ell))),\end{aligned}$$

since $k < \ell + 1$. Once more $h(T') \prec^w h(T)$, a contradiction, and we conclude that $T \simeq P_n$. $\square$

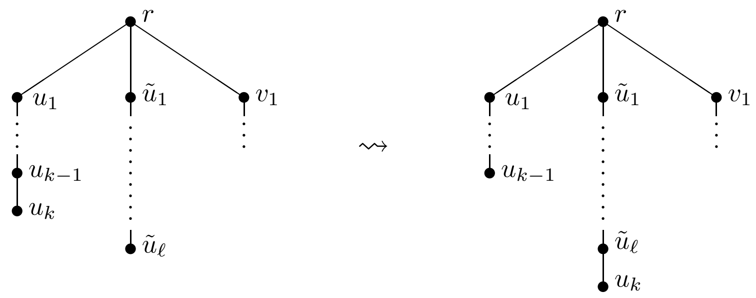

Figure 4.2: Improvement in case $\deg_T(r) \geq 3$

This result can also be proven by induction, see Entringer, Jackson and Snyder [13] or Lovász [22, exercise 6.23].

Note that we have implicitly shown that the edge height multiset $h(P_n)$ of the path P_n rooted at a barycenter is the minimum element in $(\mathcal{H}(n), \preceq^w)$. In fact, we have even proven the stronger result $h(T) \leq h(P_n)$ and $h(T) \neq h(P_n)$ for each $T \in \mathcal{T}(n)$ that is rooted at a barycenter and that is not isomorphic to P_n. This will be important for certain c-weighted distance problems in Chapter 5.

Since the path P_n is also contained in the classes $\mathcal{T}(n, q)$ and $\mathcal{T}_\Delta(n)$, we immediately infer the following results.

Corollary 4.2. *Let $T \in \mathcal{T}(n, q)$ have maximum distance. Then $T \simeq P_n$.*

Corollary 4.3. *Let $T \in \mathcal{T}_\Delta(n)$ have maximum distance. Then $T \simeq P_n$.*

4.2 Degree Sequence and Caterpillars

Consider now the maximum distance problem in the class $\mathcal{T}(\pi)$. First of all we have the following main structural result, which has also been noted by Shi [25]. Recall that a *caterpillar* is a tree T that reduces to a path if all leaves of T are deleted.

Theorem 4.4. *Let π be a tree-graphical partition and let $T \in \mathcal{T}(\pi)$ have maximum distance. Then T is a caterpillar.*

Proof. We may assume that $|\pi| \geq 4$, the other cases being trivial. Let T be rooted at a barycenter r. Then, by Theorem 2.21, $h(T) = h(r, T)$ is a minimal element of the poset $(\mathcal{H}(\pi), \preceq^w)$.

Claim 1. *Any vertex $v \neq r$ has at most one child that is not a leaf of T.*

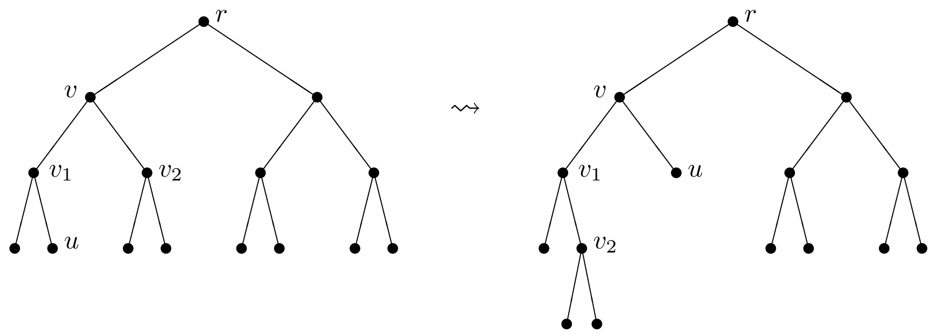

Figure 4.3: An example to Claim 1 with $\pi = (3^6, 2, 1^8)$

Proof. Assume to the contrary that v_1, v_2 are two children of v that are not leaves of T and let $u \neq v_1$ be a leaf of $T(v_1)$, see Figure 4.3. By exchanging $T(v_2)$ and u, we obtain another tree $T' \in \mathcal{T}(\pi)$ with barycenter r. Since the heights of all edges of the path from v to the parent of u in T (containing at least the edge vv_1) have been increased, $h(T)$ is not minimal in $(\mathcal{H}(\pi), \preceq^w)$, a contradiction. $\square$

Claim 2. *The root r has at most two children that are not leaves of T.*

Proof. Assume to the contrary that $u, v, \hat{v}$ are three children of the root r with $|T(\hat{v})| \geq |T(v)| \geq |T(u)| \geq 2$. By Claim 1, each of $T(u)$, $T(v)$ and $T(\hat{v})$ is a caterpillar. If all children of u are leaves, let $\tilde{u}$ be any child of u. Otherwise, let $\tilde{u}$ be the child of u that is not a leaf. Consider now the tree $T' \in \mathcal{T}(\pi)$ that is obtained from T by exchanging the subtrees $T(\tilde{u})$ and $T(v)$, i.e., by deleting the edges $u\tilde{u}$ and rv and by adding uv and $r\tilde{u}$ instead.

If r is still a barycenter of T', we have $h_T(r, ru) < h_{T'}(r, ru) \leq \frac{n}{2}$, see Figure 4.4 for an example. Since $h(r,T)$ and $h(r,T')$ differ only in this edge height, the merging lemma yields $h(r,T') \prec^w h(r,T)$, a contradiction.

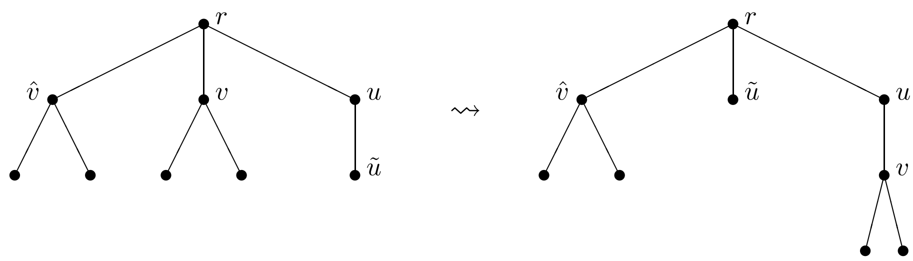

Figure 4.4: First example to Claim 2 with $\pi = (3^3, 2, 1^5)$

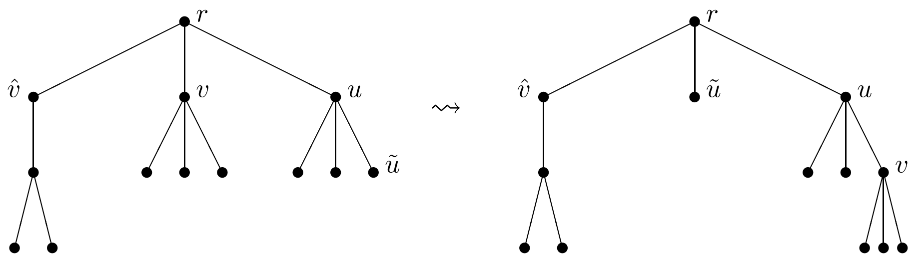

Figure 4.5: Second example to Claim 2 with $\pi = (4^2, 3^2, 2, 1^8)$

If r is no longer a barycenter of T', then $|T(v)| + \deg_T(u) - 1 > \frac{n}{2}$ by Theorem 2.17. By the same reasoning, u is identified as a barycenter of T', see Figure 4.5. Note that $h_T(r, rv) = h_{T'}(u, uv)$, $h_T(r, u\tilde{u}) = h_{T'}(u, r\tilde{u})$ and $h_T(r, e) = h_{T'}(u, e)$ for all edges $e \in (E(T) \cap E(T')) \setminus \{ru\}$. Since $h_T(r, ru) = |T(u)| < |T(\hat{v})| + |T(\tilde{u})| + 1 \leq h_{T'}(u, ru)$, the merging lemma yields $h(u, T') \prec^w h(r, T)$, again a contradiction. $\square$

These two claims immediately imply that T is a caterpillar, completing the proof of the theorem. $\square$

In some special cases, there is only one caterpillar in $\mathcal{T}(\pi)$ and the maximum distance problem is thus settled by the preceding theorem. For instance, the tree-graphical partitions $\pi_k(\Delta) = (\Delta^k, 1^{k(\Delta-2)+2})$ with $k \in \mathbb{N}$ and $\Delta \geq 2$ have this property. Using a different approach, this result has also been given by Fischermann, Hoffmann, Rautenbach, Székely and Volkmann [14].

In general, however, the class $\mathcal{T}(\pi)$ contains many caterpillars. Let us fix some notation and terminology for the remainder of this section. For any tree-graphical partition $\pi = (d_1 \geq d_2 \geq \ldots \geq d_n)$ of length $|\pi| = n \geq 3$, let $s(\pi)$ be defined by

$$s(\pi) = \max\{j : 1 \leq j \leq n,\, d_j > 1\}.$$

The path consisting of the vertices of degree $d_1, \ldots, d_{s(\pi)}$ in a caterpillar $T \in \mathcal{T}(\pi)$ will be called the *spinal path* of T. Obviously, T is completely determined by the arrangement of these degrees on the spinal path. When depicting a caterpillar, a horizontal representation of the spinal path will be chosen and the root (which will always be a barycenter) will be encircled.

Lemma 4.5. *Let π be a tree-graphical partition and let T be a caterpillar that is rooted at a barycenter r and that has maximum distance within the class $\mathcal{T}(\pi)$. Let $rv_1 \ldots v_\ell$ be a subpath of the spinal path of T for some $\ell \geq 2$. Then $\deg_T(v_i) \geq \deg_T(v_{i-1})$ for $2 \leq i \leq \ell$.*

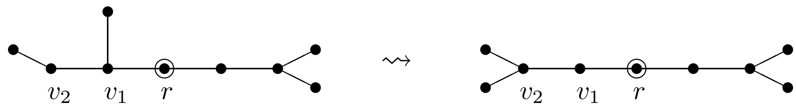

Figure 4.6: An example to Lemma 4.5 with $\pi = (3^2, 2^3, 1^4)$

Proof. Assume that there is an index i with $\delta = \deg_T(v_{i-1}) - \deg_T(v_i) > 0$. By deleting any δ children of v_{i-1} that are leaves in T and by adding them as leaves at v_i instead, we obtain another caterpillar T' in which the degrees of v_{i-1} and v_i have been exchanged, see Figure 4.6. Since r is still a barycenter of T' and since the height of $v_{i-1}v_i$ has been increased, $h(T)$ is not minimal in $(\mathcal{H}(\pi), \preceq^w)$, a contradiction. □

Thus, the trees T having maximum distance within $\mathcal{T}(\pi)$ are contained in the class of those caterpillars in $\mathcal{T}(\pi)$ that fulfill the degree constraints stated in the previous lemma. We denote this class by $\mathcal{C}(\pi)$. Note that, as in the previous section, the proofs of Theorem 4.4 and Lemma 4.5 yield the stronger result $h(T) \leq h(T')$ and $h(T) \neq h(T')$ for $T, T' \in \mathcal{T}(\pi)$ (each rooted at a barycenter) with $T' \in \mathcal{C}(\pi)$ and $T \notin \mathcal{C}(\pi)$.

As before, sometimes an optimal caterpillar can easily be identified within the class $\mathcal{C}(\pi)$. For instance, consider a tree-graphical partition π with $|\pi| = n$ and $d_1 \geq \frac{n}{2}$. Then the vertex of degree d_1 is a barycenter of T. In fact, exactly these partitions yield caterpillars in which the barycenter has only one neighbor that is not a leaf. Consequently, there is only one caterpillar in $\mathcal{C}(\pi)$, namely the one whose sequence of degrees along the spinal path is given by $d_1, d_{s(\pi)}, d_{s(\pi)-1}, \ldots, d_2$. The example $\pi = (7, 3^2, 2, 1^9)$ is depicted in the left picture of Figure 4.7. This example also indicates that the barycenter of an optimal caterpillar need not have degree $d_{s(\pi)}$.

The last observation remains true even if the barycenter r of an optimal caterpillar in $\mathcal{C}(\pi)$ has two neighbors u, v that are not leaves, see the example given in the right picture of Figure 4.7. By applying the usual technique of exchanging certain subtrees, it can be proven that in this case we either

Figure 4.7: Optimal caterpillars with $\pi = (7, 3^2, 2, 1^9)$ and $\pi = (5^3, 3, 2, 1^{12})$

have $\deg_T(r) = d_{s(\pi)}$ or $d_{s(\pi)} = \deg_T(u) < \deg_T(r) \le \deg_T(v)$ in an optimal caterpillar T. Further minor results of the same type could also be deduced. We do not go into detail here, since it is a priori difficult to predict the position of the barycenter on the spinal path, and hence these results do not help much to determine the optimal trees.

Recalling our approach, we are left with the problem of determining the caterpillars in $\mathcal{C}(\pi)$ whose edge height multiset is a minimal element in the poset $(\mathcal{H}(\pi), \preceq^w)$. For a tree-graphical partition $\pi = (d_1 \ge d_2 \ge \ldots \ge d_n)$ of length $n \ge 3$ and a fixed caterpillar $T \in \mathcal{C}(\pi)$ rooted at a barycenter r, the edge height multiset $h(T) = h(r, T)$ is easily constructed. First of all there is the term $1^{n-s(\pi)}$, corresponding to the $n - s(\pi)$ edges that are incident to leaves of T. The remaining terms of $h(T)$ are derived by moving from both endvertices of the spinal path towards the barycenter, thereby successively scanning the vertices of degree $d_1, d_2, \ldots, d_{s(\pi)}$ and collecting their contribution to the heights of the edges on the spinal path. With this consideration and Lemma 4.5 in mind, we can give an algorithm for constructing a minimal element of $(\mathcal{H}(\pi), \preceq^w)$.

Algorithm *Min_$\mathcal{H}$*(π)
Input: A tree-graphical partition $\pi = (d_1 \ge d_2 \ge \ldots \ge d_n)$ with $n \ge 3$
Output: A multiset $h^*(\pi)$

$s_1 \leftarrow d_1$
$s_2 \leftarrow 1$
$h^*(\pi) \leftarrow (1^{n-s(\pi)})$
for $i = 2$ **to** $s(\pi)$ **do**
    if $s_1 \le s_2$ **then** $s_1 \leftarrow s_1 + d_i - 1$ **else** $s_2 \leftarrow s_2 + d_i - 1$
    $h^*(\pi) \leftarrow (h^*(\pi), \min(s_1, s_2))$

It is convenient to think of s_1 and s_2 as two stacks that are built during the execution of the algorithm. Note that

$$1 + d_1 + \sum_{i=2}^{s(\pi)} (d_i - 1) = 2 + \sum_{i=1}^{n} (d_i - 1) = 2 + 2n - 2 - n = n$$

and thus we always have $\min(s_1, s_2) \le \frac{n}{2}$. In particular, at the termination of the algorithm either $\max(s_1, s_2) > \frac{n}{2} > \min(s_1, s_2)$ or $s_1 = s_2 = \frac{n}{2}$, corresponding to the cases of one and two barycenters, see Theorem 2.17.

Lemma 4.6. *Let $\pi = (d_1 \ge d_2 \ge \ldots \ge d_n)$ be a tree-graphical partition of length $n \ge 3$. Then the multiset $h^*(\pi)$ constructed by algorithm Min_$\mathcal{H}(\pi)$ is a minimal element in $(\mathcal{H}(\pi), \preceq^w)$.*

Proof. Following the steps of the algorithm, a caterpillar $T \in \mathcal{C}(\pi)$ that is rooted at a barycenter and that has $h^*(\pi)$ as its edge height multiset is easily constructed. This construction process is also depicted in Figure 4.9 for the example $\pi = (5, 3^3, 2^2, 1^8)$.

Thus $h^*(\pi) \in \mathcal{H}(\pi)$ and it remains to show that $h^*(\pi)$ is minimal in $(\mathcal{H}(\pi), \preceq^w)$. This will be done by induction on $s(\pi)$. The cases $s(\pi) \leq 2$ are trivial, since there is only one tree (and hence only one caterpillar) in $\mathcal{T}(\pi)$.

Assume now that $s(\pi) \geq 3$. Let $d = d_{s(\pi)}$ and let m denote the last term that is added to $h^*(\pi)$, i.e., $m = \min(s_1, s_2)$ at the end of the iteration $i = s(\pi)$. Let π' denote the tree-graphical partition that is derived from π by deleting the terms d and 1^{d-2}. Then $s(\pi') = s(\pi) - 1$, $n' = |\pi'| = n - (d-1)$ and $h^*(\pi) = (h^*(\pi'), 1^{d-2}, m)$.

As already remarked above, any multiset in $\mathcal{H}(\pi)$ necessarily contains the term $(1^{n-s(\pi)}) = (1^{n'-s(\pi')}, 1^{d-2})$. Since $h^*(\pi')$ is a minimal element of $(\mathcal{H}(\pi'), \preceq^w)$ by induction and m is easily seen to be maximum in view of the final values s_1', s_2' of the stacks after the execution of *Min_*$\mathcal{H}(\pi')$, we conclude that $h^*(\pi)$ is minimal in $(\mathcal{H}(\pi), \preceq^w)$. □

The multiset $h^*(\pi)$ may well be realizable by several caterpillars in $\mathcal{C}(\pi)$. Indeed, in each iteration i of *Min_*$\mathcal{H}(\pi)$ in which the stacks s_1, s_2 are equal, we are free to add a vertex of degree d_i to either side of the spinal path, thereby possibly producing non-isomorphic caterpillars. For instance, in case of $\pi = (5, 3^3, 2^2, 1^8)$ with $h^*(\pi) = (1^8, 3, 5^2, 6, 7)$, we obtain the two caterpillars depicted in Figure 4.8, following the construction shown in Figure 4.9. As indicated, both trees have two barycenters. It is easily checked that $h^*(\pi)$ is the minimum element in $(\mathcal{H}(\pi), \preceq^w)$ and thus these non-isomorphic caterpillars have maximum distance in $\mathcal{T}(\pi)$.

At first sight, it may be tempting to conjecture that $h^*(\pi)$ is not only a minimal, but always the minimum element of $(\mathcal{H}(\pi), \preceq^w)$. However, this is not true, as will be shown in our final example. Consider the tree-graphical partitions $\pi_k = (9, 7^2, 6^2, 2^k, 1^{27})$ of length $32 + k$ for $k = 1, 2, 3$. Figure 4.10 shows three pairs $T_1(\pi_k), T_2(\pi_k)$ of caterpillars in $\mathcal{T}(\pi_k)$. Each tree is rooted at a barycenter (note that $T_2(\pi_2)$ has two barycenters) and the edge height multisets $h_{i,k} = h(T_i(\pi_k))$ for $i = 1, 2$ and $k = 1, 2, 3$ are given by

$$\begin{aligned} h_{1,1} &= (1^{27}, 7, 9, 13, 14, 15), & h_{2,1} &= (1^{27}, 7, 9, 12, 15, 16), \\ h_{1,2} &= (1^{27}, 7, 9, 13, 14, 15, 16), & h_{2,2} &= (1^{27}, 7, 9, 12, 15, 16, 17), \\ h_{1,3} &= (1^{27}, 7, 9, 13, 14, 15, 16, 17), & h_{2,3} &= (1^{27}, 7, 9, 12, 15, 16, 17^2). \end{aligned}$$

Note that $h_{1,k} = h^*(\pi_k)$ for $k = 1, 2, 3$ and that $h_{1,k}$ and $h_{2,k}$ are incomparable in the superdominance order. Indeed, the multiset $h_{2,k}$ is easily identified as

Figure 4.8: Non-isomorphic optimal caterpillars with $\pi = (5, 3^3, 2^2, 1^8)$

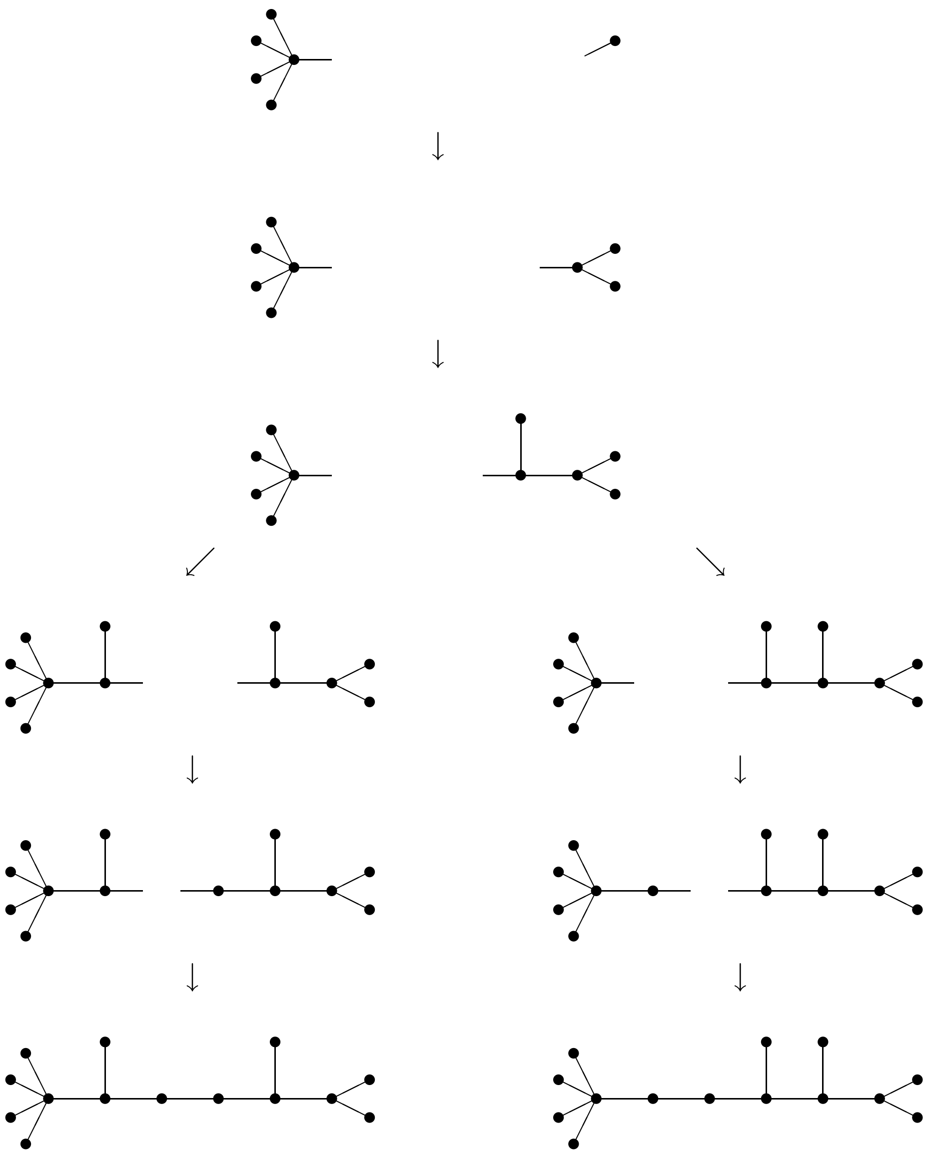

Figure 4.9: Construction of the non-isomorphic caterpillars of Figure 4.8

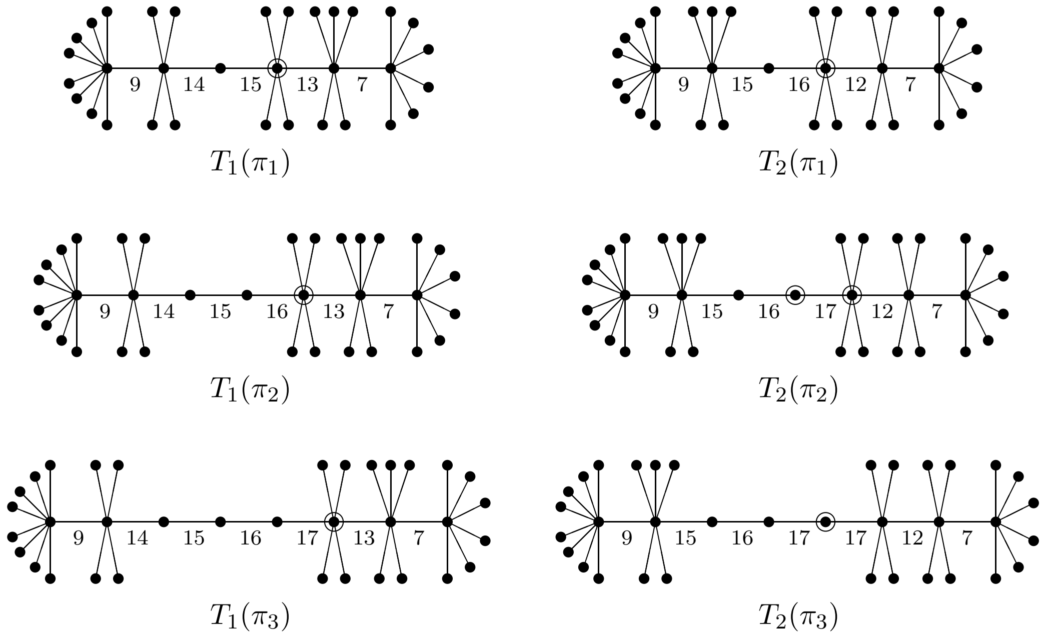

Figure 4.10: Pairs of caterpillars with $\pi_k = (9, 7^2, 6^2, 2^k, 1^{27})$ for $k = 1, 2, 3$

a minimal element of the poset $(\mathcal{H}(\pi_k), \preceq^w)$ for $k = 1, 2, 3$. Now, by applying formula (2.11) for the distance of trees, we obtain

$$\begin{aligned}
\sigma(T_1(\pi_1)) &> \sigma(T_2(\pi_1)), \quad \text{since} \quad g_{33}(13) + g_{33}(14) > g_{33}(12) + g_{33}(16),\\
\sigma(T_1(\pi_2)) &= \sigma(T_2(\pi_2)), \quad \text{since} \quad g_{34}(13) + g_{34}(14) = g_{34}(12) + g_{34}(17),\\
\sigma(T_1(\pi_3)) &< \sigma(T_2(\pi_3)), \quad \text{since} \quad g_{35}(13) + g_{35}(14) < g_{35}(12) + g_{35}(17),
\end{aligned}$$

and the trees $T_1(\pi_1)$, $T_1(\pi_2)$, $T_2(\pi_2)$ and $T_2(\pi_3)$ are easily seen to have maximum distance in $\mathcal{T}(\pi_k)$ respectively.

Summarizing these results, we conclude that there may be several minimal elements in $(\mathcal{H}(\pi), \preceq^w)$ and that not all of them may correspond to a caterpillar having maximum distance in $\mathcal{T}(\pi)$. In particular, a caterpillar with edge height multiset $h^*(\pi)$ need not be optimal, and the optimal caterpillars are not necessarily unique. These phenomena and results reveal the limitations of our approach in case of the maximum distance problem in $\mathcal{T}(\pi)$.

Chapter 5

Weighted Distance of Trees

This final chapter is devoted to two kinds of weighted distance problems in trees. The main part, consisting of the first two sections, deals with the trees that have minimum and maximum c-weighted distance in the usual four subclasses of $\mathcal{T}(n)$. In the third section the trees having an extremal degree distance are characterized. Both these weighted distance problems can be reduced to the simpler unweighted problem treated before.

5.1 Minimum c-Weighted Distance

The general framework for the minimum c-weighted distance problem has been introduced in Section 2.4. Recall that we are given a subclass $\mathcal{T}$ of $\mathcal{T}(n)$ and an $(n-1)$-multiset $c = (c_1, c_2, \ldots, c_{n-1})$ of edge weights. We ask for a tree $T \in \mathcal{T}$ and a c-valuation γ of T such that $\sigma_\gamma(T)$ is minimum. If $T = (V, E)$ is rooted at a barycenter r, then $\sigma_\gamma(T)$ is given by

$$\sigma_\gamma(T) = \sum_{e \in E} \gamma(e)\, g_n(h(e)).$$

For a fixed tree T, we already know that the minimum value $\sigma_{\min}(T, c)$ of $\sigma_\gamma(T)$ is obtained if the multisets $g_n[h(T)] = (g_n(h(e)))_{e \in E}$ and c are oppositely ordered, see Corollary 2.23. Since the parabola g_n is strictly increasing on the interval $[0, \frac{n}{2}]$, the multisets $h(T)$ and c can also be assumed to be oppositely ordered. In other words, $\sigma_{\min}(T, c)$ is obtained if the smallest (largest) weights are assigned to the edges with the largest (smallest) heights in T.

Thus, in order to solve the minimum c-weighted distance problem, all that remains is to get a clear idea of the relation between $\sigma_{\min}(T_1, c)$ and $\sigma_{\min}(T_2, c)$ for trees T_1 and T_2 from the class $\mathcal{T}$. In case of non-negative weights, the answer is given by Theorem 2.10.

Theorem 5.1. *Let $\mathcal{T}$ be a subclass of $\mathcal{T}(n)$ and let $T_i \in \mathcal{T}$ be rooted at a barycenter r_i for $i = 1, 2$. Let c be an $(n-1)$-multiset of non-negative edge weights and assume that $h(T_1) = h(r_1, T_1) \preceq^w h(r_2, T_2) = h(T_2)$. Then $\sigma_{\min}(T_2, c) \leq \sigma_{\min}(T_1, c)$.*

Proof. We may assume that the multisets $g_n[h(T_i)]$ are arranged in decreasing order for $i = 1, 2$ and that c is given in increasing order $c = (c_1 \leq \ldots \leq c_{n-1})$. Then, with $\psi_c(z) = c \cdot z$ as in Section 2.1,

$$\sigma_{\min}(T_i, c) = c \cdot g_n[h(T_i)] = \psi_c(g_n[h(T_i)]) \quad \text{for } i = 1, 2.$$

Now $h(T_1) \preceq^w h(T_2)$ implies

$$g_n[h(T_1)] \preceq^w g_n[h(T_2)] \tag{5.1}$$

by Theorem 2.6, and thus, by Theorem 2.10,

$$\sigma_{\min}(T_2, c) = \psi_c(g_n[h(T_2)]) \leq \psi_c(g_n[h(T_1)]) = \sigma_{\min}(T_1, c), \tag{5.2}$$

completing the proof. □

Obviously, one or more edge weights of value 0 have a big impact on our optimization problem as there can be equality in (5.2) even if T_1 and T_2 are not isomorphic or if $h(T_1) \prec^w h(T_2)$. In the more interesting case of positive weights, a stronger result can be obtained.

Corollary 5.2. *Let $\mathcal{T}$ be a subclass of $\mathcal{T}(n)$ and let $T_i \in \mathcal{T}$ be rooted at a barycenter r_i for $i = 1, 2$. Let c be an $(n-1)$-multiset of positive edge weights and assume that $h(T_1) = h(r_1, T_1) \prec^w h(r_2, T_2) = h(T_2)$. Then $\sigma_{\min}(T_2, c) < \sigma_{\min}(T_1, c)$.*

Proof. As in the previous proof, we may assume that the multisets $g_n[h(T_i)]$ are arranged decreasingly for $i = 1, 2$ and that c is arranged increasingly. Since $h(T_1) \prec^w h(T_2)$, Corollary 2.7 implies that $\preceq^w$ is replaced by $\prec^w$ in (5.1) and Corollary 2.5 yields

$$\sigma(T_2) = \Sigma(g_n[h(T_2)]) < \Sigma(g_n[h(T_1)]) = \sigma(T_1).$$

Since all weights are positive, all the assumptions of Corollary 2.11 are fulfilled and strict inequality in (5.2) is deduced. □

Consequently, the minimum c-weighted distance problem with positive edge weights is basically the same as the unweighted minimum distance problem treated in Chapter 3, and we deduce the following result.

Theorem 5.3. *Let c be an $(n-1)$-multiset of positive edge weights. Then the trees $K_{1,n-1}$, $T^*_{q+1}(n)$, $T^*_\Delta(n)$ and $T^*(\pi)$ are the unique trees that have minimum c-weighted distance within the classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$, $\mathcal{T}_\Delta(n)$ and $\mathcal{T}(\pi)$ respectively. In each case the weights have to be assigned to the edges according to Corollary 2.23, i.e., the multisets c and $g_n[h(\cdot)]$ have to be oppositely ordered.*

Clearly, there may still be some choice in how to assign different weights to edges of the same height, see Figure 5.1 for an example from the class $\mathcal{T}(\pi)$ with $\pi = (3^3, 2^3, 1^5)$, $h(T^*(\pi)) = (5, 3, 2^3, 1^5)$ and $c = (7^7, 6^3)$.

Not surprisingly, there is a dual version of Theorem 5.3 in case of multisets c consisting of only negative weights and the search for trees having maximum c-weighted distance.

Corollary 5.4. *Let c be an $(n-1)$-multiset of negative edge weights. Then the trees $K_{1,n-1}$, $T^*_{q+1}(n)$, $T^*_\Delta(n)$ and $T^*(\pi)$ are the unique trees that have maximum c-weighted distance within the classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$, $\mathcal{T}_\Delta(n)$ and $\mathcal{T}(\pi)$ respectively. In each case the weights have to be assigned to the edges according to Corollary 2.23, i.e., the multisets c and $g_n[h(\cdot)]$ have to be similarly ordered.*

Proof. Let $\hat{c} = (\hat{c}_i)_{i=1,\dots,n-1}$ denote the multiset defined by $\hat{c}_i = -c_i$ for $1 \le i \le n-1$ and take any tree $T \in \mathcal{T}(n)$ rooted at a barycenter. If c and $g_n[h(T)]$ are similarly ordered, $\hat{c}$ and $g_n[h(T)]$ are oppositely ordered and hence

$$\sigma_{\max}(T, c) = c \cdot g_n[h(T)] = -\,\hat{c} \cdot g_n[h(T)] = -\sigma_{\min}(T, \hat{c}).$$

Since $\hat{c}$ is a multiset of positive edge weights, the result follows from the preceding theorem. $\square$

With Corollary 5.4 just proven, it is obvious that a result on minimum c-weighted distance with negative weights will be derived as a dual version

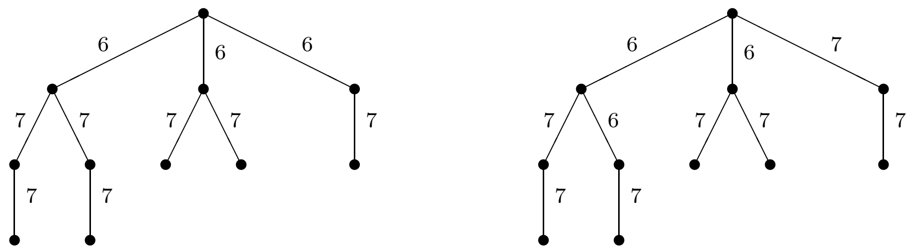

Figure 5.1: Minimum c-weighted trees with $\pi = (3^3, 2^3, 1^5)$ and $c = (7^7, 6^3)$

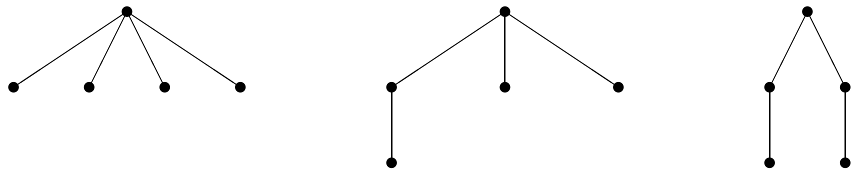

Figure 5.2: The non-isomorphic trees $K_{1,4}$, $T^\diamond$ and P_5 in $\mathcal{T}(5)$

from the solution to the maximum c-weighted distance problem with positive weights, see Corollary 5.8 in the next section.

Thus we are left with the case of multisets c consisting of both positive and negative edge weights. This is a quite complex problem and not much can be said in general, since now the structure of the optimal trees depends on c. In particular, an optimal tree need not be a tree having minimum distance any more. A simple example can already be given in the class $\mathcal{T}(5)$ consisting of the three non-isomorphic trees $K_{1,4}$, $T^\diamond$ and P_5 depicted in Figure 5.2. As indicated, each tree is rooted at a barycenter. It is easily verified that

$$g_5[h(K_{1,4})] = (4^4), \quad g_5[h(T^\diamond)] = (6, 4^3) \text{ and } g_5[h(P_5)] = (6^2, 4^2),$$

such that, for instance, the path P_5 has minimum c-weighted distance for $c = (-2, -1, 1^2)$, while $T^\diamond$ is the optimal tree for $c = (-1, 1^3)$.

5.2 Maximum c-Weighted Distance

Turning to maximum c-weighted distance problems, Corollary 2.23 implies that, for a fixed tree T of order n, the multisets c and $g_n[h(T)]$ have to be similarly ordered to obtain the maximal possible value $\sigma_{\max}(T, c)$ of $\sigma_\gamma(T)$. In other words, now the smallest (largest) weights have to be assigned to the edges with the smallest (largest) heights in T.

We have already settled the maximum c-weighted distance problem for multisets containing only negative weights in Corollary 5.4. The case of both positive and negative weights is as complex as in the minimization problem and is not pursued any further.

Thus it remains to consider a multiset c of non-negative edge weights. As remarked in Section 2.1, we do not have a result analogous to Theorem 2.10 and Corollary 2.11 for multisets c and $g_n[h(T)]$ that are similarly ordered. Consequently, the usual approach involving the superdominance order does not work here. Nonetheless, the proofs given in Chapter 4 can be combined with the elementwise vector ordering and with Lemma 2.12 to yield results similar to Theorem 5.1 and Corollary 5.2.

Theorem 5.5. *Let $T \in \mathcal{T}(n)$ and let c be an $(n-1)$-multiset of non-negative edge weights. Then $\sigma_{\max}(T, c) \le \sigma_{\max}(P_n, c)$ and this inequality is strict if all edge weights are positive and $T \not\simeq P_n$.*

Proof. Assume that $T \not\simeq P_n$ and let both T and P_n be rooted at a barycenter. Then

$$h(T) \le h(P_n) \quad \text{and} \quad h(T) \ne h(P_n), \tag{5.3}$$

see the remark following the proof of Theorem 4.1. Since g_n is strictly increasing on the interval $[0, \frac{n}{2}]$, this implies

$$g_n[h(T)] \le g_n[h(P_n)] \quad \text{and} \quad g_n[h(T)] \ne g_n[h(P_n)].$$

Let $g_n[h(T)]$, $g_n[h(P_n)]$ and c be arranged decreasingly. By Lemma 2.12,

$$\sigma_{\max}(T, c) = c \cdot g_n[h(T)] \le c \cdot g_n[h(P_n)] = \sigma_{\max}(P_n, c),$$

and this inequality is strict if all weights are positive. □

Theorem 5.6. *Let π be a tree-graphical partition of length n and let c be an $(n-1)$-multiset of non-negative edge weights. Assume that T, T' are trees in $\mathcal{T}(\pi)$ with $T' \in \mathcal{C}(\pi)$ and $T \notin \mathcal{C}(\pi)$. Then $\sigma_{\max}(T, c) \le \sigma_{\max}(T', c)$ and this inequality is strict if all edge weights are positive.*

Proof. This is proven along the same lines as the previous theorem. Just note that (5.3) is replaced by $h(T) \le h(T')$ and $h(T) \ne h(T')$, see the remark following Lemma 4.5. □

Thus, there is no great difference between the maximum c-weighted distance problem with positive edge weights and the corresponding unweighted problem, and we can summarize our previous results as follows.

Theorem 5.7. *Let c be an $(n-1)$-multiset of positive edge weights. Then the path P_n is the unique tree that has maximum c-weighted distance within the classes $\mathcal{T}(n)$, $\mathcal{T}(n, q)$ and $\mathcal{T}_\Delta(n)$. In case of the class $\mathcal{T}(\pi)$, the trees having maximum c-weighted distance can be found in the same class $\mathcal{C}(\pi)$ of caterpillars as the trees having maximum distance. In each case the weights have to be assigned to the edges according to Corollary 2.23, i.e., the multisets c and $g_n[h(\cdot)]$ have to be similarly ordered.*

Once again, an optimal c-valuation of an optimal tree need not be unique, as shown in Figure 5.3 for the path P_5 with $g_5[h(P_5)] = (6^2, 4^2)$ and weights $c = (4, 3, 2, 1)$.

In case of the class $\mathcal{T}(\pi)$ and its subclass $\mathcal{C}(\pi)$, we have already seen in Section 4.2 that the caterpillars having maximum distance need not be

Figure 5.3: Maximum c-weighted paths P_5 with $c = (4, 3, 2, 1)$

unique and that not every caterpillar in $\mathcal{C}(\pi)$ yields an optimal tree. Thus it is not surprising that the optimal structure of a caterpillar having maximum c-weighted distance also depends on c. In particular, a caterpillar having maximum distance need not have maximum c-weighted distance for all multisets c of positive edge weights. For instance, consider the tree-graphical partition $\pi = (9, 7^2, 6^2, 2, 1^{27})$ of length 33 and the two caterpillars $T_1(\pi)$ and $T_2(\pi)$ depicted in Figure 5.4. These trees, as usual rooted at a barycenter, have been studied in the last example in Chapter 4, with $T_1(\pi)$ being identified as the unique tree having maximum distance in $\mathcal{T}(\pi)$. Recall that the edge height multisets are given by

$$h(T_1(\pi)) = (15, 14, 13, 9, 7, 1^{27}), \qquad h(T_2(\pi)) = (16, 15, 12, 9, 7, 1^{27}),$$

and thus

$$g_{33}[h(T_1(\pi))] = (270, 266, 260, 216, 182, 32^{27})$$

and

$$g_{33}[h(T_2(\pi))] = (272, 270, 252, 216, 182, 32^{27}).$$

The class $\mathcal{C}(\pi)$ contains more than these two caterpillars, but, using the idea underlying the proof of Theorem 5.6, it is easily seen that only $T_1(\pi)$ and $T_2(\pi)$ can occur as trees having maximum c-weighted distance in case of positive edge weights. Consider now the multisets $c_\lambda = (\lambda, 1^{31})$ for $\lambda \geq 1$. Then

$$\sigma_{\max}(T_1(\pi), c_\lambda) - \sigma_{\max}(T_2(\pi), c_\lambda) = 270\lambda + 526 - 272\lambda - 522 = 4 - 2\lambda$$

and thus $T_1(\pi)$ is the unique tree that has maximum c_λ-weighted distance in $\mathcal{T}(\pi)$ for $\lambda \in [1, 2)$, while $T_2(\pi)$ is optimal for $\lambda > 2$. For $\lambda = 2$, both trees have maximum c_2-weighted distance.

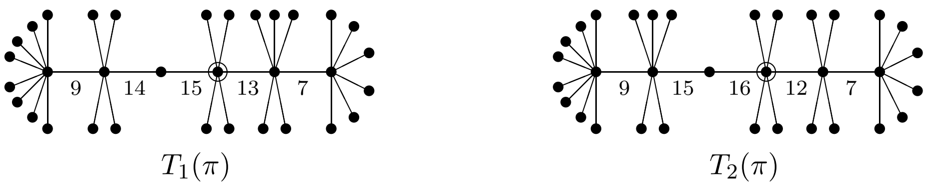

Figure 5.4: Two caterpillars in $\mathcal{C}(\pi)$ with $\pi = (9, 7^2, 6^2, 2, 1^{27})$

To close this section, let us state the dual version of Theorem 5.7. This result provides a partial solution to the remaining minimum c-weighted distance problem of Section 5.1.

Corollary 5.8. *Let c be an $(n-1)$-multiset of negative edge weights. Then the path P_n is the unique tree that has minimum c-weighted distance within the classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$ and $\mathcal{T}_\Delta(n)$. In case of the class $\mathcal{T}(\pi)$, the trees having minimum c-weighted distance can be found within the class $\mathcal{C}(\pi)$. In each case the weights have to be assigned to the edges according to Corollary 2.23, i.e., the multisets c and $g_n[h(\cdot)]$ have to be oppositely ordered.*

5.3 Degree Distance

In this final section we briefly discuss another weighted distance problem in trees. The distance of a tree has found numerous applications in chemistry and several extensions have been introduced in recent years, among them the *Schultz index*. The main part of this invariant consists of the sum

$$\sigma_{\deg}(T) = \sum_{v \in V} \deg_T(v)\, \sigma_T(v),$$

which is called the *degree distance* of T. Recall from (2.9) that the distance of T can be computed as

$$\sigma(T) = \tfrac{1}{2} \sum_{v \in V} \sigma_T(v) = \tfrac{1}{2} \sum_{v \in V} 1 \cdot \sigma_T(v).$$

As indicated, this equation can be considered to be a sum of the distances of the vertices of T with unit weights. In this sense, $\sigma_{\deg}(T)$ is another weighted distance in trees, this time using the degrees of the vertices as weights. The following result shows that the distance and the degree distance of a tree are closely related, see e.g. Dobrynin and Gutman [9] for a proof.

Theorem 5.9. *Let T be a tree of order n. Then $\sigma(T) = \frac{1}{4}[n(n-1) + \sigma_{\deg}(T)]$.*

Consequently, the optimization problems for $\sigma(T)$ and $\sigma_{\deg}(T)$ are identical in every subclass of $\mathcal{T}(n)$.

Theorem 5.10. *The trees $K_{1,n-1}$, $T^*_{q+1}(n)$, $T^*_\Delta(n)$ and $T^*(\pi)$ are the unique trees that have minimum degree distance within the classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$, $\mathcal{T}_\Delta(n)$ and $\mathcal{T}(\pi)$ respectively. The path P_n is the unique tree that has maximum degree distance in the classes $\mathcal{T}(n)$, $\mathcal{T}(n,q)$ and $\mathcal{T}_\Delta(n)$. In case of $\mathcal{T}(\pi)$, the trees having maximum degree distance are those having maximum distance. They are contained in the class $\mathcal{C}(\pi)$.*

Further results on the degree distance can be found in Tomescu [27].

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