Combinatorial Optimization with One Quadratic Term

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Zusammenfassung

Diese Arbeit befasst sich mit einer neuen Herangehensweise für binäre kombinatorische Optimierungsprobleme. Die wesentliche Idee hierbei ist, die Anzahl der quadratischen Terme in der Zielfunktion auf einen einzigen zu beschränken, und das durch eine Linearisierung entstehende Polyeder zu analysieren.

Für diesen Ansatz gibt es mehrere Motivationsgründe. Im Allgemeinen ist das ursprüngliche Problem mit beliebig vielen quadratischen Termen NP-schwer. Doch obwohl eine gute polyedrische Beschreibung mit schnellen Separierungsroutinen die Optimierung in einem Branch-and-Cut-Verfahren signifikant beschleunigen könnte, gibt es bislang nur wenige Erkenntnisse zur polyedrischen Struktur des binären quadratischen Optimierungsproblems. Betrachtet man das reduzierte Problem mit einem quadratischen Term, dann ist eine effiziente Optimierung möglich, falls die zugrundeliegende lineare Version effizient lösbar ist. Somit können hier auch die facettendefinierenden Ungleichungen effizient separiert werden. Darüberhinaus bleiben alle zulässigen Ungleichungen des reduzierten Problems zulässig für das ursprüngliche Problem. In Kombination bedeutet dies, dass Erkenntnisse zur Facettenstruktur des Problems mit einem quadratischen Term direkt zu einer verbesserten polyedrische Beschreibung des Ursprungsproblems führen.

Für eine praktische Anwendung dieses theoretischen Ansatzes betrachten wir verschiedene konkrete Optimierungsprobleme mit einem quadratischen Term und analysieren deren jeweilige polyedrische Struktur, die sich nach der Linearisierung ergibt. Konkret betrachten wir das Minimale Spannwald- und das Minimale Spannbaumproblem, das Minimale Branching- und das Minimale Arboreszenzproblem, das Minimale Assignmentproblem und das Maximale Matchingproblem. Für jedes dieser Optimierungsprobleme leiten wir neue Klassen von facettendefinierenden Ungleichungen her. Außerdem präsentieren wir für das Minimale Spannwald- und das Minimale Spannbaumproblem eine vollständige Beschreibung der jeweiligen Polytope. Für die verwandten gerichteten Probleme, das Minimale Branching- und das Minimale Arboreszenzproblem, zeigen wir zwar einerseits einige Gemeinsamkeiten mit den ungerichteten Problemen, andererseits aber auch, dass sich die polyedrischen Strukturen im gerichteten Fall durch die zusätzlichen Gradbedingungen deutlich verkomplizieren. Bei der Untersuchung des Minimalen Assignmentproblems mit einem quadratischen Term stellen wir nicht nur die Vermutung über die vollständige polyedrische Beschreibung auf, sondern kommen insbesondere zu der überraschenden Erkenntnis, dass bereits ein einziger quadratischer Term genügen kann, um die Anzahl der Facetten von polynomiell auf exponentiell zu erhöhen. Die größte Vielfalt an Facettenklassen leiten wir für das Polyeder des Maximalen Matchingproblems mit einem quadratischen Term her. Wir zeigen jedoch auch, dass diese noch nicht genügen, um die vollständige Beschreibung des Polyeders zu erhalten. Da die meisten der hergeleiteten Facettenklassen von exponentieller Größe sind, leiten wir verschiedene Routinen für eine polynomielle Separierung her. Unsere exemplarischen Rechenergebnisse für das quadratische Minimale Spannwald- und das quadratische Minimale Spannbaumproblem zeigen die praktische Relevanz unseres Ansatzes.

Abstract

This thesis deals with a new approach to tackle binary combinatorial optimization problems. Generally speaking, the idea is to reduce the number of quadratic terms in the objective function to one single, and to analyze the polyhedron which is obtained after a linearization of the quadratic term.

This approach is motivated by several reasons. The original problem with arbitrarily many quadratic terms is NP-hard in general, but although a good polyhedral description with fast separation routines could significantly speed up the optimization when using branch-and-cut algorithms, there is only few information about polyhedral structures so far. Considering the reduced problem with one quadratic term, an efficient optimization is possible if the underlying linear version is tractable. Thus, an efficient separation of the facet defining inequalities is possible in theory. Furthermore, all inequalities which are valid for the reduced problem remain valid for the original problem. In combination, the investigation of the facetial structure of the reduced problem with one quadratic term can yield a better polyhedral description of the original problem.

For a practical usage of such a theoretical approach we consider several specific optimization problems with one quadratic term and analyze their polyhedral structure after linearization. In particular, we consider the minimum spanning forest and the minimum spanning tree, the minimum branching and the minimum arborescence problem, and the minimum assignment and the maximum matching problem. For each of these problems we determine several classes of facet defining inequalities. Furthermore, for the minimum spanning forest and the minimum spanning tree problem, we present a complete description of the corresponding polytopes. For the strongly related minimum branching and the minimum arborescence problem we show on the one hand several similarities, but on the other hand we also have to state that the polyhedral structure becomes much more complicated due to directedness of the edges requiring the degree constraints. When considering the minimum assignment problem with one quadratic term we not only make a conjecture about the complete description but also discover that one single quadratic term can suffice to increase the number of facets from polynomial to exponential. For the polyhedron of the maximum matching problem with one linearized quadratic term we determine the greatest variety of facet classes but however show that they still do not suffice for a complete description. Since most of the derived facet classes are of exponential size, we propose different routines for a polynomial time separation. Our exemplary computational results on the quadratic minimum spanning forest and the quadratic minimum spanning tree problem show the practical relevance of our approach.

Contents

Introduction

Combinatorial optimization problems aim at finding an optimal solution with respect to a given objective function, where the discrete set of feasible solutions is finite. Typically, the solution set is too large for an exhaustive search, such that common solution methods are based on polyhedral or combinatorial approaches.

One famous combinatorial optimization problem is the minimum spanning tree problem. Here, a given set of points has to be connected such that no cycle is closed and such that the solution is minimal with respect to a given linear objective function. The minimum spanning tree problem appears in many practical applications, especially in the wide field of network design, such as telecommunication, internet and transport networks, electrical grids, and many others. When planning an electrical grid, the power station has to be connected with all places to which energy needs to be transported. The costs mainly depend on the length of the cables, such that the objective is to minimize the total length of cables under the restriction that all places are connected with each other and that no cycles are closed.

Now consider the situation that the combination of two electric cables induces additional costs. If, for instance, local conditions necessitate transmission lines to change from over- to underground in some places, supplementary costs occur in any such case. The changeover from one to another cable can be modeled by a quadratic term, such that the supplementary cost only appears in the model if both cables are chosen in the solution. The resulting optimization problem is a minimum spanning tree problem with quadratic terms in the objective function, thus called quadratic minimum spanning tree problem. Since all variables in the model are binary, it belongs to the class of binary quadratic optimization problems.

There are many other practical applications which can be modeled by a binary quadratic optimization problem. Considering networks for oil or water transmission, including changeover costs for different kinds of pipes, the flow direction has to be respected in the model, which leads to a quadratic minimum arborescence problem, the directed version of the quadratic minimum spanning tree problem. One of the most famous binary quadratic optimization problems is the quadratic assignment problem. Here, the optimal allocation of facilities to locations is desired, where construction costs and costs for transferring goods between the facilities determine the quality of a solution. The problem of the transportation itself, where additional costs occur if the conveyance is changed e. g. from truck to train, can be modeled by the quadratic spanning tree problem, or, if a round trip is planned, by the quadratic traveling salesman problem.

Unfortunately, as wide as the range of applications is, as high is the problem complexity. Since binary quadratic optimization problems are NP-hard in general, there exist particular problems of small dimension which are not exactly solvable in reasonable computation times, even if the solution method is well custom-tailored. The high complexity has two reasons, the quadratic objective as well as the binarity of the variables. Standard approaches to overcome these difficulties are a linearization of the quadratic terms and a relaxation of the binarity, but unfortunately this typically results in non-integral solutions. Branch-and-bound algorithms provide a remedy by iteratively excluding fractional solutions, but the runtime of such algorithms highly depends on the quality of the initial polyhedral description or on separation routines. The aim of this thesis is to extend such polyhedral knowledge in order to provide new tools for the optimization of binary quadratic problems.

Due to the problem complexity it is impossible to identify a polynomial time separation algorithm for the complete polyhedral description. Thus, we tackle the problem from another direction, which to the best of our knowledge was not investigated so far. The basic idea is to reduce the number of quadratic terms in the objective function to one, linearize the problem and investigate the resulting polyhedron. This approach is motivated by a combination of two facts. On the one hand, if the underlying linear problem is polynomially solvable, this is also the case when one quadratic term is added to the objective function, which allows integral polyhedral descriptions with polynomial time separation routines. On the other hand, all valid inequalities for this problem remain valid for the original quadratic problem, such that the gained information also improves the polyhedral description of the latter.

Considering binary quadratic optimization problems in general, it is possible to formulate a complete description and a generic separation approach. This, however, is much too general for specific optimization problems and practical applications. This provides the main motivation of this thesis, the investigation of several specific optimization problems with one quadratic term in the objective function. Especially, we study their polyhedral structures, determining facet defining inequalities and aiming at complete descriptions.

Outline

This thesis is divided into two main parts. Providing a base for the essential research contribution presented in Part II, we recapitulate fundamental information about polyhedral combinatorics in Part I. First of all, we present basic definitions about graph theory, linear programming as well as polyhedral theory. As we analyze several quadratic optimization problems in the following, we define the corresponding linear versions in Chapter 2, where we also discuss related solution and separation approaches. In Chapter 3 we summarize relevant information about binary quadratic optimization problems in general, present several linearization approaches, cutting planes and lower bounding approaches.

In Part II we present the main results of our research concerning combinatorial optimization with one quadratic term. First of all, we motivate the subsequent investigations by presenting the main intention of our research approach. We explain in detail the idea of considering only one quadratic term in the objective function and present our results with respect to general combinatorial optimization problems. After that, we present our problem-related results when applying our approach to different specific optimization problems.

The first of the analyzed optimization problems are the strongly related minimum spanning forest and the minimum spanning tree problem, which we both consider in Chapter 4. Being the corresponding directed versions, we then apply and extend our findings to the minimum branching and the minimum arborescence problem in Chapter 5. In Chapter 6 and 7 we analogously investigate the minimum assignment and the maximum matching problem. Since several of the derived facet classes are of exponential size we present custom-tailored polynomial time separation approaches at the end of each chapter.

To show the practical relevance of our approach, we exemplarily present some computational results on the quadratic minimimum spanning forest and on the quadratic minimum spanning tree problem in Chapter 8. This thesis is concluded with a summary of our results and a brief discussion on open questions and further promising research directions regarding the approach considered here.

Partial publications and collaboration partners

The polyhedral results on the quadratic minimum spanning forest and the quadratic minimum spanning tree problem in Chapter 4 and the corresponding practical results in Chapter 8 have already been published in [27, 30].

The results on the quadratic assignment problem in Chapter 6 were obtained in productive cooperation with Dr. Anja Fischer (TU Dortmund). In another fruitful collaboration with Professor Dr. Frauke Liers and Lena Hupp (Universität Erlangen-Nürnberg), we carried out the studies of the matching problem with one quadratic term presented in Chapter 7.

A first investigation on the matching problem with one quadratic term was carried out in the bachelor thesis of Ewald Tews [165]. In her diploma thesis [122], Katharina Lechtenberg adapted the results of [27, 30] to branchings and arborescences under the supervision of the author of the present thesis, see Chapter 5.

Part I

Basics of Polyhedral Combinatorics

Chapter 1

Basic Definitions

1.1 Graphs and networks

In the wide field of combinatorial optimization, there are various definitions of graphs and related problems. For the sake of consistency, the notation and basic definitions used in this thesis are presented in the following. Moreover, relevant background information and theorems which are adressed in the following chapters are mentioned.

An **undirected graph** is a tuple $G = (V, E)$ with finite sets V and $E \subseteq \binom{V}{2}$, where $\binom{V}{2}$ here denotes the set of unsorted 2-pairs of different elements of V. The elements $v \in V$ are called **nodes** or **vertices**, the elements $e := \{u, v\} \in E$ **edges**. If the two nodes of an edge are ordered, we write $e = (u, v)$ and sometimes call the edges **arcs** and the graph **directed** or **digraph**. For an arc $e = (u, v)$ we say e **points from u to v** and that e is an **outgoing edge** of u and an **ingoing edge** of v. Since we mostly consider undirected graphs in the following, all graphs are meant to be undirected unless mentioned explicitly.

Two vertices $u, v \in V$ are said to be **adjacent** if there exists an edge $e = \{u, v\} \in E$. If all nodes are pairwise adjacent, the graph is said to be **complete** and is denoted with $K_{|V|}$. The set of all adjacent edges of one vertex $v \in V$ is denoted with $\delta(v) \subseteq E$ and if $\delta(v) \neq \emptyset$, v is **covered**. If the graph is directed, it is **complete** if $(u, v), (v, u) \in E$ for all $u, v \in V$ and the set of all ingoing edges of a vertex v is denoted with $\delta^{in}(v)$ and the set of all outgoing edges with $\delta^{out}(v)$. An edge $e = \{u, v\}$ or $e = (u, v)$ is **incident** to its **endnodes** u and v and two edges which share a vertex are called **adjacent**. For a subset $S \subseteq V$ we write $\delta(S)$ for the set of all edges with exactly one endnode in S and analogously $\delta^{in}(S)$ and $\delta^{out}(S)$ in the directed case. $\delta(S)$ is a **cut** in G, which is **induced by S**.

A **subgraph** of a graph $G = (V, E)$ is a graph $H = (V', E')$ with $V' \subseteq V$ and $E' \subseteq E$. H is **induced** by subset $V' \subseteq V$ if $E' = \{\{u, v\} \in E \mid u, v \in V'\}$. We then write $H = G[V']$ and denote the edge set of the induced subgraph with $E(G[V'])$. H is called **spanning** if $V' = V$.

A **path** of **length** k is a subgraph $H = (\{v_1, \dots, v_{k+1}\}, \{\{v_1, v_2\}, \{v_2, v_3\}, \dots, \{v_k, v_{k+1}\}\})$ of G, where $v_i \neq v_j$ for all $i \neq j$. v_1 and v_{k+1} are called **endpoints** of the path and the path is then called **v_1-v_{k+1}-path**. If it only holds that $v_i \neq v_j$ for all $i \neq j$ except for $i = 1$ and $j = k + 1$, i. e. $v_1 = v_{k+1}$, H is called a **cycle**.

In a **connected** graph there exists a u-v-path for all $u, v \in V$. The node set of a **bipartite** graph can be separated into two disjoint subsets $V_a \dot{\cup} V_b = V$ such that $E(G[V_a]) = E(G[V_b]) = \emptyset$. In a **weighted** graph $G = (V, E, c)$ a function $c : E \to \mathbb{R}$ defines **weights** or **costs** on the edges; we usually write c_e instead of $c(e)$. A directed weighted graph $G = (V, E, u, s, t)$ with two specified vertices s and t and a weight function $u : E \to \mathbb{R}^+$ defining the **capacity** of each edge is called **network** with **source** s and **sink** t. A function $f : E \to \mathbb{R}^+$ satisfying the **capacity constraints** $f_e \leq u_e$ for all $e \in E$ is called **flow**. If at each vertex except s and t **flow conservation** $\sum_{e\in\delta^{out}(v)} f_e = \sum_{e\in\delta^{in}(v)} f_e$ is given, the flow is an ***s*-*t*-flow** with value $val(f) = \sum_{e\in\delta^{out}(s)} f_e - \sum_{e\in\delta^{in}(s)} f_e$. An ***s*-*t*-cut** is an edge set $\delta^{out}(S)$ where S contains s but not t.

A cycle-free graph, i. e. a graph $G = (V, E)$ without a cycle as a subgraph, is called a **forest**. A connected forest is a **tree** and if a tree connects all vertices of the graph it is called **spanning tree**. A directed graph with $\delta^{in}(v) \leq 1$ for all vertices $v \in V$ and whose underlying undirected graph is a forest (tree) is called **branching** (**arborescence**). A vertex with $\delta^{in}(v) = 0$ is a **root node** and by definition each arborescence contains exactly one root node.

A graph with no adjacent pair of edges is a **matching** and if additionally all vertices are covered, the matching is **perfect**.

A subgraph $H = (V, E')$ of $G = (V, E)$ can be represented by an **incidence vector** $x \in \{0, 1\}^{|E|}$ as follows. Each entry of x, x_e, represents edge e in the edge set of E. Now x_e is set to one if e is an edge in the subgraph, i. e. if $e \in E'$, otherwise it is set to zero. If H is a weighted graph with cost function $c : E' \to \mathbb{R}$ and x is the corresponding incidence vector, the overall edge weight of H is $c(H) = \sum_{e\in E'} c_e$.

1.2 Linear programming

A **linear program** (LP) is an optimization problem defined by a matrix $A \in \mathbb{R}^{m\times n}$, column vectors $b \in \mathbb{R}^m$ and $c \in \mathbb{R}^n$ and a direction of optimization, say minimization. The task is to find a vector $x \in \mathbb{R}^n$ which minimizes the **objective function** $c^\top x$ and satisfies the **constraint** $Ax \leq b$, or, to decide that the problem is either unbounded or infeasible. The problem is said to be **unbounded** if for arbitrary $\alpha \in \mathbb{R}$ there exists a vector $x \in \mathbb{R}^n$ with $Ax \leq b$ and $c^\top x < \alpha$. If $\{x \in \mathbb{R}^n \mid Ax \leq b\} = \emptyset$, the problem is **infeasible**, otherwise **feasible**. A vector x is said to be a **(feasible) solution** if it satisfies $Ax \leq b$. An **optimal solution** is a vector x^* with $c^\top x^* \leq c^\top x$ for all solutions x. An LP is often written in the following way.

$$\text{(LP)} \qquad \begin{aligned} \min \quad & c^\top x \\ \text{s. t.} \quad & Ax \leq b \\ & x \in \mathbb{R}^n \end{aligned} \tag{1.1}$$

Note that it is possible to reformulate LPs containing linear equations or inequalities with $\geq$, objective functions with additional constant terms or a inverse optimization direction. For instance, if the objective is to maximize $c^\top x$ one can equivalently minimize the negated function $-c^\top x$ and afterwards multiply the optimal objective value with -1. For more details on the reformulations see, e. g., [117].

The three most common approaches for solving an LP problem are the simplex, the ellipsoid and the interior point methods. The first of the three, the simplex method, was devised by Dantzig in 1951 [50]. Although up to now there exists no pivot rule for a polynomial running time, it is quite efficient on average as the worst-case rarely appears in practice. Secondly, the ellipsoid method, developed by Yudin and Nemirovskiĭ [171] and Shor [160], was adapted by Khachiyan in 1979 to the first polynomial time algorithm for solving LPs [114]. Nonetheless the ellipsoid method is not practical due to the high average running time. Karmarkar then showed in 1984 that also the interior point method has a polynomial running time and that there exist efficient implementations being competitive with the simplex algorithm in practical terms [110, 111].

A fundamental theorem about separation provides the basis for the theory of polyhedra and duality. It is due to the research of Farkas and Minkowski in the 19th century [65, 66, 133] and is formulated here in a version for convex and closed sets.

Theorem 1.2.1 (Separation Theorem for convex sets)**.**
Let $C \subseteq \mathbb{R}^n$ be a convex and closed set. Either $z \in C$ or there exists a vector $\alpha \in \mathbb{R}^n$ with $\alpha^\top z < 0$ and $\alpha^\top c \geq 0$ for all $c \in C$.

Proofs of this theorem are based on elementary analysis and topology [24, 157]. A direct but very important consequence is the following.

Theorem 1.2.2.
Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Let $z \in \mathbb{R}^n$ violate $Az \leq b$. Then, there exists a vector $\alpha \in \mathbb{R}^n$ with $\alpha^\top z > \beta := \max\{\alpha^\top x \mid x \in \mathbb{R}^n, Ax \leq b\}$. □

The set $\{x \in \mathbb{R}^n \mid \alpha x = \beta\}$ is called **separating hyperplane** which separates the vector z from all vectors $x \in \mathbb{R}^n$ which satisfy $Ax \leq b$, see Figure 1.1.

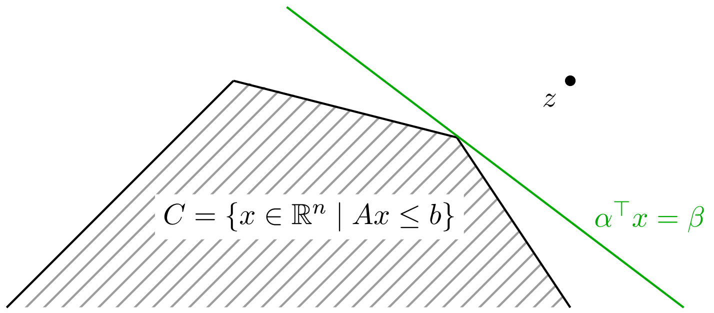


Figure 1.1: The green hyperplane $\alpha^\top x = \beta$ separates the point z from the set C

A direct consequence of Theorem 1.2.2 are the different variants of **Farkas' Lemma** [65,66,133], which characterize feasibility of a linear program and lay the foundation for the duality theory.

Lemma 1.2.3 (Farkas' Lemma I)**.**
Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Then, the system $Ax = b$ has a solution $x \geq 0$, if and only if $y^\top b \geq 0$ for each vector $y \in \mathbb{R}^m$ with $y^\top A \geq 0$.

Proof. Necessity follows directly by $y^\top b = y^\top Ax \geq 0$ for all $x \geq 0$ and for all $y \geq 0$ with $y^\top A \geq 0$. Sufficiency can be proven by contradiction: suppose that there exists no $x \geq 0$ with $Ax = b$. Define $C := \{\sum_i \lambda_i a_i \mid \lambda_i \geq 0\}$. Then, $b \notin C$ and by Theorem 1.2.1 there exists a vector $y \in \mathbb{R}^n$ satisfying $y^\top A \geq 0$ but $y^\top b < 0$. □

Lemma 1.2.4 (Farkas' Lemma II)**.**
Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Then, the system $Ax \leq b$ has a solution $x \in \mathbb{R}^n$, if and only if $y^\top b \geq 0$ for each vector $y \in \mathbb{R}^m, y \geq 0$ with $y^\top A = 0$.

Proof. Define matrix $A' = [A \ -A \ \ I_m]$. Then, Lemma 1.2.3 is applicable to the system $A'x' = b$ since $Ax \leq b$ has a solution $x \in \mathbb{R}$ if and only if $A'x' = b$ has a solution $x' \geq 0$. □

1.2.1 Duality

The **dual** LP of (1.1) is defined as

$$\begin{aligned} \text{(DP)} \qquad \max \quad & y^\top b \\ \text{s. t.} \quad & y^\top A = c^\top \\ & y \geq 0. \end{aligned} \tag{1.2}$$

The dual of (DP) is equivalent to the original problem (LP). To see this, split up the equation into two inequality constraints and dualize,

$$\begin{aligned} -\min \quad & -b^\top y \\ \text{s. t.} \quad & \begin{bmatrix} A^\top \\ -A^\top \\ I \end{bmatrix} y \leq \begin{bmatrix} c \\ -c \\ 0 \end{bmatrix} \end{aligned} \qquad \rightsquigarrow \qquad \begin{aligned} -\max \quad & z_1^\top c - z_2^\top c \\ \text{s. t.} \quad & \begin{bmatrix} A & -A & I \end{bmatrix} \begin{pmatrix} z_1 \\ z_2 \\ w \end{pmatrix} = -b \\ & z_1, z_2, w \geq 0 \end{aligned}$$

and finally replace $z_2 - z_1$ by x and eliminate the slack variables w. (LP) and (DP) are said to be a **primal-dual pair** and they are related in a very strong way which is provided in the most important theorem in LP theory, the Duality Theorem.

Theorem 1.2.5 (Duality Theorem [76, 169])**.**
If there exists a feasible solution $x \in \mathbb{R}^n$ for (LP) and a feasible solution $y \in \mathbb{R}^m$ for (DP), then

$$\min \left\{ c^\top x \;\middle|\; Ax \leq b \right\} = \max \left\{ y^\top b \;\middle|\; y^\top A = c^\top, y \geq 0 \right\}.$$

Proof. One direction is directly given by inserting the constraints: $c^\top x = y^\top Ax \leq y^\top b$. For the other direction it is to show that there exist solutions x and $y \geq 0$ such that $Ax \leq b$, $y^\top A = c^\top$ with $c^\top x \geq y^\top b$, i. e. it is to show that

$$\text{there exist } x \text{ and } y \geq 0 \text{ with} \begin{bmatrix} A & 0 \\ -c^\top & b^\top \\ 0 & A^\top \\ 0 & -A^\top \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \leq \begin{bmatrix} b \\ 0 \\ c^\top \\ -c^\top \end{bmatrix}.$$

By Farkas' Lemmata I and II, i. e. Lemma 1.2.3 and Lemma 1.2.4, this is equivalent to show that

$$u^\top b + v^\top c^\top - w^\top c^\top \geq 0 \text{ for all } u, \lambda, v, w \geq 0 \text{ with } u^\top A - \lambda\, c^\top = 0 \text{ and } \lambda\, b^\top + v^\top A^\top - w^\top A^\top \geq 0.$$

So assume that $u, \lambda, v, w \geq 0$ satisfy the constraints $u^\top A - \lambda c^\top = 0$ and $\lambda b^\top + v^\top A^\top - w^\top A^\top \geq 0$. Either $\lambda > 0$,then

$$u^\top b = \lambda^{-1} \lambda\, b^\top u = \lambda^{-1} (w - v)^\top A^\top u = \lambda^{-1} (w - v)^\top \lambda\, c = (w - v)^\top c.$$

Otherwise, if $\lambda = 0$, let x_0 be an arbitrary solution of (LP) and let $y_0 \geq 0$ be an arbitrary solution of (DP). Then,

$$u^\top b \geq u^\top A x_0 = 0 \geq (w - v)^\top A^\top y_0 = (w - v)^\top c.$$

Hence, in both cases all u, λ, v, w satisfying the premises also satisfy $u^\top b + v^\top c^\top - w^\top c^\top \geq 0$. □

As a result of the first proof direction, (DP) is infeasible if (LP) is unbounded. Moreover, feasibility of one problem depends on the other as follows.

Theorem 1.2.6.
(LP) is feasible if and only if $y^\top b \geq 0$ *for all* $y \geq 0$ *with* $y^\top A = 0$.

Proof. One direction follows immediately by inserting the constraints: if there exists a vector x with $Ax \leq b$, then for all $y \geq 0$ with $y^\top A = 0$ we have $0 = y^\top Ax \leq y^\top b$. Conversely, let $y^\top b \geq 0$ for all $y \geq 0$ with $y^\top A = 0$. Then, consider the LP $\min\{y^\top b \mid y^\top A = 0, 0 \leq y \leq 1\}$. One feasible solution is $y = 0$, and its dual problem is $\max\{(1, \ldots, 1)w \mid Ax - w \leq b, w \geq 0\}$, which has the feasible solution $x = 0, w = |b|$. By Theorem 1.2.5, the optimal values of both LPs are equal, which can be 0 only if there exists an x with $Ax \leq b$. □

Clearly, both problems can be infeasible at a time, but if a problem has an optimal solution, the corresponding dual has an optimal solution, too. In this case, the optimal solutions are related as follows.

Corollary 1.2.7.
Let $\min\{c^\top x \mid Ax \leq b, x \geq 0\}$ *and* $\max\{y^\top b \mid y^\top A \leq c^\top, y \leq 0\}$ *be a primal-dual pair of LPs and let* x *and* y *be feasible solutions. Then, the following statements are equivalent:*

(a) x *and* y *are both optimal solutions*

(b) $c^\top x = y^\top b$

(c) $(c^\top - y^\top A)x = 0$ *and* $y^\top(b - Ax) = 0$.

Proof. The equivalence of (a) and (b) follows from Duality Theorem 1.2.5. For the equivalence of (b) and (c) note that for all feasible solutions x and y we have $y^\top(b - Ax) \leq 0 \leq (c^\top - y^\top A)x$. Thus, $y^\top(b - Ax) = y^\top b - y^\top Ax = c^\top x - y^\top Ax = (c - y^\top A)x$ if and only if $c^\top x = y^\top b$. □

The conditions in (c) are called **complementary slackness constraints** and are an important tool for proving optimality of a solution or integrality of a polyhedron, such as in Theorems 4.2.4 and 4.2.5 below. In order to prove optimality it suffices to show for all variables of a feasible solution that either the variable equals zero or that the associated dual inequality is satisfied with equality.

1.2.2 Integer linear programming

If the solution of an LP is required to be integral, i. e., $x \in \mathbb{Z}^n$, the LP is called **integer linear program** (ILP). All combinatorial optimization problems can be formulated as ILP problems [117]. Therefore, it is not surprising that no polynomial-time algorithm is known to solve an ILP as otherwise this algorithm could solve even NP-hard optimization problems [77].

Defining duality similar to (1.2) but with integrality constraints, the duality relation

$$\min\{c^\top x \mid Ax \leq b, x \text{ integer}\} \geq \max\{y^\top b \mid A^\top y = c, y \geq 0, y \text{ integer}\}$$

is obtained, but, other than in the continuous case, strict inequality holds in general and is called **weak duality**.

A common method to tackle an ILP problem is to relax it by removing the integrality constraint and solve the resulting LP. Of course, in the majority of cases the optimal fractional solution x^* is not integral, i. e. not feasible for ILP and can only give a lower bound on the optimal integral solution x_I^*.

1.2.3 Branch-and-bound

One option to successively delete fractional solutions is a **branch-and-bound** (B&B) approach, which was first presented by Land and Doig in 1960 [120]. The name of the approach is based on the branching tree structure which appears by successively partitioning the problem and on the pruning of certain branches via a dual bound.

More precisely, the B&B scheme starts with solving the relaxed version of the ILP problem, LP_0, yielding an optimal solution x_0^*. If x_0^* is not integral, one fractional variable $(x_0^*)_j$ is chosen and new branches of the B&B tree are created. In each of these branches appropriate constraints are added to LP_0 to exclude solutions with the same fractional value of $(x_0^*)_j$. It is understood that these constraints have to be feasible for all integral solutions of the original ILP. Individually, the extended LPs are solved again, and if again the optimal solution of such an LP, say LP_i, contains a fractional variable $(x_i^*)_k$, the set of constraints is enlarged by the same rules. By this, the branching tree is extended gradually. A branch node is called **active** if the corresponding LP is not solved so far, otherwise it is **explored**.

Typical constraints force the fractional variable to the next lower or higher integral value, such that in the first branch of node i LP_i is extended by the inequality $x_j \leq \lfloor (x_i^*)_j \rfloor$ and in the second branch by $x_j \geq \lceil (x_i^*)_j \rceil$. This strategy is called **variable dichotomy**. In case of binary variables this strategy fixes the value of x_j to zero and one respectively. If x_j has a lower and an upper bound such that it can take l different values, a **multiple branch** strategy creates l branches in each of which x_j is fixed to one of these values. The multiple branch strategy is the original strategy proposed by Land and Doig [120] but only pays off if l is fairly small, e. g. if $x_j \in \{-1, 0, 1\}$ with $l = 3$. The selection of index j follows some branching rule, such as the **most/least infeasible integer variable** rule; an overview of the most common branching strategies is given in, e. g., [1, 123].

The objective function value of the best integral solution found so far is called **primal bound** and the objective value of the current solution x_i^* is called **dual bound**. **Pruning** a branch node i means to cease branching from this node. This is possible if either the dual bound is worse than the primal, if LP_i is infeasible or if x_i^* is integral. In the latter case the primal bound is updated if x_i^* has a better objective value. Optimality is obtained if the branching tree is pruned in all of its leaves, i. e., if there is no active node left. The sequence of active node consideration is provided by a node selection rule. There are strategies like **depth-first search**, choosing a child node of the previous node or, if pruned, the most recently created active node, **best bound** chosing the active node with the best LP objective value, and many others [123].

The B&B approach terminates if the feasible set of the relaxed problem $\{x \in \mathbb{R}^n \mid Ax \leq b\}$ is bounded [157]. Its running time mainly depends on the quality of its bounds. The better the primal and dual bound, the earlier a branch is prunable. Therefore, in many cases additional heuristics are applied in advance or within the B&B search tree to find good feasible solutions. The quality of the dual bound depends on the relaxation quality, which can be improved by the (iterative) application of cutting planes, see Section 1.3.1.

1.3 Polyhedra and polytopes

A **polyhedron** is a subset $P \subseteq \mathbb{R}^n$ which can be described by $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$ for some matrix $A \in \mathbb{R}^{m \times n}$ and some vector $b \in \mathbb{R}^m$. If P is bounded, it is called **polytope**.

A system $Ax \leq b$ is **minimal** if each proper subsystem contains a solution which violates $Ax \leq b$. For the following definitions assume that P is always described by a minimal system. The **affine hull** of a polyhedron P is the set of solutions of the maximal subsystem $A'x \leq b'$ which is satisfied with equality for all feasible solutions x. The **dimension** of P is defined as $\dim(P) := n - \text{rank}(A')$. A polytope with $\dim(P) = n$ is **fulldimensional**. A **face** of P is a subset $F \subseteq P$ if there exists a subsystem $A'x \leq b'$ with $F = \{x \in P \mid A'x = b'\}$; then $A'x \leq b$ **induces** face F. A 0-dimensional face of P is called **vertex** of P. A **facet** of P is an inclusionwise maximal face of P with $F \neq P$. The dimension of a facet is $\dim(P) - 1$ by definition.

The convex hull of all integral vectors of a polyhedron P is called **integral hull** P_I of P. Obviously, $P_\text{I} \subseteq P$. A polyhedron P is **integral** if each non-empty face $F \subseteq P$ contains an integral point. As a consequence a polytope is integral if each of its vertices is integral. In this case, $P_\text{I} = P$ and at least one optimal solution of $\min\{c^\top x \mid x \in P\}$ is integral for arbitrary $c \in \mathbb{R}^n$ [81, 103], i. e. $\min\{c^\top x \mid x \in P_\text{I}\} = \min\{c^\top x \mid x \in P\}$.

1.3.1 Branch-and-cut

In case P is not integral, a common way to approximate the integral hull of a polyhedron is to add **cutting planes**, i. e., separating hyperplanes $w^\top x = \beta$ such that all feasible points of the integral problem P_I lie the corresponding **half-space** $\{x \mid w^\top x \leq \beta\}$, whereas $w^\top x' \nleq \beta$ for at least one fractional point $x' \in P$. By Theorem 1.2.2, such cutting planes must exist if $P_i \neq P$. If throughout the B&C algorithm cutting planes are generated and added to LP_i, the algorithm is called **branch-and-cut** (B&C) [53, 87, 88]. A cutting plane $w_1^\top x = \beta_1$ is **stronger** than another cutting plane $w_2^\top x = \beta_2$ with respect to a polyhedron P, if $P \cap \{w_1^\top x \leq \beta_1\} \subseteq P \cap \{w_2^\top x \leq \beta_2\}$. In other words, a stronger cutting plane cuts off more infeasible points from P and thus yields a better approximation of the integral hull P_I. Stronger cutting planes naturally lead to faster approaches and the strongest possible cutting planes are the facets of P_I.

The difference between B&B and B&C lies in the method how to speed up the calculation of the optimal solution. The philosophy of the B&B algorithm is a preferably fast reoptimization in each branch node, whereas the B&C approach puts great effort in each branch node to gain powerful dual bounds and to prune as early as possible. Although the worst case is a complete enumeration of the branching tree, both, the branch-and-bound and the branch-and-cut methods are quite practical as they "often produce acceptable solutions in reasonably short amount of time" [17]. A detailed discussion on whether and how to branch or to cut can be found in [134].

1.3.2 Separation

Let $x \in \mathbb{R}^n$ and $P \subseteq \mathbb{R}^n$ be a polyhedron. A **separation algorithm** decides whether $x \in P$ or not, and, in the latter case, returns a violated inequality showing that $x \notin P$. Separation algorithms are applied e. g. in the context of problems with implicite constraints or if the number of constraints is exponential. For the latter, the computational time of solving the LP with all constraints is exponential which especially in B&B and B&C schemes leads to tremendous running times as one or more LPs have to be solved in each branch node.

For those problems with exponentially many constraints, the separation reduces the LP by omitting certain (classes of) inequalities and separate them sequentially. More precisely, the reduced LP is solved and the optimal solution is separated. If a violated inequality is found, it is added to the current LP and the procedure is repeated. Therefore, in each step only LPs with a polynomial number of constraints have to be solved. Having a separation algorithm running in polynomial time, each step can be performed in polynomial time. This motivates the idea of a very famous result of Grötschel, Lovász and Schrijver about the equivalence of the optimization and the separation problem: if there exists a polynomial time separation algorithm for P, the optimization problem is solvable in polynomial time for an arbitrary objective function $c^\top x$, and vice versa [90, 92].

1.4 Facets

Let $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$ be a polyhedron and $a_i^\top x \leq b_i$ be an inequality from $Ax \leq b$. There are several ways to show that $a_i^\top x \leq b_i$ induces a facet of P out of which the three most common are presented in the following as they are applied in several facet proofs in this thesis. Assume that P is fulldimensional, otherwise it additionally has to be shown that the inequality is not an implicite equation, e. g. by proving that there exists a vector $x' \in P$ with $a_i^\top x' < b_i$.

One straightforward idea is to show that the inequality is needed in the corresponding minimal system of P. This can be done by displaying a vector $\bar{x}$ which violates $a_i^\top x \leq b_i$ but satisfies all other inequalities in $Ax \leq b$. Then each subset of $Ax \leq b$ that still defines P, including the corresponding minimal system, must include $a_i^\top x \leq b_i$. A second method, if P is the convex hull of a finite set $\mathcal{S}$ of combinatorial objects, is proving that the face $\mathcal{F} = \{s \in \mathcal{S} \mid a^\top x_{\mathcal{S}} = b\}$ is not contained in another larger proper face of P. For instance by comparison of the coefficients of a, b, c and d, show that for each proper face $\{x \in \mathbb{R}^n \mid c^\top x = d\}$ of P containing $\mathcal{F}$, $c^\top x \leq d$ is a positive scalar multiple of $a^\top x \leq b$, or, if P is not fulldimensional, differs by a linear combination of the implicit equations of P. Finally, it is also possible to show the correct dimension of the face induced by $a^\top x \leq b$ by presenting $\dim P$ many affinely independent vectors $x \in P$ with $a^\top x = b$.

A set of vectors $v^1, \ldots, v^k$ is **affinely independent** if for $\lambda_1, \ldots, \lambda_k \in \mathbb{R}^n$ with $\sum_{i=1}^k \lambda_i = 0$ and $\sum_{i=1}^k \lambda_i v^i = 0$ the only feasible assignment is $\lambda_i = 0$ for all $i \in \{1, \ldots k\}$.

Lemma 1.4.1.

Let the vectors $v^1, \ldots, v^k \in \mathbb{R}^n$ with $k < n$ be affinely independent and let $v^{k+1} \in \mathbb{R}^n$. If there exists a vector $a \in \mathbb{R}^n$ and a scalar $b \in \mathbb{R}$ with

$$a^\top v^i = b \qquad \textit{for all } i \in \{1, \ldots, k\} \tag{1.3}$$

and

$$a^\top v^{k+1} \neq b, \tag{1.4}$$

then $v^1, \ldots, v^{k+1}$ are affinely independent.

In other words, a vector v^{k+1} is affinely independent from affinely independent vectors $v^1, \ldots, v^k$ if there exists an equation which is satisfied by all $v^1, \ldots, v^k$ but not by v^{k+1}. An iterative application of this result leads to constructive dimension proofs, which are used in several places in this thesis.

Proof. Let $v^1, \ldots v^k$ be affinely independent and let $a \in \mathbb{R}^n$ and $b \in \mathbb{R}$ such that (1.3) is satisfied. We show that (1.4) does not hold if v^{k+1} is affinely dependent from $v^1, \ldots, v^k$.

By affine dependence of v^{k+1} there exist $\lambda_1, \ldots, \lambda_{k+1}$ not all zero with $\sum_{i=1}^{k+1} \lambda_i = 0$ and $\sum_{i=1}^{k+1} \lambda_i v^i = 0$. Note that $\lambda_{k+1} \neq 0$ as otherwise $\sum_{i=1}^k \lambda_i = 0$ and $\sum_{i=1}^k \lambda_i v^i = 0$, a contradiction to the affine independence of $v^1, \ldots, v^k$. We affinely combine the equalities (1.3) with respect to $\lambda_1, \ldots, \lambda_k$ and obtain

$$\lambda_{k+1} b = -\sum_{i=1}^k \lambda_i b = -\sum_{i=1}^k \lambda_i (a^\top v^i) = -a^\top \sum_{i=1}^k \lambda_i v^i = -a^\top(-\lambda_{k+1} v^i_{k+1}) = \lambda_{k+1} a^\top v^i_{k+1}$$

Due to $\lambda_{k+1} \neq 0$ we obtain $a^\top v^i_{k+1} = b$. □

Chapter 2

Some Combinatorial Optimization Problems

In this chapter we introduce the main combinatorial optimization problems which we consider in the remainder of this thesis. As several of the separation routines reduce to a maximum flow problem, we start with the definition of and some facts about this problem. Afterwards we introduce important basics about some linear optimization problems. These optimization problems reappear in the second part of this thesis as they are investigated concerning a quadratic objective function.

2.1 Maximum flows

In a given network $G = (V, E, u, s, t)$ the **maximum flow problem** asks for an s-t-flow with maximal value. By definition, a straightforward LP formulation is to maximize $val(f)$ subject to the flow conservation, the capacity and nonnegativity constraints as formulated in Section 1.1.

Besides the LP approach there exist various polynomial time combinatorial algorithms, such as the augmenting path algorithm of Edmonds and Karp [61] or the push-relabel algorithm of Goldberg and Tarjan [86], where either flow is sent from vertices which are labeled in a certain way (push) or vertices are relabeled, until flow conservation is given for all vertices except s and t.

By flow conservation, the value of a flow f equals $\sum_{e\in\delta^{out}(S)} f_e - \sum_{e\in\delta^{in}(S)} f_e$ for all subsets S containing s but not t [117]. In other words, the flow value cannot exceed the value of a minimum s-t-cut. This leads to the main theorem stated in 1956 by Ford and Fulkerson [70], Dantzig and Fulkerson [52] and Elias, Feinstein and Shannon [64].

Theorem 2.1.1 (Max-Flow-Min-Cut).
In a network the value of a maximal s-t-flow equals the value of a minimum s-t-cut.

The proof bases on the observation that an s-t-flow is maximal if and only if there exists no augmenting path in the residual graph which is generated within each step of the algorithm of Ford and Fulkerson. Given a flow f, a vertex $v \in V\setminus\{s\}$ is reachable from s if there exists an s-v-path with a positive residual capacity $u(e) - f(e) > 0$ for all edges along the path. Since the set S that includes all reachable vertices forms a minimum s-t-cut, most types of cut problems are reduced to a max-flow problem.

2.2 Minimum spanning trees and forests

A spanning tree can be defined in various equivalent ways. The following theorem quoted from [117] gives an overview over the equivalent definitions.

Theorem 2.2.1.
Let $G = (V, E)$ be a graph with $|V| = n$ vertices. Then, the following statements are equivalent:

a) G is a tree.

b) $|E| = n - 1$ and G is cycle-free.

c) $|E| = n - 1$ and G is connected.

d) G is a minimal connected graph.

e) G is a maximal cycle-free graph.

f) G contains a unique path between any pair of vertices.

For connected graphs, Theorem 2.2.1 d) guarantees the existence of a spanning tree. In the following we consider connected graphs as a basis for the MST problem since otherwise no feasible solution exists. If additionally a cost function for the edges of the graph is defined, the various spanning trees can be of different values. To find a spanning tree of e. g. minimal value can be formulated as an optimization problem.

Definition 2.2.2.
Let $G = (V, E)$ be a connected graph with cost function $c : E \to \mathbb{R}$. The **minimum spanning tree problem** *(MST problem) is to find a spanning tree of minimal cost, i. e. a subgraph T of G with $E(T) \subseteq E$ which is a spanning tree and whose sum of costs $\sum_{e \in E(T)} c_e$ is minimal.*

Leaving out the connectivity constraint, a minimum spanning forest problem can be formulated similarly.

Definition 2.2.3.
Let $G = (V, E)$ be a graph with cost function $c : E \to \mathbb{R}$. The **minimum spanning forest problem** *(MSF problem) is to find a spanning forest of minimal cost, i. e. a subgraph F of G with $E(F) \subseteq E$ which is a spanning forest and whose sum of costs $\sum_{e \in E(F)} c_e$ is minimal.*

If the graph is connected and if $c_e < 0$ for all $e \in E$, the two problems are equivalent as each optimal forest contains as many edges with negative costs as possible, leading to a spanning tree of $n - 1$ edges. Otherwise, the MST problem reduces to a MSF problem by subtracting the value $M := \max\{c_e \mid e \in E\} + 1$ from the cost vector c such that all costs become negative. The optimal value of the original problem is obtained by adding $(n - 1)M$.

The search for a maximal spanning tree or a maximal spanning forest can easily be formulated as an MST or an MSF problem by negating the cost function.

2.2.1 Combinatorial approaches and ILP formulations

For both, the MST and the MSF problem, there exist polynomial time combinatorial optimization algorithms. The first known algorithm for the MST problem is from O. Borůvka [23]; the more common ones are the algorithms of J. Kruskal [118] and R.C. Prim [151]. Since Kruskal's algorithm iteratively chooses the cheapest edge which does not form a cycle, it can easily be adapted for the MSF problem by eliminating all edges of positive cost in advance.

Another way to tackle the two problems is to formulate them as integer linear programs. The first ILP approach for the MST problem is based on matroid theory and was formulated by Edmonds [60], which later was established in the following way (see e. g. [48]).

Proposition 2.2.4.

Let $G = (V, E)$ be a connected graph with $|V| = n$ vertices and let $c : E \to \mathbb{R}$ be the cost function on the edges of G. The MST problem can be formulated as an integer linear program as follows:

$$
\begin{aligned}
(\mathrm{ILP}_{\mathrm{MST}}) \qquad \min \quad & \sum_{e \in E} c_e\, x_e \\
\text{s.t.} \quad & \sum_{e \in E} x_e = n - 1 && (2.1)\\
& \sum_{e \in E(G[S])} x_e \leq |S| - 1 \qquad \forall\, \emptyset \neq S \subseteq V && (2.2)\\
& x_e \in \{0, 1\} \qquad \forall\, e \in E && (2.3)
\end{aligned}
$$

Proof. Let $x \in \{0,1\}^m$ be a feasible solution of $\mathrm{ILP}_{\mathrm{MST}}$. Due to the binary constraints (2.3) we can consider x as the incidence vector of a subgraph T of G, i. e. if $x_e = 1$, edge e is in edge set of T, otherwise not. Equation (2.1) guarantees that T contains exactly $n - 1$ edges whereas the inequalities (2.2) ensure that each subset S does not contain more than $|S| - 1$ edges, i. e. excluding cycles. With 2.2.1 b), T is a spanning tree. The objective function guarantees minimal edge costs. □

Equation (2.1) is called **cardinality constraint** and the inequalities (2.2) are the **subtour elimination constraints**, also called **cycle** or **rank inequalities**. The ILP formulation ($\mathrm{ILP}_{\mathrm{MSF}}$) for the MSF problem equals the one for the MST problem except that the cardinality constraint (2.1) is left out since a spanning forest is not required to be connected.

2.2.2 Polyhedral descriptions

An attractive property of spanning trees and spanning forests is that not only the optimization problems are easy to solve, e. g. with one of the mentioned combinatorial algorithms, but that they also have nice polyhedral structures. We define the **spanning tree polytope**

$$P_T(G) := \left\{ x \in [0,1]^m \;\middle|\; (2.1),\, (2.2) \right\}$$

and the **spanning forest polytope**

$$P_F(G) := \left\{ x \in [0,1]^m \;\middle|\; (2.2) \right\}.$$

When the context leads to the correct association, we sometimes shortly write P_T and P_F instead of $P_T(G)$ and $P_F(G)$.

Proposition 2.2.5.

Let $G = (V, E)$ be a complete graph with n vertices and $m = \frac{n(n-1)}{2}$ edges. Then,

$$\dim(P_T(G)) = m - 1$$

and

$$\dim(P_F(G)) = m.$$

Proof. For proving the statement on the dimension of $P_T(G)$, we list m feasible and affinely independent vectors $x \in [0,1]^n$. As $P_T(G)$ is the spanning tree polytope, we can restrict ourselves to binary variables $x \in \{0,1\}^n$ and consider x as incidence vector of a subgraph of G. We show by complete induction over the number of vertices in G the existence of m affinely independent vectors $x \in \{0,1\}^n$ satisfying the constraints of $P_T(G)$.

$n = 2$: G consists of only two vertices and one edge; the incidence vector of the unique spanning tree G satisfies the requirements.

$n \to n+1$: Let $G_n = (V_n, E_n)$ be the graph with vertices $v_1, \ldots, v_n$ and $G_{n+1} = (V_{n+1}, E_{n+1})$ the extension of G_n by one vertex v_{n+1}, i. e. $V_{n+1} := V_n \cup \{v_{n+1}\}$. By induction hypothesis there exist $m_n := |E_n|$ affinely independent incidence vectors corresponding to spanning trees $T_n^1, \ldots, T_n^{m_n}$ in G_n. Define $e_j := \{v_j, v_{n+1}\}$ for $j = 1, \ldots, n$ and let h be an edge in the cycle of $T_n^1 \cup \{e_1, e_2\}$. We construct $m_{n+1} := |E_{n+1}|$ valid and affinely independent incidence vectors of trees $T = (V, E(T))$ as follows:

1. For $i = 1, \ldots, m_n$ let $E(T) := E(T_i^n) \cup \{e_1\}$.
   By 2.2.1 b), the generated graphs form spanning trees: on the one hand we have a correct number of edges $\sum_{e \in E(T)} x_e = \sum_{e \in E(T_i^n)} x_e + 1 = n$, and on the other hand no cycles by induction hypothesis. More precisely, the subtour elimination constraints hold for all $S \subset V_n$ due to the hypothesis and since v_{n+1} is a new vertex and not connected to any of the trees T_i^n, the insertion of edge e_1 does not create a cycle. The corresponding incidence vectors are pairwise affinely independent as they are lifted affinely independent vectors.
2. For $j = 2, \ldots, n$ let $E(T) := E(T_1^n) \cup \{e_j\}$
   By the same argument, these graphs are spanning trees. They are pairwise affinely independent as each of them contains an edge which none of the other ones contains. In other words, each vector satisfies $x_{e_j} = 0$ except the one corresponding to the tree containing edge e_j. With Lemma 1.4.1 pairwise affine independence and also affine independence with respect to the vectors in 1. follows.
3. Let $E(T) := (E(T_1^n) \setminus \{h\}) \cup \{e_1, e_2\}$
   T is a spanning tree as edge h is chosen such that its exchange with e_2 does not create a cycle in T. The incidence vector does not satisfy the equation $\sum_{e \in \delta(v_{n+1})} x_e = 1$, which all vectors in 1. and 2. do. With Lemma 1.4.1 affine independence follows.

In summary, we obtain

$$m_n + (n-1) + 1 = \frac{n(n-1)}{2} + n = \frac{n^2 - n + 2n}{2} = \frac{(n+1)n}{2}$$

affinely independent vectors satisfying the constraints of $P_T(G)$.

In the case of spanning forests, the zero-vector can be added to the m vectors above as it is affinely independent and valid in $P_F(G)$. □

Note that this statement does not hold for graphs which are not complete. Consider, e. g., a connected graph G with $n > 2$ vertices and exactly $m = n - 1$ edges. The graph itself is a spanning tree and, in particular, the only one. The dimension of the corresponding polytope is thus zero and not m.

The convex hull of all (integral) solutions of MST and MSF equals the polytope arising from the relaxed version of (ILP_{MST}) and (ILP_{MSF}), respectively.

Theorem 2.2.6.
Let $G = (V, E)$ be a complete graph. $P_T(G)$ and $P_F(G)$ both are integral. The vertices of the spanning tree (forest) polytope are exactly the incidence vectors of spanning trees (forests) of G.

Proof. The proof for the spanning tree case can be found e. g. in [117]. Since its idea is resumed in the further course of this thesis, i. e. in some proofs concerning facet defining inequalities for the quadratic MST and MSF problems, we present a short version of the slightly adapted proof for the spanning forest case, giving a base for the following.

The second statement of the theorem follows from Proposition 2.2.4. It remains to show integrality of P_F. For that purpose let $c : E \to \mathbb{R}$ be an arbitrary cost function and let F^* be an optimal solution. Let the edges $E(F^*) = \{f_1, \dots, f_{m-1}\}$ be sorted by ascending costs, i. e. $c_{f_1} \leq \dots \leq c_{f_{m-1}}$. Let finally $S_k \subseteq V$ be the connected component of the subgraph $(V, \{f_1, \dots, f_k\})$ containing edge f_k.

As F^* is a minimal spanning forest, for each of its edges the optimality criterion

$$c_{f_k} \leq 0 \qquad \forall\, k \in \{1, \dots, m-1\} \tag{2.4}$$

is satisfied, since edges with positive costs are not considered in an optimal solution, and for all edges not contained in the forest we have the optimality criteria

$$c_e \geq \begin{cases} c_f & \forall\, e \notin E(F^*) \text{ leading to a cycle } \mathcal{C}_e \text{ in } E(F^*) \cup \{e\} \text{ and } \forall\, f \in \mathcal{C}_e \\ 0 & \forall\, e \notin E(F^*) \text{ otherwise} \end{cases} \tag{2.5}$$

as otherwise the insertion of e, eventually with a removal of f, would yield a better feasible solution.

We will show that the incidence vector x^* of F^* is an optimal solution of the relaxed version of (ILP_{MSF}), i. e. of

$$\begin{array}{lll} (\text{LP}_{\text{MSF}}) & \min \displaystyle\sum_{e \in E} c_e\, x_e & \\ & \text{s. t.} \displaystyle\sum_{e \in E(G[S])} x_e \leq |S| - 1 & \forall\, \emptyset \neq S \subseteq V \\ & \qquad x_e \in [0, 1] & \forall\, e \in E. \end{array}$$

By the complementary slackness constraints 1.2.5 (c), x^* is optimal in (LP_{MSF}) if there exists a solution z^* of the dual problem of (LP_{MSF}) with the property that the dual constraint is satisfied with equality whenever the corresponding primal variable is strictly positive, and, vice versa, that the subtour elimination constraint is tight if the corresponding dual variable obtains a value strictly greater than zero. The dual problem of (LP_{MSF}) reads

$$\begin{array}{lll} (\text{DP}_{\text{MSF}}) & \max \ - \displaystyle\sum_{\emptyset \neq S \subseteq V} (|S| - 1) & \\ & \text{s. t.} \ - \displaystyle\sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S \leq c_e & \forall\, e \in E \\ & \qquad z_S \geq 0 & \forall\, \emptyset \neq S \subseteq V \end{array}$$

where a dual variable z_S is defined for each set $\emptyset \neq S \subseteq V$.

A dual solution satisfying the complementary slackness constraints can now be constructed as follows. For $k \leq m-2$, assign $z^*_{S_k} := c_{f_l} - c_{f_k}$, where l is the first index greater than k for which $f_l \cap S_k \neq \emptyset$. Additionally, set $z^*_{S_{m-1}} := -c_{f_{m-1}}$ and $z^*_S := 0$ for all $S \notin \{S_1, \dots, S_{m-1}\}$.

Note that by this construction we have $z_S \geq 0$ for all $S \subseteq V$ due to the ascending sorting and due to (2.4). If the end vertices of an edge e are in the same connected component of F^*, this construction yields

$$-\sum_{\substack{S\subseteq V\\ e\in E(G[S])}} z_S = c_{f_i},$$

where i is the smallest index with $e \subseteq S_i$. If otherwise the end vertices are in different connected components of F^*, we have

$$-\sum_{\substack{S\subseteq V\\ e\in E(G[S])}} z_S = 0.$$

The solution z^* is thus dual feasible by (2.5). Moreover, the dual constraint corresponding to an edge e is satisfied with equality whenever $x^*_e > 0$, whereas $z^*_S > 0$ implies that the corresponding subtour elimination constraint is tight. In summary, the complementary slackness constraints are satisfied by x^* and z^* which proves integrality of P_F. □

With this polyhedral result, both the MST and the MSF problem can be solved to optimality by optimizing over the corresponding LP. The exponential number of the subtour elimination constraints (2.2) can be dealt with using a polynomial time separation algorithm developed by Padberg and Wolsey [141] which is presented in the following. It is based on minimal cuts, which by Theorem 2.1.1 can be computed by a maximal flow algorithm.

2.2.3 Separation of the subtour elimination constraints

Basically, the values of a given solution $x^* \in [0,1]^{|E|}$ are considered as edge weights in an extended graph such that a minimal cut gives information about feasibility or violated constraints. More detailed, rewrite (2.2) in a cut formulation as follows. For a given vector $x^* \in [0,1]^{|E|}$ define $d_i := 2 - \sum_{e\in\delta(i)} x^*_e$ for $i \in V$ and rewrite

$$\begin{aligned} 2\sum_{e\in E(G[S])} x^*_e &= 2\sum_{e\in E(G[S])} x^*_e + \sum_{e\in\delta(S)} x^*_e - \sum_{e\in\delta(S)} x^*_e \\ &= \sum_{i\in S}\sum_{e\in\delta(i)} x^*_e - \sum_{e\in\delta(S)} x^*_e \end{aligned}$$

as each edge in the inner sum is counted twice when both end nodes are in S and once when only one end node is in S. By definition of d_i,

$$\sum_{i\in S}\sum_{e\in\delta(i)} x^*_e = \sum_{i\in S}(2-d_i) = 2|S| - \sum_{i\in S} d_i.$$

Partitioning the sum by positive and negative d_i values and putting together the equations above yields

$$\begin{aligned} \sum_{e\in E(G[S])} x^*_e - |S| &= -\frac{1}{2}\Big(\sum_{e\in\delta(S)} x^*_e + \sum_{i\in S} d_i\Big) \\ &= -\frac{1}{2}\Big(\underbrace{\Big(\sum_{e\in\delta(S)} x^*_e + \sum_{\substack{i\in S\\ d_i>0}} d_i - \sum_{\substack{i\in V\setminus S\\ d_i<0}} d_i\Big)}_{=:f(S)} + \underbrace{\sum_{\substack{i\in V\\ d_i<0}} d_i}_{=:\kappa}\Big). \end{aligned}$$

Now there exists a violated subtour elimination constraint, corresponding to some set S, if and only if there exists a nonempty set $S \subseteq V$ with

$$\sum_{e \in E(G[S])} x_e^* - |S| > -1. \tag{2.6}$$

As κ is a constant, this can be decided by minimizing $f(S)$ over all $\emptyset \neq S \subseteq V$. For this purpose, construct a directed network $G' := (V', E', c)$: double all edges of G, direct them reversely and set capacities $c_{(i,j)} = c_{(j,i)} = x^*_{\{i,j\}}$. Add two vertices s and t with directed edges from s to i if $d_i > 0$ and from i to t if $d_i < 0$. Set the capacities on these edges to $c_{\{s,i\}} = d_i$ and $c_{\{i,t\}} = -d_i$. Then,

$$f(S) = \sum_{e \in \delta^{in}_{E'}(S \cup \{t\})} c_e,$$

which is the value of a cut set in G' containing t and which is to minimize. As S must not be empty, for each vertex $i \in V$ a minimal cut has to be computed with i being linked to t by setting $c_{\{i,t\}} = \infty$. The construction of the network and the fixing of one vertex to t is visualized in Figure 2.1. By Theorem 2.1.1 this construction leads to $|V|$ maximum s-t-flow problems, one for each vertex $i \in V$. Each of the corresponding $|V|$ sets satisfying (2.6) yields a violated subtour elimination constraint. If no such set satisfies (2.6), then x^* is valid for (2.2).

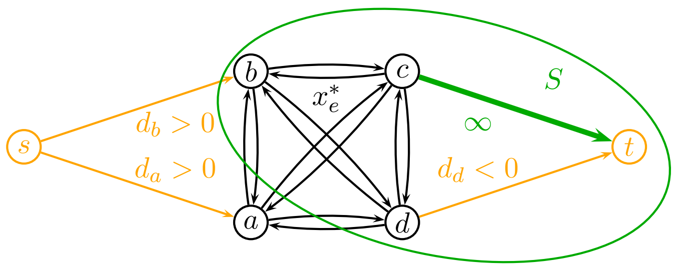


Figure 2.1: Each vertex is once fixed to t (here vertex c) and a minimal cut S in the extended graph containing t and the fixed vertex is calculated. If in none of the cases inequality (2.6) is satisfied, then x^* is valid with respect to the subtour elimination constraints.

2.3 Minimum branchings and arborescences

Considering the underlying undirected graph, branchings and arborescences are nothing but spanning forests and trees. In the directed graph nevertheless they additionally need to satisfy $\delta^{in}(v) \leq 1$ in each vertex. Connectivity of the graph thus does not guarantee the existence of an arborescence. For sake of simplicity, we thus only consider complete directed graphs when studying branching and arborescence problems with cost structures. A cost structure again is given by a cost function $c : E \to \mathbb{R}$ and the corresponding optimization problems are defined as follows.

Definition 2.3.1.

Let $G = (V, E)$ be a complete directed graph with cost function $c : E \to \mathbb{R}$.
The **minimum arborescence problem** *(MArb problem) is to find an arborescence of minimal cost, i. e. a subgraph $A = (V, E(A))$ of G with $E(A) \subseteq E$ which is an arborescence and whose sum of costs $\sum_{e \in E(A)} c_e$ is minimal.*
The **minimum branching problem** *(MBra problem) is to find a branching of minimal cost, i. e. a subgraph $B = (V, E(B))$ of G with $E(B) \subseteq E$ which is a branching and whose sum of costs $\sum_{e \in E(B)} c_e$ is minimal.*

Due to the similarity to minimal spanning tree and forest problems only the most important facts about minimal arborescence and branching problems are mentioned in the following without going into detail.

Since at most one arc is allowed to point to each vertex, the greedy strategies of Prim and Kruskal are not usable in this context. Chu and Liu [43] and Edmonds [59] independently developed a combinatorial approach for solving the MBra or the MArb problem in polynomial time. Stated on matrices instead of graphs a very similar algorithm was presented by Bock [22]. The main idea of the algorithms is to choose an ingoing edge of minimal cost for each vertex except the root node and to shrink resulting cycles to supernodes. This procedure is done until no cycles are left such that finally all supernodes can be extended and one edge in each cycle is deleted to obtain an arborescence. If the objective is to find a minimal branching, all edges of nonnegative cost are deleted in advance.

The corresponding ILP formulation results from a straightforward combination of the subtour elimination constraints (2.2) to avoid cycles and the additional **degree constraints**

$$\sum_{e \in \delta^{in}(v)} x_e \leq 1 \qquad \forall\, v \in V, \tag{2.7}$$

and the cardinality constraints (2.1) for arborescences. We analogously define the **arborescence polytope**

$$P_{Arb}(G) := \left\{ x \in [0,1]^m \;\middle|\; (2.1),\ (2.2),\ (2.7) \right\}$$

and the **branching polytope**

$$P_{Bra}(G) := \left\{ x \in [0,1]^m \;\middle|\; (2.2),\ (2.7) \right\}$$

which we sometimes shortly call P_{Arb} and P_{Bra}. They both are integral and the vertices of $P_{Arb}(G)$ and $P_{Bra}(G)$ are exactly the incidence vectors of arborescences and branchings of G [59]. The dimensions of the polytopes are $\dim(P_{Arb}(G)) = |E|-1$ and $\dim(P_{Bra}(G)) = |E|$, which implies that a set of $|E|$ affinely independent incidence vectors of arborescences exists. Moreover the following lemma proves that this set can be chosen in a certain way which will be useful in Chapter 5.

Lemma 2.3.2.

Let $G = (V, E)$ be a complete directed graph with $|E| =: m$. There exists a set $\mathcal{A}$ of m affinely independent incidence vectors of arborescences such that each vertex $v \in V$ is root node of at least one of the arborescences in $\mathcal{A}$.

Proof. We prove the result by induction over the number n of vertices $V = \{v_1, \ldots, v_n\}$ in G. For $n = 2$ the incidence vectors of the two arborescences $A_1 = \{(v_1, v_2)\}$ and $A_2 = \{(v_2, v_1)\}$ are affinely independent and both vertices v_1 and v_2 are root nodes in one case. Now let the statement hold for a certain $n \in \mathbb{N}$ and consider the complete graph $G' = (V' = V \cup \{v_{n+1}\}, E')$ with $|E'| =: m'$. By induction hypothesis there exists a set $\mathcal{A}$ of m affinely independent incidence vectors of arborescences in $G[V]$, $A_1, \ldots, A_m$, such that each vertex $v_1, \ldots, v_n$ is a root node once. Adding the edge (v_1, v_{n+1}) to each element of $\mathcal{A}$ yields m arborescences in G', see Figure 2.2. The induction hypothesis guarantees affine independence and the root property for each vertex $v_1, \ldots, v_n$.

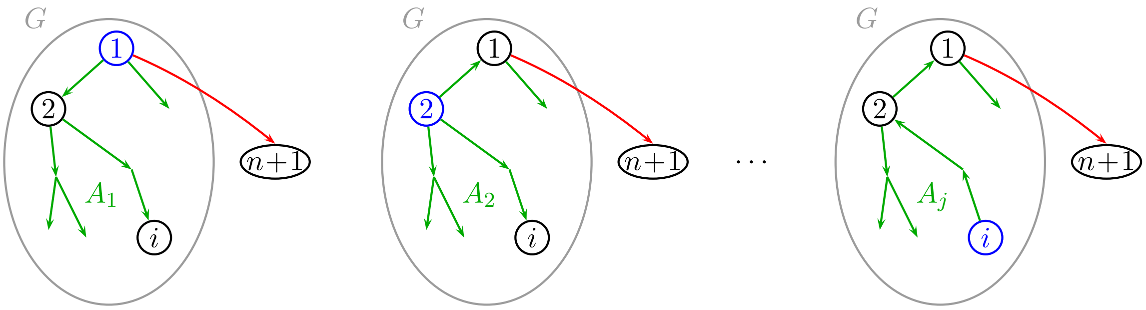


Figure 2.2: For each vertex $v_i \in V$ there exists an arborescence A_j in G having v_i as root node, colored in blue. Each of it can be extended to an arborescence in G' by adding edge (v_1, v_{n+1}) to A_j.

It is also guaranteed by the induction hypothesis that, in a second step, we can add each edge $e \in \delta(v_{n+1}), e \neq (v_1, v_{n+1})$ to an element $A_j \in \mathcal{A}$ such that $A_j \cup \{e\}$ is an arborescence in G', see Figure 2.3. By this we obtain $2n - 1$ arborescences in G' whose incidence vectors are pairwise affinely independent by Lemma 1.4.1.

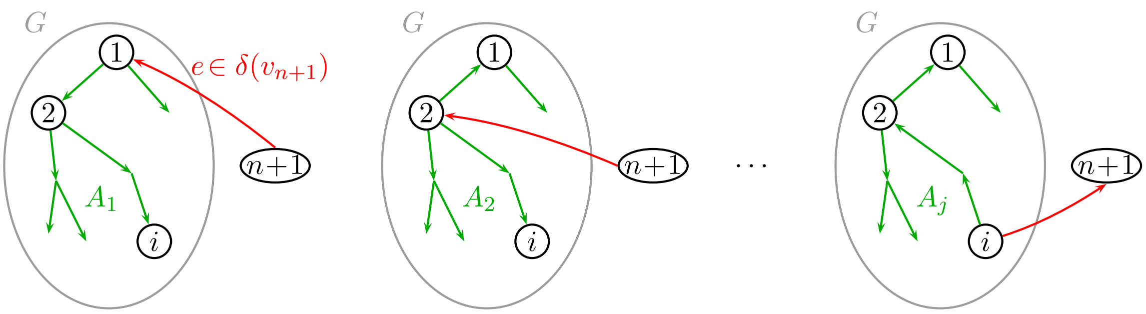


Figure 2.3: For each edge $e \in \delta(v_{n+1})$ there exists an arborescence A_i in G which can be extended to an arborescence in G' by adding e to A_i.

Finally, we add the incidence vector of the arborescence $A_1 \setminus (v_i, v_j) \cup (v_{n+1}, v_i) \cup (v_{n+1}, v_j)$ in G' where v_i is root node of A_1 and (v_i, v_j) is an edge in A_1. Then, v_{n+1} also is a root node such that we obtain a total number of $m + (2n - 1) + 1 = m'$ many affinely independent incidence vectors of arborescences in G' such that each vertex is root node of at least one arborescence.

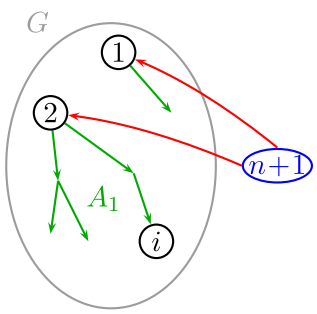


Figure 2.4: A_1 is splitted by removing edge (v_1, v_2) and an arborescence with v_{n+1} being root node in the extended graph results from adding (v_{n+1}, v_1) and (v_{n+1}, v_2).

□

2.4 Minimum assignments and maximum matchings

A perfect matching in a bipartite graph $G = (V_a \dot\cup V_b, E)$ is called **assignment**. The existence of an assignment is only possible if $|V_a| = |V_b|$ and if the distribution of the edges in the graph is appropriate. It can be tested by solving the **cardinality matching problem** in G which returns a matching M of maximal cardinality $|E(M)|$. This matching is perfect, i. e. an assignment, if and only if $|E(M)| = |V_a| = |V_b|$. The cardinality matching problem is solvable in polynomial time by directing all edges $e \in E$ from V_a to V_b and extending the graph by additional arcs from a new source vertex s to all vertices in V_a and additional arcs from all vertices in V_b to a new sink vertex t. A maximal s-t-flow in this network directly leads to a matching of maximal cardinality in G.

Since we want to analyze weighted cases of assignment and matching problems, we only consider complete (bipartite) graphs in the following to ensure the existence of an assignment.

Definition 2.4.1.

Let $G = (V_a \dot\cup V_b, E)$ be a complete bipartite graph with $|V_a| = |V_b|$ and a cost function $c : E \to \mathbb{R}$. The **minimum assignment problem** *(AP) is to find an assignment of minimal cost, i. e. a subgraph A of G with $E(A) \subseteq E$ which is an assignment and whose sum of costs $\sum_{e \in E(A)} c_e$ is minimal.*

Remark. *Another common definition for AP is by considering the assignment as a permutation π of the numbers $1, \dots, n$ such that $\sum_i c_{i\pi(i)}$ is minimized, where c_{ij} is the $(i, j)^{th}$ entry of the cost matrix $C \in \mathbb{R}^{n \times n}$.*

Changing the optimization direction, i. e., finding an assignment of maximal weight, can be reduced to the minimization problem by negating the cost function via setting $c_e = -c_e$ for all $e \in E$. A change of the graph structure to a non-bipartite graph in turn yields a fairly different problem, the **minimum weight perfect matching problem** (PMP). This problem is equivalent to the following to which we refer in this thesis when discussing matching problems.

Definition 2.4.2.

Let $G = (V, E)$ be a complete graph with a cost function $c : E \to \mathbb{R}$. The **maximum (weight) matching problem** *(MP) is to find a matching of maximal cost, i. e. a subgraph M of G with $E(M) \subseteq E$ which is a matching and whose sum of costs $\sum_{e \in E(M)} c_e$ is maximal.*

The two problems MP and PMP reduce to each other by a simple graph extension and slight changes of the cost function, see e. g. [117]. Since the matching not necessarily has to be perfect, the cost function can be restricted w. l. o. g. to only map to nonnegative values.

2.4.1 Combinatorial approaches and ILP formulations

The easier of the two problems is the assignment problem since the bipartiteness simplifies the structure significantly. The graph can be extended to a network as in the cardinality matching algorithm described at the beginning of this section. Here, the edges from s to $|V_a|$ and from $|V_b|$ to t obtain zero costs, the others retain the original costs c_e and all edge capacities are set to one. By this construction, any integral s-t-flow of value $|V_a| = |V_b|$ corresponds to an assignment of equal costs and vice versa. Thus, a minimum cost flow yields a minimum assignment and therefore, the polynomial runtime of the flow algorithm determines the runtime of an algorithm for AP.

The ILP formulation of AP is straightforward as the only constraint for an assignment is the degree of one for each vertex.

Proposition 2.4.3.
Let $G = (V_a \dot\cup V_b, E)$ be a complete bipartite graph with $|V_a| = |V_b|$ and let $c : E \to \mathbb{R}$ be the cost function on the edges of G. The minimum assignment problem can be formulated as an integer linear program as follows:

$$
\begin{aligned}
(\mathrm{ILP_{AP}}) \qquad & \min \sum_{e \in E} c_e x_e \\
& \text{s. t.} \sum_{e \in \delta(v)} x_e = 1 \qquad \forall\, v \in V && (2.8) \\
& \qquad\qquad x_e \in \{0, 1\} \qquad \forall\, e \in E && (2.9)
\end{aligned}
$$

□

The constraints (2.8) are called **degree constraints** in the following. The ILP formulation ($\mathrm{ILP_{MP}}$) for MP equals the one for AP except that the degree constraints (2.8) are relaxed to inequality constraints

$$\sum_{e \in \delta(v)} x_e \leq 1 \qquad \forall\, v \in V. \tag{2.10}$$

Also the maximum weight matching problem is polynomially solvable, even though the arbitrary graph structure complicates the calculation significantly. The weighted matching algorithm developed by Edmonds [58] is a primal-dual approach and is presented for the equivalent minimum weighted perfect matching problem. It uses the fact that at least one matching edge has to be in the cut of any odd-cardinality subset of vertices. With $\mathcal{S} := \{S \subseteq V \mid |S| \text{ odd}\}$, each perfect matching satisfies the **(outer) blossom inequalities**

$$\sum_{e \in \delta(S)} x_e \geq 1 \qquad \forall\, S \in \mathcal{S}, \tag{2.11}$$

and thus, these inequalities can be added to the ILP formulation of PMP. We obtain ($\mathrm{ILP_{AP}}$) combined with (2.11) and denote the resulting integer program with ($\mathrm{ILP_{PMP}}$) and its relaxation with ($\mathrm{LP_{PMP}}$). The dual of ($\mathrm{LP_{PMP}}$) reads

$$
\begin{aligned}
(\mathrm{DP_{PMP}}) \qquad & \max \sum_{S \in \mathcal{S}} z_S \\
& \text{s. t.} \sum_{\substack{S \in \mathcal{S} \\ e \in \delta(S)}} z_S \leq c_e \qquad \forall\, e \in E \\
& \qquad\qquad z_S \geq 0 \qquad \forall\, S \in \mathcal{S} \text{ with } |S| > 1.
\end{aligned}
$$

Edmonds' weighted matching algorithm now starts with an empty matching and a feasible dual solution where $z_s = \frac{1}{2} \min\{c_e \mid e \in \delta(S)\}$ for all $|S| = 1$ and $z_S = 0$ else, and iteratively extends the matching until it is perfect, where in each step the dual solution is adapted accordingly such that the complementary slackness constraint 1.2.5 (c) is satisfied. Since z_S always remains feasible in ($\mathrm{DP_{PMP}}$), both primal and dual optimality is guaranteed when the algorithm terminates.

2.4.2 Polyhedral descriptions

Let $G = (V_a \dot\cup V_b, E)$ be a complete bipartite graph with $|V_a| = |V_b|$ and with m edges. We define the **assignment polytope** as

$$P_A(G) := \left\{ x \in [0, 1]^m \;\middle|\; (2.8) \right\},$$

The following theorem of Birkhoff [21] guarantees that $P_A(G)$ equals the convex hull of all assignments, therefore, $P_A(G)$ is also known as the **Birkhoff polytope**. The convex hull of assignments is given as follows. Consider (ILP_{AP}) and relax the binary constraints to $x_e \geq 0$ for all $e \in E$. Denote the resulting problem with (LP_{AP}).

Theorem 2.4.4 (Birkhoff)**.**
Let $G = (V_a \dot\cup V_b, E)$ be a complete bipartite graph with $|V_a| = |V_b|$ and a cost function $c : E \to \mathbb{R}$. The minimum weight of an assignment is equal to the optimal value of (LP_{AP}).

Proof. Since the graph is bipartite, the incidence matrix of G is totally unimodular. Since additionally the right-hand side of (2.8) is integral, the corresponding polyhedron is integral [104]. □

A second way to prove Birkhoff's Theorem is to adapt Edmonds' primal-dual matching algorithm to the bipartite case, such that the shrinking steps can be omitted. This bipartite version is called **Hungarian Algorithm** and was first developed by Kuhn [119] and Munkres [135].

Another direct consequence of the primal-dual weighted matching algorithm is that the **perfect matching polytope**

$$P_{PMP}(G) := \left\{ x \in [0,1]^m \;\middle|\; (2.8),\ (2.11) \right\}$$

is integral and that its vertices are exactly the incidence vectors of perfect matchings of a complete graph G. On complete bipartite graphs with $|V_a| = |V_b| = n$, the dimension of the polytopes $P_A = P_{PMP}$ is equal to $m - 2n + 1$ [129].

Although the maximum weight matching problem can be formulated as a mimimal perfect matching problem, the blossom inequalities (2.11) are not valid for maximum weight matchings as any matching can be an optimal solution of MP. Edmonds [58] and Pulleyblank [152] proved that nevertheless odd subsets are needed to define the matching polytope: in each set $S \subseteq V$ with $|S|$ odd there are at most $(|S| - 1)/2$ edges in a matching. Thus, any matching satisfies the **(inner) blossom inequalities**

$$\sum_{e \in E(G[S])} x_e \leq \frac{|S| - 1}{2} \qquad \forall\, S \in \mathcal{S}. \tag{2.12}$$

In [48, 158] it is shown that these blossom inequalities are facet defining if S satisfies two conditions. On the one hand, $G[S]$ must be **two-connected**, i. e. $G[S]$ is connected and for each vertex $v \in S$ the subgraph $G[S \backslash \{v\}]$ remains connected. On the other hand $G[S]$ must be **hypomatchable**, i. e. for each $v \in S$, $G[S \backslash \{v\}]$ has a perfect matching. Note that these conditions are always satisfied in complete graphs such that in this case all blossom inequalities are facet inducing. The proof is based on the idea that the face induced by one of the inequalities is not contained in any larger proper face of the polytope. A modified version is presented in Section 7.2.

Indeed, the degree constraints for matchings and the inner blossom inequalities for odd sets yield a complete description of the matching polytope [58].

Theorem 2.4.5 (Edmonds)**.**
Let $G = (V, E)$ be a complete graph. The **matching polytope**

$$P_{MP}(G) := \left\{ x \in [0,1]^m \;\middle|\; (2.10),\ (2.12) \right\}$$

is integral and its vertices are exactly the incidence vector of all matchings in G.

Proof. Obviously, the incidence vector of any matching satisfies (2.10) and (2.12). Conversely, we show that each vector $x \in P_{MP}(G)$ is a convex combination of incidence vectors of matchings. For this, create a copy $G' = (V', E')$ of G and connect each vertex $v \in V$ with its copy $v' \in V'$. Define the vector $\tilde{x} \in \mathbb{R}^{2|E|+|V|}$ with $\tilde{x}_e := x_e$ for all original and copied edges $e \in E \cup E'$ and with $\tilde{x}_{\{v,v'\}} := 1 - \sum_{e\in\delta(v)} x_e$ for all $v \in V$. Then, x is the incidence vector of a matching in G if $\tilde{x}$ is the incidence vector of a perfect matching in the extended graph $\tilde{G}$. Obviously, $\tilde{x}$ is nonnegative and satisfies (2.8) with respect to $\tilde{G}$. It remains to show that $\tilde{x}$ also satisfies (2.11), since then, $\tilde{x} \in P_{PMP}(\tilde{G})$. For this, let $S \subseteq V \cup V'$ with $|S|$ odd. Define $A := \{v \in V \mid v \in S, v' \notin S\}$, $B := \{v \in V \mid v, v' \in S\}$ and $C := \{v \in V \mid v \notin S, v' \in S\}$. Since $|S|$ is odd, either $|A|$ or $|C|$ are odd, too, w.l.o.g. let A have odd cardinality such that (2.12) holds. We obtain

$$\begin{aligned}
\sum_{e\in\delta(S)} \tilde{x}_e &\geq \sum_{v\in A}\sum_{e\in\delta(v)} \tilde{x}_e - 2\sum_{e\in E(\tilde{G}[A])} \tilde{x}_e - \sum_{\substack{e=\{a,b\}\\ a\in A, b\in B}} \tilde{x}_e - \sum_{\substack{e=\{a',b'\}\\ a\in A, b\in B}} \tilde{x}_e \\
&= \sum_{v\in A}\sum_{e\in\delta(v)} \tilde{x}_e - 2\sum_{e\in E(G[A])} x_e \\
&\geq |A| - (|A| - 1) = 1.
\end{aligned}$$

□

With the use of the (relaxed) degree constraints and the blossom inequalities, the matching problems can also be solved by an LP approach. The exponential number of the blossom inequalities requires a polynomial time separation algorithm.

2.4.3 Separation of the blossom inequalities

The idea of a blossom separation algorithm origins from Padberg and Rao [140]. Later it was reused in an approach of Letchford et al. [126] and modified to a more general algorithm structure. Both approaches are motivated by the **slack** $s_i := 1 - \sum_{e\in\delta(i)} x_e$ of the degree inequality (2.10) of each vertex $i \in V$. For all $S \in \mathcal{S}$, inequality (2.12) can be re-written as follows.

$$\begin{aligned}
& & |S| - 2\sum_{e\in E(G[S])} x_e &\geq 1 \\
&\Leftrightarrow & \sum_{i\in S} 1 - 2\sum_{e\in E(G[S])} x_e &\geq 1 \\
&\Leftrightarrow & \sum_{i\in S}(s_i + \sum_{e\in\delta(i)} x_e) - 2\sum_{e\in E(G[S])} x_e &\geq 1 \\
&\Leftrightarrow & \sum_{i\in S} s_i + \underbrace{\sum_{i\in S}\sum_{e\in\delta(i)} x_e - 2\sum_{e\in E(G[S])} x_e}_{(*)} &\geq 1
\end{aligned}$$

Consider $(*)$. The double sum counts all adjacent edges of vertices in S, that is once all edges with only one endnode in S and twice all edges with both endnodes in S. The last sum contains exactly the latter edges and is subtracted twice. Hence we obtain those edges with one endnode in S, i.e., the cut of S, and equivalently write

$$\sum_{i\in S} s_i + \sum_{e\in\delta(S)} x_e \geq 1. \tag{2.13}$$

Let $x^* \in [0,1]^m$ satisfy the degree inequalities. Extend $G = (V, E)$ to $G_d = (V_d, E_d)$ by a new dummy vertex d and additional edges $\{d, i\}$ for each node $i \in V$. Assign the weight x^*_e to each edge $e \in E$ and the weight $s^*_i = 1 - \sum_{e \in \delta(i)} x^*_e$ to each of the new edges $\{d, i\}$. Then, the left-hand side of (2.13) equals the value of an odd cut in G_d, i.e. a cut $S \subseteq V_d \setminus \{d\}$ with $|S|$ odd.

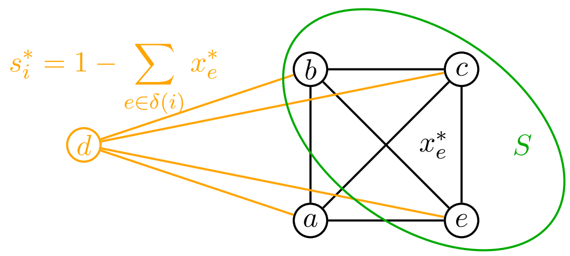


Figure 2.5: The value of an odd cut $S \in V_d \setminus \{d\}$ is equal to the value of the left-hand side of inequality (2.13).

As a consequence, inequality (2.13) is violated if there exists an odd-cut S in G_d not containing the dummy vertex d. This can be verified by using T-odd cuts. For a set T of even cardinality a cut $\delta(S)$ is called ***T*-odd cut** if $|T \cap S|$ is odd. Therefore, we define $T := V$ if $|V|$ is even, and $T := V_d$ otherwise, such that T has even cardinality in both cases. If the **minimum *T*-odd cut** in G_d, i.e. the T-odd cut of minimal cost with respect to the weight function, has a value less than 1, (2.13) is violated and so is (2.12). A minimum T-odd cut in turn can be calculated in polynomial time e.g. by the Gomory-Hu algorithm [89] which leads to a polynomial time separation algorithm for the blossom inequalities (2.12).

Chapter 3

Binary Quadratic Optimization Problems

A **quadratic program** (QP) optimizes a quadratic objective function over a polyhedron. Similar to linear and integer linear programs a QP is defined by a matrix $Q \in \mathbb{R}^{n\times n}$ for the quadratic objective function, a matrix $A \in \mathbb{R}^{m\times n}$ and a vector $b \in \mathbb{R}^m$ for the linear side constraints and the optimization direction. A feasible solution $x \in \mathbb{R}^n$ satisfies the side constraints $Ax \leq b$ and an optimal solution x^* optimizes the objective function $x^\top Qx$. In a **binary quadratic program** (BQP) each entry of x is required to be zero or one. The diagonal entries q_{ii} of Q represent the coefficients where the variable x_i is multiplied with itself. A squared binary variable always has the same value as the variable itself, i. e. Q implicitly includes the linear terms on the diagonal. For the sake of convenience, we extract these linear terms, write them in an extra column vector $c \in \mathbb{R}^n$ and only consider matrices Q with $Q_{ii} = 0$ for all $i \in \{1, \ldots, n\}$. Similar to the ILP formulation we write

$$\text{(BQP)} \qquad \begin{aligned} \min \quad & c^\top x + x^\top Qx \\ \text{s.t.} \quad & Ax \leq b \\ & x \in \{0,1\}^n \end{aligned}$$

The **underlying** linear problem optimizes over the same constraints but only a linear objective function $\bar{c}^\top x$. In the following we denote the corresponding polyhedron with

$$P_{\{0,1\}} := \operatorname{conv}\Big\{x \in \{0,1\}^n \;\Big|\; Ax \leq b\Big\}$$

and the polyhedron of the relaxed problem with

$$P := \operatorname{conv}\Big\{x \in [0,1]^n \;\Big|\; Ax \leq b\Big\}.$$

Binary quadratic problems are NP-complete in general [77, 167]. The high complexity has two reasons, corresponding to two NP-hard subproblems. On the one hand, the binary constraints are hard to deal with, already in the linear case, i. e., the underlying linear problem is NP-hard in general. On the other hand, even the unconstrained problem which minimizes the objective function $c^\top x + x^\top Qx$ over arbitrary $x \in \{0,1\}^n$ is NP-hard as it is equivalent to the max cut (MC) problem [14, 55]. MC searches for the maximal cut in a weighted graph and is NP-hard [112] even if the edge costs are restricted to be exactly 1 [78]. Note that this is not the case for BQP since this problem becomes trivial in the case where all costs are positive.

The complexity of BQP is even reflected in practice by high computing times and by only few instance classes which are polynomially solvable, e. g. if Q is positive semidefinite with fixed rank [13] or if the elements of Q are non-positive [150]. Actually BQP remains hard if Q is positive definite or if Q is negative definite and linear costs c do exist [5]. Since quadratic formulation with binary variables is very powerful, nevertheless there exist many approaches, see e. g. [142].

In this thesis we restrict ourselves to BQP problems whose underlying linear problems are efficiently solvable, whether by a combinatorial algorithm, a separation routine or an LP formulation. Due to the complexity of unconstrained BQP, the quadratic versions nevertheless become NP-hard in general. As concrete problems we mainly consider the quadratic versions of minimum spanning trees and forests, refine the results for the directed versions, i. e. minimum arborescences and branchings, and also develop results for minimum weight assignments and maximum weight matchings.

3.1 Linearization

Most approaches to tackle BQP first of all get rid of the quadratic terms $x_i x_j$ in the objective function as they are one reason for the high complexity. Note that a quadratic term exists if the corresponding entry in Q is non-zero. We denote the set of all pairs appearing in a quadratic monomial in the objective function with $\mathcal{Q} := \{\{i,j\} \in N \times N \mid Q_{ij} + Q_{ji} \neq 0\}$, where $N := \{1, \ldots, n\}$.

A common way is to replace the monomials by auxiliary variables which yields a linear description in a higher dimension. The first approaches restricted the new variables to be binary, see e. g. [10, 51, 71, 121], which then was extended to approaches with continuous positive variables out of which we particularly consider the classical method of Glover and Woolsey [84], called **standard linearization**, in the following. Here, for each monomial $x_i x_j$ with $\{i,j\} \in \mathcal{Q}$ one auxiliary variable y_{ij} is introduced. Note that by this definition y_{ij} and y_{ji} denote the same variable. For the ease of notation we also define $q_{ij} = Q_{ij} + Q_{ji}$. The new **product variables** y_{ij} are linked to the original linear variables by adding the following linear inequalities to BQP.

$$y_{ij} \leq x_i, x_j \qquad \forall\ \{i,j\} \in \mathcal{Q} \tag{3.1}$$

$$y_{ij} \geq x_i + x_j - 1 \quad \forall\ \{i,j\} \in \mathcal{Q} \tag{3.2}$$

Additionally, the auxiliary variables have to be nonnegative. For the ease of notation we write $y \in \{0,1\}^{|\mathcal{Q}|}$ in the following.

The first set of inequalities, (3.1), makes sure that the product variable obtains a value of zero if one or both of the corresponding linear variables is zero. If both linear variables x_i and x_j are set to one, (3.2) leads to $y_{ij} \geq 1$ and with binarity of y to a value of one. Hence the value of every y_{ij} is exactly the product of x_i and x_j whenever $x \in \{0,1\}^n$.

We denote the resulting linearized problem with LBQP, which then is equivalent to BQP in terms of the x-variables and of the objective value. In other words, an optimal solution of LBQP directly leads to an optimal solution of BQP by projecting out the auxiliary y-variables, and, vice versa, each optimal solution can be lifted to an optimal solution of LBQP by setting $y_{ij} = x_i x_j$ for all $\{i,j\} \in \mathcal{Q}$. The dimension of LBQP thus rises by the number of product terms. We denote the convex hull of all integral solutions with

$$P^{ql}_{\{0,1\}} := \operatorname{conv}\left\{(x,y) \in \{0,1\}^{n \times |\mathcal{Q}|} \;\middle|\; Ax \leq b, (3.1), (3.2)\right\}$$

and the polytope of the relaxed problem with

$$P^{ql} := \operatorname{conv}\left\{(x,y) \in [\,0,1\,]^{n \times |\mathcal{Q}|} \;\middle|\; Ax \leq b, (3.1), (3.2)\right\}.$$

If the underlying BQP is unconstrained, $P^{ql}_{\{0,1\}} = \text{conv}\{(x, y) \in \{0,1\}^{n\times|\mathcal{Q}|} \mid (3.1), (3.2)\}$ is called **boolean quadric polytope**, which was introduced and widely analyzed by Padberg [139].

By reasons of complexity one cannot expect that $P^{ql}_{\{0,1\}} = P^{ql}$. Nevertheless the optimal value of P^{ql} defines a lower bound which was shown to be equal to other lower bounds mentioned in the literature [98]. Other linearization approaches are motivated by maintaining the number of auxiliary variables possibly small, such as the compact linearizations of Glover [83], of Adams, Forrester and Glover [2] and of Hansen and Meyer [101]. They achieve the same lower bounds as the standard linearization [101].

To gain better bounds, Adams and Sherali [4] investigated additional possibilities to strenghten the standard linearization (3.1) and (3.2) as much as possible. They proposed to strengthen the linear constraints by multiplying with linear variables, exploiting their binarity. More precisely, in a first step, each inequality $\sum_{i\in N} a_i x_i \le b$ is multiplied with x_j separately for each $j \in N$. Then, all resulting products $x_i x_j$ are replaced by the corresponding linearization variables y_{ij} if $i \ne j$, and the product $x_i x_i$ is simply replaced by x_i due to the binarity of x. Hence, the stronger inequalities

$$\sum_{i\in N\setminus\{j\}} a_i y_{ij} + (a_j - b)x_j \le 0 \qquad \forall\, j \in N$$

are obtained, which even dominate the original ones. The same holds for a multiplication with the complement $1 - x_f$, separately for each $f \in E$:

$$\sum_{i\in N\setminus\{j\}} a_i(x_i - y_{ij}) + bx_j \le b \qquad \forall\, j \in N.$$

The same procedure can be applied for all equations of BQP. Here, the multiplication with x_j suffices; a multiplication with $1 - x_j$ yields the same results. Therefore, also the equations

$$\sum_{i\in N\setminus\{j\}} a_i y_{ij} + (a_j - b)x_i = 0 \qquad \forall\, j \in N$$

can be added to LBQP. Due to the authors we call this method **Sherali-Adams reformulation** or **linearization**. The advantage of this method are the significantly stronger bounds resulting from the combination of several linearization variables in each inequality. Moreover, the standard linearization is implicitely contained in the Sherali-Adams reformulation when also multiplying the bounds $x_i \ge 0$ and $x_i \le 1$ with $1 - x_j$ for all $\{i, j\} \in \mathcal{Q}$.

Applying this procedure $d \le n$ times yields the **Sherali-Adams reformulation of order d**: Let $J_1, J_2 \subseteq N$ be disjoint subsets with $|J_1 \cup J_2| = d$, then each original inequality is multiplied with d many variables or complements,

$$\Big(\sum_{i\in N} a_i x_i - b\Big) \cdot \Big(\prod_{j\in J_1} x_j\Big)\Big(\prod_{j\in J_2} (1 - x_j)\Big) \le 0,$$

and, after a replacement of each product term $\Pi_{j\in J} x_j$ by a linearization variable y_J, the convex hull of the feasible solutions is denoted with P_d. Sherali and Adams proved that its projection $P_{Pd} := \{x \in [0,1]^{|E|} \mid (x, y) \in P_d\}$ yields a better approximation of the original polytope with increasing d, and, moreover, that the reformulation of order n is exactly the convex hull of all integer points of P. This yields

$$P \supseteq P_{P1} \supseteq P_{P2} \supseteq \ldots \supseteq P_{Pn} = P_{\{0,1\}},$$

and an exact linear reformulation of the quadratic problem. By reasons of complexity it follows that the LP size increases exponentially in order d. But even more, the number of additional constraints depends on both the number of linear variables and the number of the original constraints such that this approach becomes too complex in practice even for small d. Note that even in the case of $d = 1$ the number of constraints can become extremely high.

Moreover, the multiplication with d linear variables creates $\sum_{i=1}^{d} \binom{n}{i}$ linearization variables and lifts the corresponding polytope P_d in an extremely high dimension. In the case of $d = 1$, only variables of quadratic terms are created, which also is done when applying the standard linearization. But in case that not all quadratic terms appear in the objective function of (BQP), i. e., if $|\mathcal{Q}|$ is small, the reformulation technique creates additional quadratic terms respective linearization variables when variables are multiplied where no corresponding quadratic term exists. By this, the problem size is artificially increased and especially in the case with very few or even a single quadratic term this method obviously becomes inefficient.

Another strengthening of the standard linearization was presented by Caprara in [37]. Here, the fact is used that $x_i = 1$ implies $y_{ij} = x_j$, such that $(y_{ij})_{j\in N} \in P_{\{0,1\}}$ with $y_{ii} = x_i$. With the definition

$$P^{x_i}_{\{0,1\}} := \begin{cases} \{0^n\} & \text{if } x_i = 0 \\ P_{\{0,1\}} & \text{if } x_i = 1 \end{cases}$$

and the linear constraints defining $P_{\{0,1\}}$, we can write equivalently

$$P^{x_i}_{\{0,1\}} = \left\{ (y_{ij})_{j\in N} \in \{0, x_i\}^n \;\middle|\; \sum_{j\in N\setminus\{i\}} a_{kj} y_{ij} + (a_{ki} - b_k) x_i \leq 0,\ \forall\, k \in \{1, \dots, m\} \right\}$$

and obtain the linearization

$$\begin{aligned}
(\text{LIN}_{\text{sep}}) \qquad \min \quad & \sum_{i\in N} c_i x_i + \sum_{i\neq j\in N} q_{ij} y_{ij} \\
\text{s.t.} \quad & x \in P_{\{0,1\}} \\
& (y_{ij})_{j\in N} \in P^{x_i}_{\{0,1\}} && \forall\, i \in N \\
& y_{ij} \leq x_i && \forall\, i \neq j \in N \\
& y_{ij} \geq x_i + x_j - 1 && \forall\, i \neq j \in N
\end{aligned}$$

which is stronger than the standard linearization. By relaxing the latter constraints the problem gets tractable and leads to good dual bounds, see Section 3.3. The disadvantage again is that in the case where originally only few quadratic terms appear in the objective function a large number of additional linearization variables are created which would not be necessary in the standard linearization approach.

In addition there exist several other linearization approaches, which mostly are established for special cases of BQPs, such as the quadratic knapsack problem [20] and variants of the quadratic assignment problem [3, 113, 127]. A survey of linearization approaches can be found, e. g., in [100]. As it fits best for our purpose, we concentrate on the standard linearization and the corresponding polyhedra $P^{ql}_{\{0,1\}}$ and P^{ql}.

3.2 Cutting planes

The idea to add cutting planes to approach the polyhedron $P^{ql}_{\{0,1\}}$ and the optimal solutions with respect to a certain objective function is as obvious as complex. There mainly exist highly problem specific approaches, out of which we present the ones for the optimization problems which we investigate in Part II of this thesis in the respective chapters. One semi-specific approach is presented in [28, 29] where a variant of local cuts (c. f. [7]), so-called **target cuts**, is introduced. Here, the problem structure is exploited for a projection to a lower dimensional space in which the generation of the cutting planes is performed problem-independently.

Other approaches are mainly focused on the unconstrained case, respectively on the equivalent max cut problem. This special case is nevertheless productive as any cutting plane developed for the cut polytope P_C, which is the convex hull of all cuts in a given graph, is also a valid cutting plane of $P^{ql}_{\{0,1\}}$ after a simple transformation. A basic class of cutting planes are the **triangle inequalities** $x_{uv} - x_{uw} - x_{vw} \leq 0$ and $x_{uv} + x_{uw} + x_{vw} \leq 2$ for pairwise distinct vertices $u, v, w \in V$ in a graph $G = (V, E)$. In a complete graph these inequalities are satisfied by any cut since each cycle of exactly three edges $\{u, v\}, \{u, w\}, \{v, w\}$ is cut either twice or not at all. The **cycle inequalities** $\sum_{e \in F} x_e - \sum_{e \in C \setminus F} x_e \leq |F| - 1$ on arbitrary cycles C in the graph and subsets $F \subseteq C$ of odd cardinality define the **semimetric polytope** P_{SM}. Each cycle inequality is valid for any cut and, if the graph is complete, they are in accordance with the triangle inequalities. Therefore, $P_C \subseteq P_{SM}$ and the cycle inequalities are valid cutting planes for BQP. More cutting planes for $P^{ql}_{\{0,1\}}$ are hypermetric, gap, clique-web inequalities and others, detailed studies with facet defining properties and an explanation of corresponding separation routines can be found in [56, 57, 72].

3.3 Lower bounds

To solve a BQP exactly via a branch-and-bound approach, good lower bounds on the objective value are needed such that branches of the B&B tree can be truncated preferably fast. As a matter of course such bounds can be attained by relaxing, e. g., the integrality constraints of the ILP formulation. The addition of cutting planes might improve these bounds.

An alternative approach is a semidefinite program (SDP) formulation for instance for the max cut problem. The underlying graph can be characterized by its Laplace matrix L, leading to the problem formulation

$$\max\{x^\top Lx \mid x \in \{-1, 1\}^n\},$$

which, by the use of $x^\top Lx = tr(L(xx^\top))$, leads to the SDP relaxation

$$\max\{\langle \frac{1}{4}L, X\rangle \mid \operatorname{diag}(X) = e, X \succeq 0\}.$$

The resulting optimal value is a good lower bounds for the original problem. Also here, additional cutting planes might improve the bounds, such as in the case of added triangle inequalities, yielding a very fast algorithm [143, 154]. This approach is also applied successfully for other BQP such as the quadratic knapsack problem [102] or the quadratic linear ordering problem [31]. The strength of a cutting plane not only depends on the underlying problem which is modeled as an SDP but also on quadratic reformulations of the constraints, c. f. a study on the different reformulations for the quadratic knapsack problem in [102].

A widely used approach for generating lower bounds is **Lagrangean relaxation**. The idea is to move constraints of a given problem into the objective function and to multiply each of them with a nonnegative penalty factor, the **Lagrangean multiplier** λ, such that a violation of a relaxed constraint is penalized with additional costs, depending on the violation and λ [69, 80]. For a problem (P) with two sets of constraints $Ax \leq b$ and $Cx \leq d$ the Lagrangean relaxation of the latter set

$$(\mathrm{R}_\lambda) \qquad \begin{aligned} \min \quad & f_\lambda(x) = f(x) + \lambda^\top (Cx - d) \\ \text{s. t.} \quad & Ax \leq b \\ & x \in \{0, 1\}^n \end{aligned}$$

provides a lower bound for (P) for each $\lambda \geq 0$ since

$$f_\lambda(x^*) \leq f_\lambda(x) = f(x) + \underbrace{\lambda^\top}_{\geq 0} \underbrace{(Cx - d)}_{\leq 0} \leq f(x)$$

for an optimal solution x^* in (R_λ) and any vector x which is feasible in (P). The value of λ therefore determines the quality of the relaxation on the one hand, as a greater Lagrangean multiplier yields stronger penalties for violations, but it also determines the quality of the lower bound such that the choice of λ always is a trade-off between bounds and feasibility. The ideal choice thus is the multiplier λ which yields the greatest lower bound, i. e. the solution of $\max\{\mathrm{val}(\mathrm{R}_\lambda) \mid \lambda \geq 0\}$. This problem is called the **Lagrangean dual** of (P) with respect to the relaxed constraints $Cx \leq d$ [79]. Lagrangean relaxation is widely applied for binary quadratic problems such as in [138] and [149] for the quadratic minimum spanning tree (QMST) problem, which will be discussed in Chapter 4, or in [73] and [125] for the quadratic assignment problem (QAP), see Chapter 6.

A classical lower bound is the **Gilmore-Lawler bound** (GLB) for the QAP. The name is dedicated to the ideas of Gilmore [82] and Lawler [121], who independently proposed to relax the quadratic function to a linear one and simply take the value of the optimal solution of the resulting linear assignment problem as a lower bound. One definition of the QAP, c. f. Chapter 6, is to find an optimal permutation π on the numbers $1, \dots, n$ with respect to the cost defining matrices $A, B \in \mathbb{R}^{n \times n}$, such that the objective is to find a permutation minimizing

$$\sum_{i=1}^{n} \sum_{j=1}^{n} b_{ij} c_{\pi(i)\pi(j)}.$$

Let a_i and b_i be the row vectors of the matrices A and B and $\bar{a}_i$ and $\bar{b}_i$ be the column vectors without the element a_{ii} and b_{ii}, respectively. With the definition of the minimal permuted vector product $\langle u, v\rangle := \min\{\pi \text{ permutation} \mid \sum_{i=1}^{n} u_i v_{\pi(i)}\}$ for $u, v \in \mathbb{R}^n$, the GLB bound obtains the value of the minimal linear assignment with respect to the linear function

$$l_{ij} := a_{ii} b_{jj} + \langle \bar{a}_i, \bar{b}_j \rangle.$$

To compute the minimal permuted vector product, a linear AP has to be solved for each fixed pair $\{i, j\}$ with $i \neq j \in \{1, \dots, n\}$, leading to about n^2 assignment problems.

Caprara [37] generalized the method of calculating the Gilmore-Lawler bound to arbitrary BQP. Again, the quadratic objective function is reduced to linear functions such that lower bounds are obtained by solving the underlying linear problem. If the objective function of (BQP) is expressed as

$$\min \sum_{i=1}^{n} \underbrace{\left(\sum_{j=1}^{n} q_{ij} x_j \right)}_{(\star)} x_i$$

with $q_{jj} = c_j$, and if $x_i = 1$, ($\star$) cannot be smaller than $p_i := \min\{\sum_{j=1}^{n} q_{ij} x_j \mid x \in P_{\{0,1\}}, x_i = 1\}$. For all i the value of p_i can be computed by n linear optimizations over $P_{\{0,1\}}$ with the respective fixing $x_i = 1$ and the lower bound for BQP is obtained by solving the linear problem

$$L_0 := \min \left\{ \sum_{i=1}^{n} p_i x_i \;\middle|\; x \in P_{\{0,1\}} \right\}$$

To improve this lower bound, note that it is affected by different subdivision of the quadratic costs into $q'_{ij} + q'_{ji} = q_{ij}$. Therefore, Caprara proposed to find the subdivision which maximizes L_0 [37]. For this, consider again the reformulation ($\mathrm{LIN}_{\mathrm{sep}}$) introduced in Section 3.1. The linearization variables are separated into y_{ij} and y_{ji} for each $i < j$ and constrained to be equal. The linear problem then reads

$$
\begin{aligned}
(\text{LIN'}_{\text{sep}}) \qquad \min \quad & \sum_{i=1}^{n} c_i x_i + \sum_{i \neq j=1}^{n} q_{ij} y_{ij} && && (3.3)\\
\text{s.t.} \quad & x \in P_{\{0,1\}} && && (3.4)\\
& (y_{ij})_{j \in \{1,\dots,n\}} \in P_{\{0,1\}}^{x_i} && \forall\, i \in \{1,\dots,n\} && (3.5)\\
& y_{ij} \leq x_i && \forall\, i < j \in \{1,\dots,n\} && (3.6)\\
& y_{ij} \geq x_i + x_j - 1 && \forall\, i < j \in \{1,\dots,n\} && (3.7)\\
& y_{ij} = y_{ji} && \forall\, i < j \in \{1,\dots,n\}. && (3.8)
\end{aligned}
$$

Although this operation doubles the number of variables, this reformulation has two advantages. On the one hand the optimal solution of this reformulation without constraints (3.7) and (3.8) equals the lower bound L_0. On the other hand, the problem becomes tractable when omitting these two classes of constraints. As a result, a natural improvement of L_0 can be obtained by a Lagrangean relaxation of (3.7) or (3.8), or both.

The idea of calculating underestimators for each fixation $x_i = 1$ was already presented by Assad and Xu in [8] for a certain class of BQP. This class consists of those problems which are constrained by an equation $\sum_i x_i = K$ for some $K \in \mathbb{Z}$ and whose underlying linear problem is efficiently solvable, such as the QAP and the QMST. The idea is to change the matrix entries by a vector $u \in \mathbb{R}^n$ to

$$
\begin{aligned}
c_i(u) &:= c_i - (K-1)u_i\\
q_{ij}(u) &:= q_{ij} + u_j,
\end{aligned}
$$

which leaves the value of the objective function unchanged for all $x \in P_{\{0,1\}}$ such that it can be expressed as

$$
\min \sum_i \underbrace{\Big(c_i(u) + \sum_j q_{ij}(u) x_j \Big)}_{(\blacktriangle)} x_i .
$$

The term $(\blacktriangle)$ is not smaller than $f_i(u) := \min\{c_i(u) + \sum_j q_{ij}(u)x_j \mid x \in P_{\{0,1\}}, x_i = 1\}$. Thus, a lower bound $b(u)$ for BQP can be found by minimizing $\sum_i f_i(u)x_i$ with $x \in P_{\{0,1\}}$ and the best lower bound is again the one corresponding to the optimal vector $\bar{u}$, which can be calculated by solving $\bar{b} = \max\{b(u) \mid u \in \mathbb{R}^n\}$, e. g. by standard subgradient techniques or the leveling procedure proposed in [8].

Furthermore there are several approaches to underestimate the quadratic objective function by a convex function such that the optimal value with respect to the underestimator yields a lower bound for the original problem. One example is the widely discussed strategy of rising the diagonal entries of matrix Q by the smallest eigenvalue of Q to obtain positive semidefiniteness [18,39,99,132]. A very current approach is the **quadratic convex reformulation** (QCR) technique [19]. It also yields an equivalent binary problem $(P_{\alpha,u})$ with a convex quadratic objective function $g_{\alpha,u}$. This function equals the original objective function for all $x \in P$ but depends on two parameters α and u, which have to be chosen appropriately to guarantee convexity. Then, the problem can be solved by a B&B algorithm based on continuous relaxation. To obtain the best root bound of the branching tree, which in turn equals the optimal value of the continuous relaxation of $(P_{\alpha,u})$, the idea is to optimize

$$
\begin{aligned}
\max_{\alpha,u} \quad & \min_{x \in P} g_{\alpha,u}(x)\\
\text{s.t.} \quad & Q_{\alpha,u} \succeq 0
\end{aligned}
$$

where $Q_{\alpha,u}$ is a transformation of Q depending on α and u. The best choice $\bar{\alpha}, \bar{u}$ is obtained by a semidefinite program. Finally the continuous relaxation of the problem minimizing $g_{\bar{\alpha},\bar{u}}$, which can be calculated efficiently by software tailored for convex problems, yields a strong lower bound.

An even more recent development on underestimators is presented in [30], where the underestimating function g_t is required to be separable but not necessarily convex. By exploiting binarity, the quadratic underestimator is reduced to a linear function l_t such that lower bounds are obtained by optimizing the original problem with respect to a linear objective function. Here, any algorithmic knowledge about the underlying problem structure can be exploited directly. The definition of the underestimator depends on a parameter $t \in \mathbb{R}^n$, which is constrained by $Q \succeq \mathrm{Diag}(t)$. Its choice is similar to the one of α and u in the QCR approach, i. e. $\bar{t}$ is chosen such that it induces a maximal lower bound for BQP, respecting the constraints,

$$\begin{array}{ll} \max\limits_{t} & \min\limits_{x \in P} g_t(x) \\ \text{s. t.} & Q \succeq \mathrm{Diag}(t). \end{array}$$

A subgradient algorithm efficiently provides the parameter t of the optimal separable underestimator. The difference to the QCR method lies in the point of relaxation. In the QCR approach, the reformulation yields an equivalent quadratic integer convex problem, which then is relaxed to obtain convexity for an efficient computation. The separable underestimator in turn relaxes the objective function but then is transformed to an equivalent linear function which can be optimized efficiently over the set of binary feasible solutions by the given assumptions.

Part II

Combinatorial Optimization with One Quadratic Term

In the remainder of this thesis, we present a new method to get stronger bounds for BQP. We strengthen the standard linearization by additional cutting planes which we generate by considering a reduced BQP. More precisely, we study BQP with only **one quadratic term** in the objective function, but still take all side constraints into account. After the application of the standard linearization we call the problem BQP_1 and investigate the polyhedral description of its convex hull.

The main reasons for this approach are the following. First of all, cutting planes which are valid for the convex hull of BQP_1 remain valid in the original problem. They potentially improve the straightforward model obtained from the relaxation of the standard linearization, since the product variable is considered in combination with all side constraints. Moreover, considering only one quadratic term of binary variables leads to a polynomial time approach. Note that the underlying linear problem is supposed to be efficiently solvable (this was required in Chapter 3). Due to this, there exist several strategies to solve BQP_1 in polynomial time.

Denote the two variables in the quadratic term with $x_{\mathring{e}_1}$ and $x_{\mathring{e}_2}$ and the product variable with $y_{\mathring{e}_1\mathring{e}_2}$ or simply y. Then the problem reads

$$
\begin{aligned}
(\text{BQP}_1) \qquad \min \quad & \sum_{e\in E} c_e x_e + q_{\mathring{e}_1\mathring{e}_2} y_{\mathring{e}_1\mathring{e}_2} \\
\text{s.t.} \quad & Ax \le b \\
& y_{\mathring{e}_1\mathring{e}_2} \le x_{\mathring{e}_1}, x_{\mathring{e}_2} \\
& y_{\mathring{e}_1\mathring{e}_2} \ge x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1 \\
& x \in \{0,1\}^n \\
& y_{\mathring{e}_1\mathring{e}_2} \in \{0,1\}.
\end{aligned}
$$

The most intuitive strategy is a distinction of cases. As the variables are binary, there are four different cases how the quadratic term can be composed, which in each case leads to a fixed impact of the product variable and the additional quadratic costs.

$$
\begin{aligned}
&x_{\mathring{e}_1} = x_{\mathring{e}_2} = 1, \quad y = 1 && \qquad x_{\mathring{e}_1} = 1, \ x_{\mathring{e}_2} = 0, \quad y = 0 \\
&x_{\mathring{e}_1} = x_{\mathring{e}_2} = 0, \quad y = 0 && \qquad x_{\mathring{e}_1} = 0, \ x_{\mathring{e}_2} = 1, \quad y = 0
\end{aligned}
$$

As the linear problem is efficiently solvable, the optimal solution of BQP_1 can be obtained in polynomial time by calculating the four optimal linear solutions fixing $x_{\mathring{e}_1}$ and $x_{\mathring{e}_2}$ to the respective values, adding the quadratic cost $c_{\mathring{e}_1\mathring{e}_2}$ in the case of $x_{\mathring{e}_1} = x_{\mathring{e}_2} = 1$ and choosing the solution with the lowest cost.

Although this is a very efficient strategy to solve BQP_1, it does not provide further information for the original problem BQP since no generalization to more quadratic terms is possible. But nevertheless it establishes that the optimization problem for BQP_1 is efficiently solvable, and thus, by the result of Grötschel, Lovász and Schrijver (c. f. Section 1.3), also the separation problem is solvable in polynomial time. The resulting cutting planes remain valid for $P^{ql}_{\{0,1\}}$, the polytope of the linearized BQP. Nonetheless, it is a very indirect way, calling the optimization routine several times in each separation step, and thus very time-consuming and not usable in practice.

Therefore, we propose another strategy which combines case distinction and the aim of generating cutting planes. It adopts the idea of disjunctive cuts for (mixed) 0-1 programs presented by Balas et al. [11,12]. Given an infeasible solution $\bar{x}$ with $\bar{x}_e \notin \{0,1\}$, a disjuctive cut is a cutting plane which is valid for the convex hull of the two disjoint sets where $\bar{x}_e$ is set to zero and one, respectively.

The proposed strategy again considers the feasible values of the two product variables and the corresponding quadratic variable, but here consists of the three cases

$$x_{\mathring{e}_1} = x_{\mathring{e}_2} = 1, \quad y = 1 \qquad\qquad x_{\mathring{e}_1} = 0, \quad y = 0 \qquad\qquad x_{\mathring{e}_2} = 0, \quad y = 0.$$

Note that the three cases are not disjoint as it is not necessary in this approach.

Since the underlying linear problem is efficiently solvable, there exists an exact LP formulation of the problem $\min\{c^\top x \mid Ax \leq b, x \in [0,1]^n\}$, which either is polynomially sized or for which efficient separation routines exist. For the sake of clarity, we continue to use the notation $Ax \leq b$ for the set of inequalities which is necessary for a complete formulation of the problem, even though it might be different from the binary formulation. For the following construction we furthermore include the bounds for the x-variables in the matrix notation such that we consider the underlying linear problem

$$\min\{c^\top x \mid Ax \leq b\}.$$

For each of the three cases $i \in \{1,2,3\}$ a new set of variables $x^{(i)} \in [0,1]^n$ is introduced, which is supposed to copy the original linear variables and therefore is restricted by the original constraints, i. e. $Ax^{(i)} \leq b$, plus the fixings of the respective case. The quadratic variable is not explicitely considered as its value is implicitly given by the case distinction. A feasible solution $x^{(i)}$ with respect to the problem of case i directly leads to a feasible solution of the original problem by setting $x = x^{(i)}$.

By this construction, the set of all feasible solutions of the three cases yields all feasible solutions x of the original problem such that the feasible solutions (x, y) of BQP_1 are convex combinations of the three cases, extended by the value of the product term y.

$$\begin{pmatrix} x \\ y \end{pmatrix} = \lambda_1 \begin{pmatrix} x^{(1)} \\ 1 \end{pmatrix} + \lambda_2 \begin{pmatrix} x^{(2)} \\ 0 \end{pmatrix} + \lambda_3 \begin{pmatrix} x^{(3)} \\ 0 \end{pmatrix} \qquad \text{for } \lambda_1, \lambda_2, \lambda_3 \geq 0 \text{ with } \sum_{i=1}^{3} \lambda_i = 1$$

By replacing the auxiliary variables $x^{(i)}$ by $\tilde{x}^{(i)} := \lambda_i x^{(i)} \in [0,1]^n$ we can construct an LP which is equivalent to the original problem BQP_1.

$$\begin{aligned}
\min \quad & \sum_{i=1}^{n} c_e x_e + c_{\mathring{e}_1 \mathring{e}_2} y \\
\text{s.t.} \quad & \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \tilde{x}^{(1)} \\ \lambda_1 \end{pmatrix} + \begin{pmatrix} \tilde{x}^{(2)} \\ 0 \end{pmatrix} + \begin{pmatrix} \tilde{x}^{(3)} \\ 0 \end{pmatrix} \\
& A\tilde{x}^{(1)} \leq \lambda_1 b, \qquad \tilde{x}^{(1)}_{\mathring{e}_1} = \tilde{x}^{(1)}_{\mathring{e}_2} = \lambda_1 && (3.9) \\
& A\tilde{x}^{(2)} \leq \lambda_2 b, \qquad \tilde{x}^{(2)}_{\mathring{e}_1} = 0 && (3.10) \\
& A\tilde{x}^{(3)} \leq \lambda_3 b, \qquad \tilde{x}^{(3)}_{\mathring{e}_2} = 0 && (3.11) \\
& \sum_{i=1}^{3} \lambda_i = 1, \qquad \lambda_1, \lambda_2, \lambda_3 \geq 0
\end{aligned}$$

Due to the requirement that the underlying linear problem is efficiently solvable, the constraints (3.9) to (3.11), which are exactly the constraints of the linear problem enriched by the respective fixing, are efficiently separable. On the whole, this construction yields new cutting planes in polynomial time, which remain valid in the general BQP problem.

As a matter of fact the complexity of solving a problem with one quadratic term in the objective is at least as complex as solving the underlying linear problem, and the practical hardness usually increases significantly. To solve a specific optimization problem with quadratic objective function by this generic strategy therefore is probably too difficult. Nevertheless the former results indicate that it can be worth investigating the approach of one single quadratic term as they grant the possibility for an understanding of the complete description of the BQP_1 polytope.

This promising fact provides the main motivation of this thesis. In the following we consider specific quadratic optimization problems whose underlying linear problems are efficiently solvable, and investigate them concerning an objective function with exactly one quadratic term. The problems of choice are the quadratic MSF and the quadratic MST problem and their directed variants, followed by the quadratic assignment and the quadratic matching problem. We analyze the polyhedra of the respective linearized problems in the context of dimensions, valid and facet defining inequalities and, if possible, present complete polyhedral descriptions. For practical applications, exemplarily in the case of the quadratic MSF, we study the impact of such BQP_1 cutting planes for the optimization of general quadratic problems.

Chapter 4

Quadratic Spanning Forests and Trees

We start the investigation of specific quadratic optimization problems with the **quadratic minimum spanning forest** (QMSF) and the **quadratic minimum spanning tree** (QMST) problem, i. e., the MSF and the MST problem with additional quadratic terms q_{ef} for pairs of different edges $e, f \in E$ in the objective function. The objective then reads

$$z(x) := \sum_{e \in E} c_e x_e + \sum_{\{e,f\} \in \mathcal{Q}} q_{ef} x_e x_f, \tag{4.1}$$

where again $\mathcal{Q}$ is the set of all edge pairs $e \neq f \in E$ with $q_{ef} \neq 0$.

The QMST problem was introduced by Xu [170] and has a variety of applications, see the seminal work of Assad and Xu [9] and the papers [49, 74, 75, 149]. The most common applications occur in the field of network design, where the linear costs model the investment for building the edges and the quadratic costs model the interference costs within the network. Popular examples are electric supply networks, where the grid consists of different types of cables such that additional costs appear when switching types, e. g. from over- to underground cables. These additional costs can be modelled by the quadratic part of the cost function. Other related examples are oil or water transmission networks with different kinds of pipes, or transportation networks with varying means of conveyances, where changeover or reload costs are given when changing from one conveyance to another [74, 75]. The QMST also finds application in wireless telecommunication or sensor networks, where the aim is to design a communication spanning tree which minimizes the interferences of radio transmissions [149].

In many applications interference costs only occur for adjacent edges in the corresponding graph model. This leads to a special case, the adjacent-only quadratic minimum spanning tree (AQMST) problem, where $q_{ef} = 0$ if edges e and f are not adjacent. The adjacent-only case is important in problems where the costs depend on connections of different kinds, besides supply or transmission problems one can think of design problems with bending losses or routing problems with turn delays. The more general case with quadratic costs for arbitrary pairs of edges in turn occurs in problems with only little relation between the topology of the network and its physical layout, such as in cases of radio transmissions or in fiber-optic networks [49].

4.1 Properties and algorithms

4.1.1 Formulation

Similar to the ILP formulations of MSF and MST, the quadratic problems can be formulated as integer programs with the same linear constraints but quadratic objective functions. After the application of the standard linearization, i. e. after the replacement of the quadratic terms $x_e x_f$ by y_{ef} and the addition of the linking inequalities (3.1) and (3.2), the equivalent linear formulation for the QMSF problem reads

$$(\mathrm{LQP_{QMSF}}) \qquad \min \sum_{e\in E} c_e x_e + \sum_{\{e,f\}\in\mathcal{Q}} q_{ef} y_{ef}$$

$$\text{s.t.} \sum_{e\in E(G[S])} x_e \le |S|-1 \qquad \forall\, \emptyset \ne S \subseteq V \tag{4.2}$$

$$y_{ef} \le x_e, x_f \qquad \forall \{e,f\} \in \mathcal{Q} \tag{4.3}$$

$$y_{ef} \ge x_e + x_f - 1 \qquad \forall \{e,f\} \in \mathcal{Q} \tag{4.4}$$

$$x \in \{0,1\}^{|E|}$$

$$y \in \{0,1\}^{|\mathcal{Q}|}$$

and the linearized formulation of QMST, denoted with $(\mathrm{LQP_{QMSF}})$, equals the former plus the additional cardinality constraint

$$\sum_{e\in E} x_e = |V| - 1. \tag{4.5}$$

Let P_F^{ql} and P_T^{ql} denote the convex hulls of the linearized QMSF and the linearized QMST problem, i. e., of all binary vectors (x, y) satisfying (4.2) to (4.4) and, in the tree case, also (4.5).

4.1.2 Complexity

As mentioned in Section 2.2, the linear problems MSF and MST are efficiently solvable and MST polynomially reduces to MSF by a simple change of the cost function. The idea of reduction can be carried over to the quadratic versions, only that the linear costs need to be reduced by a modified value M which has to be big enough such that the objective value decreases each time an edge is added to a forest with less than $|V| - 1$ egdes.

Lemma 4.1.1.

QMST polynomially reduces to QMSF.

Proof. Consider a QMST instance on a connected graph $G = (V, E)$ with objective function $z(x) = c^\top x + x^\top Qx$. With $c_{\max} := \max\{c_e \mid e \in E\}$ and $q_{\max} := \max\{q_{ef} \mid e, f \in E\}$ define $M := \max\{c_{\max}, q_{\max}, 0\}+1$ and new linear costs $\tilde{c}_e := c_e - M(|V|-1)$. By this construction, the objective values $z(x)$ and $\tilde{z}(x) := \tilde{c}^\top x + x^\top Qx$ of each forest F differ by $|E(F)| \cdot M(|V| - 1)$. Furthermore, any optimal forest with respect to $\tilde{z}$ is connected, since adding an arbitrary edge $e \in E\backslash E(F)$ to a forest F with less than $|V| - 1$ edges changes the objective value by the additional term

$$\tilde{c}_e + \sum_{f\in E(F)} q_{ef} = (\underbrace{c_e}_{<M} - M(|V|-1)) + \underbrace{\sum_{f\in E(F)} q_{ef}}_{<(|V|-2)M} < 0$$

and thus improves the solution. Therefore, an optimal spanning forest F^* with respect to $\tilde{z}$ always is a tree, which furthermore is optimal with respect to the original objective function z and has the value $z(x^*) = \tilde{z}(x^*) - (|V| - 1)M$. □

The complexity of QMSF and QMST in turn rises significantly compared to the linear versions as the NP-hardness of general BQP is carried over. There are only few special cases which have been shown to be tractable, e. g., the case of a multiplicative objective function with positive factors [153]. Even the special case of the adjacent-only versions become NP-complete. This property can be shown by a polynomial transformation of the Hamiltonian path (HP) problem to AQMST [9]. A HP is a path which passes each vertex of a given graph exactly once, and the HP problem is the corresponding decision problem and proven to be NP-complete (see, e. g. [77]).

Theorem 4.1.1.
AQMSF and AQMST are NP-complete.

Proof. For a given connected graph $G = (V, E)$ define $c_e = 0$ for all $e \in E$, $q_{ef} = 1$ if edges e and f are adjacent, and $q_{ef} = 0$ else. Let T^* be an optimal spanning tree with incidence vector x^*, moreover let $d_v := |\delta(v)|$. Then, for each vertex $v \in V$ there are $d_v(d_v - 1)$ ordered edge pairs in $E(T^*)$ which share vertex v. With $q_{ef} = 1$ for all these pairs, they contribute $d_v(d_v - 1)$ to the objective function, such that

$$z(x^*) = \sum_{v \in V} d_v(d_v - 1).$$

The sum is minimal if the tree is a path, say from u to w, such that $d_u = d_w = 1$ and $d_v = 2$ for all $v \in V \backslash \{u, w\}$. Therefore, $z(x) \geq 2(n - 2)$ for any incidence vector x of a tree, and equality holds if and only if the tree is an Hamiltonian path in G. By this construction the existence of a HP can be proven by solving an AQMST problem. By Lemma 4.1.1 AQMSF is NP-complete, too. □

Since the adjacent-only problems are special cases, QMSF and QMST with arbitrary quadratic costs are at least as hard as the adjacent-only problems. The alternative proof for the NP-hardness shows that actually one of the practically hardest problems in quadratic optimization, the NP-complete quadratic assignment problem, which searches for an assignment minimizing a quadratic objective function and which we investigate in Chapter 6, is reducable to QMST.

Theorem 4.1.2.
QMSF and QMST are NP-complete.

Proof. Consider a QAP instance on a bipartite graph $G = (V_a \dot{\cup} V_b, E)$ with disjoint vertex sets $V_a = \{a_1, \ldots, a_n\}$ and $V_b = \{b_1, \ldots, b_n\}$ and with linear costs c_e for $e \in E$ and quadratic costs q_{ef} for non-adjacent edges $e, f \in E$. Extend G to a non-bipartite graph $\tilde{G} = (V, E \cup \tilde{E})$ with auxiliary edge set $\tilde{E} = \{\{b_i, b_{i+1}\} \mid i \in \{1, \ldots, n-1\}\}$, see Figure 4.1, and define the QMST costs analogous to the QAP costs plus $q_{ef} = \infty$ for adjacent edges $e, f \in E$ and $q_{ef} = 0$ for the remaining pairs of edges, i. e., for all $e \in \tilde{E}$ and $f \in E \cup \tilde{E}$. Then, any assignment A in G can be extended to a spanning tree T in $\tilde{G}$ by adding the $n - 1$ auxiliary edges in $\tilde{E}$, where the QAP costs of A and the QMST costs of T are equal by construction. Conversely, each spanning tree T with an objective value less than ∞ contains only edges $e \in E$ which are pairwise not adjacent plus the $n-1$ edges in $\tilde{E}$. The edges in E then define an assignment in G with the same objective value as T. Thus, an optimal solution of QMST with finite objective value directly yields an optimal QAP solution. □

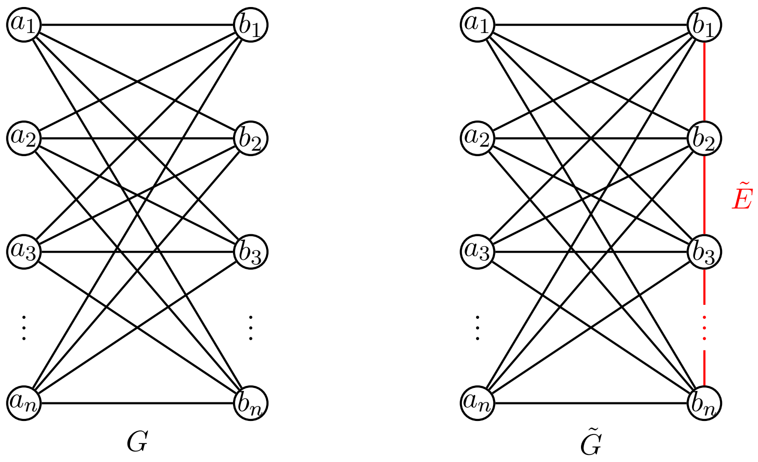


Figure 4.1: The original bipartite graph G and its extension $\tilde{G}$.

4.1.3 Lower bounds

Due to the high complexity of the QMSF and the QMST problem few literature on exact algorithms exists. Indeed, current B&B approaches can only solve dense QMST instances up to 15 and sparse instances up to 20 vertices although much effort is put into the calculation of good bounds. Of course all lower bounds mentioned in Section 3.3 are applicable, and especially two of them are used in performance studies, the Gilmore-Lawler bound and the bound proposed by Assad and Xu, which in the case of a QMST problem both have to solve several linear MST problems. A combination of several approaches leads to another lower bound for QMST and is presented in [149]. Here, a partial application of the first RLT level for a QMST formulation replaces the quadratic terms $x_e x_f$ by auxiliary variables y_{ef} but instead of the constraints of the standard linearization the following constraints are added.

$$\begin{aligned}
\sum_{e \in E} y_{ef} &= (|V|-1)\, x_f && \forall\, f \in E \\
\sum_{e \in E(G[S])} y_{ef} &\leq (|S|-1)\, x_f && \forall\, \emptyset \neq S \subseteq V \text{ and } \forall\, f \in E \\
y_{ee} &= x_e && \forall\, e \in E \\
y_{ef} &= y_{fe} && \forall\, e \neq f \in E \\
y_{ef} &\geq 0 && \forall\, e \neq f \in E
\end{aligned}$$

A Lagrangean relaxation of the equation $y_{ef} = y_{fe}$ then leads to the lower bound, which for a Lagrangean multiplier $\lambda = 0$ provides the Gilmore-Lawler bound and improves with increasing λ.

Cordone and Passeri proposed in [49] to calculate a set of lower bounds, one for each branching step in the B&B tree. In each step, the quadratic objective function is relaxed by an under-estimating linear function, which contains the original linear costs, the quadratic costs of all edges fixed in the tree, and the cheapest quadratic costs for a suitable set of edges which are not fixed so far. For this, let X_1 be the set of all variables fixed to one and let X_0 be the set of all variables fixed to zero in the current branching step. For an edge $e \in E \backslash \{X_1 \cup X_0\}$ let F be set of edges whose adding to $X_1 \cup \{e\}$ does not close a cycle. Within F choose k edges f having minimal quadratic costs q_{ef} with respect to e and define the resulting set with F^k_{e,X_1,X_0}. Then, the relaxed objective is defined as

$$\min \sum_{e \in E} \tilde{c}_e x_e$$

with the approximate costs

$$\tilde{c}_e := c_e + \sum_{f \in X_1} q_{ef} + \sum_{f \in F_{e,X_1,X_0}^{n-2-|X_1|}} q_{ef}$$

yielding a lower bound for the current subproblem. This bound can be strenghtened by constraining the k edges from F not to close a cycle with each other, too. The bound becomes even stronger by additionally applying the idea of Assad and Xu for lower bounds: the original objective function does not change by a cost replacement $c_e(u) := c_e - (n-2)u_e$ and $q_{ef}(u) := q_{ef} + u_f$ for a vector $u \in \mathbb{R}^n$. However the presented lower bound is affected and can be strengthened by a good choice of u. A leveling procedure proposed in [149] yields the best u and the strongest bound.

Apparently it is necessary for all kinds of practical applications to solve problems of much higher dimensions than $n = 15$ or $n = 20$. For this purpose, Assad and Xu already proposed two heuristics for the QMST [9]. The first of them, called the Average Contribution Method, estimates the average contribution

$$p_e = c_e + \frac{n-2}{|E|-1} \sum_{f \neq e} q_{ef}$$

of each edge $e \in E$ to the objective function and then solves the linear MST problem with respect to the costs p_e. The second heuristic is called Sequential Fixing Method and improves the calculation of the average contribution by also considering the influence of already fixed edges such that the average contribution is calculated as

$$p_e = c_e + \frac{n-2-|U|}{|F|-1} \sum_{f \in F} q_{ef},$$

where $U \subseteq E$ is the set of fixed edges and $F \subseteq E \backslash U$ the set of free edges, which are those edges which are neither fixed nor closing a cycle with the edges in U. The running times of both heuristics are quadratic in the number of edges and by this they outperform all subsequent heuristics in terms of running times.

In terms of accuracy in turn, the more recent heuristics have much better performances. Common heuristics are the Random Local Search with Tabu Thresholding (RLS-TT) algorithm of Öncan and Punnen [138], and the Tabu Search (TS) and the Variable Neighborhood Search (VNS) algorithms of Cordone and Passeri [49], which all search on similar neighborhoods. The considered k-neighborhood structures consist of spanning trees with exactly k different edges compared to the current solution. For reasons of running times, k needs to be very small which makes the algorithm vulnerable for getting stuck in a local optimum. To avoid this, RLS-TT includes random moves within the k-neighborhood, VNS applies a shaking procedure and TS allows slight worsenings of solutions. Out of the three, TS seems to outperform the others both in terms of running time and accuracy [49]. Heuristics based on artificial intelligence such as the Artificial Bee Colony (ABC) heuristic of Sundar and Singh [164] and the Edge-Window-Decoder strategy of Soak et al. [161] lead to competitive results with RLS-TT [138] and TS [49]. More heuristics for the QMST problem are presented, e. g., in [144, 174] and [130].

4.1.4 The boolean quadric forest polytope

Coming back to the main focus of this work, which is the investigation of polyhedral structures of quadratic optimization problems, we again consider the polytopes of the linearized quadratic MSF and MST problems (LQP_{QMSF}) and (LQP_{QMST}). The former of the two, P_F^{ql}, is called **boolean quadric forest polytope** and was introduced by Lee and Leung [124]. They determined facet inducing inequalities and related them to the boolean quadric polytope $P_{\{0,1\}}^{ql}$ (c. f. Section 3.1) as well as the forest polytope P_F (c. f. Section 2.2). If the underlying graph is a forest, the boolean quadric forest polytope equals the boolean quadric polytope. Otherwise it is equal to the intersection of $P_{\{0,1\}}^{ql}$ and the half-spaces defined by the subtour elimination constraints, i. e.

$$P_F^{ql} = P_{\{0,1\}}^{ql} \cap \left\{ (x,y) \in \{0,1\}^{|E| \times |\mathcal{Q}|} \;\middle|\; \sum_{e \in E[G(S)]} x_e \leq |S| - 1, \quad \forall \emptyset \neq S \subseteq V \right\},$$

where $\mathcal{Q}$ is the set of all edge pairs $e \neq f \in E$ since the polyhedral point of view is independent of cost structures. By enumerating $\binom{m+1}{2} + 1$ affinely independent vectors which all lie in the polytope, P_F^{ql} is proven to be of full dimension.

Theorem 4.1.3 (Lee and Leung)**.**

$$\dim(P_F^{ql}) = \binom{m+1}{2}.$$

□

In the next theorems we state a list of facet defining inequalities also presented by Lee and Leung.

Theorem 4.1.4 (Lee and Leung)**.**
The inequalities

a) $$y_{\{ef\}} \geq 0 \qquad \forall \{e,f\} \in \mathcal{Q}$$

b) $$(|S|-2)x_e \geq \sum_{f \in E(G[S]) \setminus \{e\}} y_{ef} \qquad \forall S \subseteq V,\ |S| \geq 3 \text{ and } e \in E[G(S)]$$

c) $$(|S|-1)x_e \geq \sum_{f \in E(G[S])} y_{ef} \qquad \forall S \subseteq V,\ |S| \geq 2 \text{ and } e \in E[G(V \setminus S)]$$

d) $$(|S|-1)(1-x_e) \geq \sum_{e \in E(G[S])} x_e + \sum_{f \in E(G[S])} y_{ef} \qquad \forall S \subseteq V,\ |S| \geq 3 \text{ and } e \in E[G(V \setminus S)] \text{ or } \forall S \subseteq V,\ |S| \geq 3 \text{ and } e \in \delta(S)$$

define facets of P_F^{ql}.

Proof. Validity of *a)* is obvious. The construction of *b)* – *d)* can be explained by the Sherali-Adams reformulation of the subtour elimination constraints (4.2). The facet defining property can be proven either by the direct method, listing $\dim(P_F^{ql})$ affinely independent and feasible vectors, or by the indirect method, showing that the inequality is a positive multiple of another facet defining inequality. The details of the proofs can be found in [124]. □

Note that the inequalities of type *c)* with $e \in \delta(S)$ are valid but not facet defining since they are dominated by the inequalities $(|S|-1)x_e \geq \sum_{f \in E(G[S \cup \{v\}])} y_{ef}$ where v is the end vertex of e which is not in S. These inequalities are of type *b)* again.

If the underlying graph contains $n = 3$ vertices and $m = 3$ edges, inequalities $a), c)$ and $d)$ are sufficient for a complete description of the quadric forest polytope. More precisely, consider the graph $G_3 = (\{u, v, w\}, E)$ with $E = \{e = \{u, v\}, f = \{u, w\}, g = \{v, w\}\}$. The corresponding quadric forest polytope $P_F^{ql}(G_3)$ can be described by the inequalities

$$\begin{aligned} y_{ef}, y_{eg}, y_{fg} &\geq 0 \\ x_e &\geq y_{ef} + y_{eg} \\ x_f &\geq y_{ef} + y_{fg} \\ x_g &\geq y_{eg} + y_{fg} \\ x_e + x_f + x_g &\leq y_{ef} + y_{eg} + y_{fg} + 1. \end{aligned}$$

If otherwise the graph contains more than three vertices, the polyhedral description becomes much more complicated as can be seen by the following three theorems which list several facet defining inequalities presented by Lee and Leung [124]. Note that these inequalities still do not suffice for a complete description for the quadric forest polytope with $|V| \geq 4$.

Theorem 4.1.5 (Lee and Leung)**.**
Let T be a subset of E and let the rank of T, $\rho(T)$, be the maximal cardinality of a forest in T. Then for any given positive integer $\alpha \leq \rho(T) - 1$ the inequality

$$\alpha \sum_{e \in T} x_e - \sum_{e \neq f \in T} y_{ef} \leq \frac{\alpha(\alpha + 1)}{2} \tag{4.6}$$

defines a facet of P_F^{ql} if

a) for every edge $e \notin T$, there exists a subset $S \subset T$ with $|S| = \alpha + 1$ such that $S \cup \{e\}$ is a forest, and

b) if $|T| \geq 3$, then for any three distinct edges $s, t_1, t_2 \in T$, there exists a subset $S \subset T \backslash \{s, t_1, t_2\}$ with $|S| = \alpha - 1$, such that both $S \cup \{s, t_1\}$ and $S \cup \{s, t_2\}$ are forests.

Proof. Let x be the incidence vector of a forest F in G. For a subset $T \subseteq E$ let $\varphi := \sum_{e \in T} x_e$ be the number of edges of F in T. Moreover let $\delta := \varphi - \alpha$. Then, validity of (4.6) follows by writing

$$\begin{aligned} \alpha \sum_{e \in T} x_e - \sum_{e \neq f \in T} y_{ef} &= \alpha\varphi - \binom{\varphi}{2} \\ &= \alpha(\alpha + \delta) - \frac{(\alpha + \delta)(\alpha + \delta - 1)}{2} \\ &= \frac{\alpha(\alpha + 1)}{2} + \underbrace{\frac{\delta - \delta^2}{2}}_{\leq 0 \ \forall \delta \in \mathbb{N}} \\ &\leq \frac{\alpha(\alpha + 1)}{2}. \end{aligned}$$

The proof for the facet defining property uses the indirect method. It can be found in [124]. □

Theorem 4.1.6 (Lee and Leung)**.**
Let S and T be disjoint subsets of E with $|S| \geq 1$ and $|T| \geq 2$. Define $\mathcal{T}$ as the set of two-element subsets of T and let $B = (S \dot\cup \mathcal{T}, E(B))$ be a bipartite graph with edge set

$$E(B) := \{(s, \{t_1, t_2\}) \mid s \in S, \{t_1, t_2\} \in \mathcal{T}, \text{ and } \{s, t_1, t_2\} \textit{ is cycle-free in } G\},$$

see Figure 4.2. Then the inequality

$$\sum_{e \in S} x_e + \sum_{e \neq f \in T} y_{ef} \geq \sum_{e \in S, f \in T} y_{ef} - \sum_{e \neq f \in S} y_{ef} \tag{4.7}$$

defines a facet of P_F^{ql} if

a) B is connected and

b) for all $s_1, s_2 \in S$, there exist $t_1, t_2 \in T$ such that $\{s_1, s_2, t_1, t_2\}$ is a forest in G.

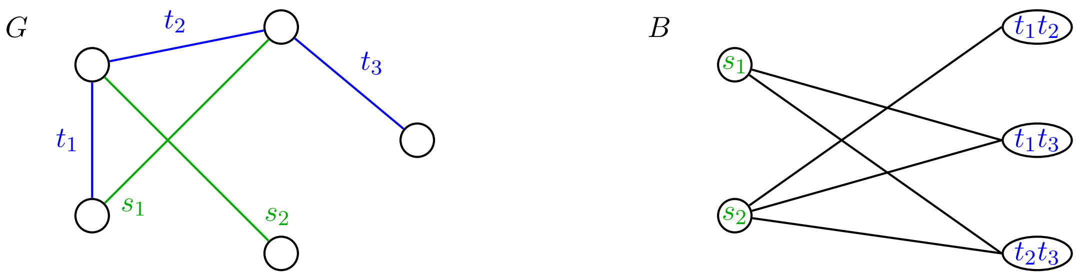


Figure 4.2: Construction of the bipartite graph B (right) from the graph G (left) with $n = 5$ vertices and subsets $S = \{s_1, s_2\}$, colored in green, and $T = \{t_1, t_2, t_3\}$, colored in blue.

Proof. We again restrict ourselves to the validity proof for (4.7). For the proof of the facet defining property we again refer to [124]. Let $F \subseteq E$ be the edge set of a forest in G and let (x^F, y^F) be the corresponding vector with

$$x_e^F = \begin{cases} 1 & \text{if } e \in F \\ 0 & \text{else} \end{cases} \quad \text{and} \quad y_{ef}^F = \begin{cases} 1 & \text{if } e,f \in F \\ 0 & \text{else.} \end{cases}$$

Set $s := |F \cap S|$ and $t := |F \cap T|$. Then,

$$\sum_{e \in S} x_e^F + \sum_{e \neq f \in T} y_{ef}^F - \sum_{e \in S, f \in T} y_{ef}^F + \sum_{e \neq f \in S} y_{ef}^F = s + \frac{t(t-1)}{2} - st + \frac{s(s-1)}{2} = \frac{1}{2}(t-s)(t-s-1),$$

which is nonnegative for all integer values of s and t. □

Theorem 4.1.7 (Lee and Leung)**.**
Let S and T be disjoint subsets of E with $|S| \geq 1$ and $|T| \geq 2$. Define $\mathcal{T}$ as in Theorem 4.1.6. Then the inequality

$$\sum_{e \in S} x_e + \sum_{e \neq f \in T} y_{ef} \geq \sum_{e \in S, f \in T} y_{ef} \tag{4.8}$$

defines a facet of P_F^{ql} if

a) B is connected and

b) for all forests F in G with $|F \cap T| \geq 2$ the inequality $|F \cap S| \leq \frac{1}{2}|F \cap T|$ holds.

Proof. Validity follows by the same arguments as in the proof of Theorem 4.1.6 with $s := |F \cap S|$ and $t := |F \cap T|$ for a forest F in G with $t \geq 2$. Then,

$$\sum_{e \in S} x_e^F + \sum_{e \neq f \in T} y_{ef}^F - \sum_{e \in S, f \in T} y_{ef}^F = s + \frac{t(t-1)}{2} - st = \frac{1}{2}(t-1)(t-2s),$$

which is nonnegative since $t \geq 2$ and $s \leq \frac{1}{2}t$ hold. □

The results of Lee and Leung show that the polyhedral description of the quadratic minimum spanning forest problem becomes very complex. To obtain P_F^{ql}, it does not suffice to simply combine the subtour elimination constraints (4.2), which indeed yield a complete description of the linear forest polytope P_F, with the complete description of the boolean quadric polytope $P_{\{0,1\}}^{ql}$. Moreover, while all inequalities (4.2) are facet defining for P_F, this does not remain true for P_F^{ql}. In the following section we will see that both negative statements concerning P_F^{ql} hold true even in the case of a single product term in the objective function, and in Section 4.3 we will carry over these statements to P_T^{ql}.

4.2 Spanning forests with one quadratic term

When considering a quadratic objective function with a single quadratic term, we have to distinguish between two cases. In the first case, the quadratic term consists of variables corresponding to two adjacent edges. Throughout the thesis, we denote these edges by $\mathring{e}_1 := \{\mathring{u}, \mathring{v}\}$ and $\mathring{e}_2 := \{\mathring{v}, \mathring{w}\}$ and the product of their variables is called a **connected monomial**. The corresponding problem is denoted by QMSF^c in the following. In the second case, the edges of the product variables are non-adjacent in the graph, therefore, the edges are $\mathring{e}_1 := \{\mathring{u}, \mathring{v}\}$ and $\mathring{e}_2 := \{\mathring{w}, \mathring{z}\}$ with pairwise distinct vertices $\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z} \in V$. In this case, we refer to a **disconnected monomial** and denote the problem by QMSF^d. Whenever the context leads to the correct association, we shortly denote the linearization variable $y_{\mathring{e}_1 \mathring{e}_2}$ by y.

Our aim is thus to investigate the polytope corresponding to QMSF^c, defined as

$$P_F^c := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies (4.2) and } y = x_{\mathring{u}\mathring{v}} x_{\mathring{v}\mathring{w}}\right\}$$

and the polytope corresponding to QMSF^d, defined as

$$P_F^d := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies (4.2) and } y = x_{\mathring{u}\mathring{v}} x_{\mathring{w}\mathring{z}}\right\}.$$

and we will devise complete polyhedral descriptions of both.

In the following we assume $|V| \geq 4$. Proposition 2.2.5 proves that the dimension of the (linear) spanning forest polytope P_F is $|E|$. Clearly, the additional linearization variable y increases the dimension by at most one. In fact, we have

Theorem 4.2.1.

$$\dim(P_F^c) = \dim(P_F^d) = \dim(P_F) + 1 = |E| + 1.$$

Proof. For each of the two polytopes P_F^c and P_F^d we list $|E|+2$ feasible and affinely independent vectors.

Let $\bar{z} \in V \backslash \{\mathring{u}, \mathring{v}, \mathring{w}\}$ be an arbitrary but fixed vertex in the connected case and $\bar{z} = \mathring{z}$ in the disconnected case. Let S_1 be a set of vertices containing both $\mathring{u}$ and $\mathring{w}$, but neither $\mathring{v}$ nor $\bar{z}$. Define $S_2 := V \backslash S_1$ and $\bar{e} := \{\mathring{u}, \bar{z}\}$. Choose $r_1 := |E(G[S_1])|$ trees $T_1^1, \dots, T_1^{r_1}$ on the subgraphs induced by the set of vertices $G[S_1]$ and $r_2 := |E(G[S_2])|$ trees $T_2^1, \dots, T_2^{r_2}$ on the subgraph induced by $G[S_2]$ whose incidence vectors are pairwise affinely independent. Let $\bar{h}_1 \in T_1^1$ and $\bar{h}_2 \in T_2^1$ be fixed edges in the paths in T_1^1 from $\mathring{u}$ to $\mathring{w}$ and in T_2^1 from $\mathring{v}$ to $\bar{z}$, respectively; see Figure 4.3 for an illustration.

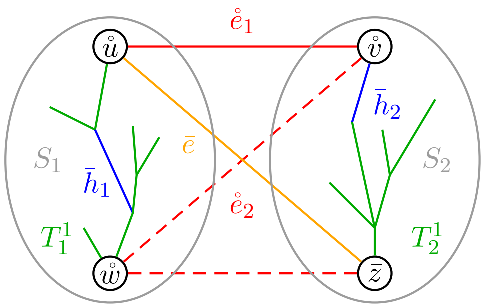


Figure 4.3: Illustration of the fixed trees and edges. The dashed lines represent the two different cases for edge $\mathring{e}_2$: in the connected case, $\mathring{e}_2$ is the edge from vertex $\mathring{w}$ to vertex $\mathring{v}$; in the disconnected case, $\mathring{e}_2$ connects $\mathring{w}$ and $\mathring{z}$.

The x-components of all vectors constructed below are incidence vectors of forests, whereas the y-entry is determined by $y = x_{\mathring{e}_1} x_{\mathring{e}_2}$. Due to Lemma 1.4.1, the incidence vectors of the forests F listed in 1 to 7 are affinely independent, as every new vector violates some (trivial) equation which all former vectors satisfy. Here, the y-variable in the corresponding incidence vector is always set to zero, since not both product edges $\mathring{e}_1$ and $\mathring{e}_2$ belong to F. The incidence vector of the forest in 8 is affinely independent, as $y = 1$ since $\mathring{e}_1, \mathring{e}_2 \in F$.

1. $F = T_1^1 \cup T_2^1$
2. $F = T_1^1 \cup T_2^1 \cup \{\bar{e}\}$
3. $F = T_1^i \cup T_2^1 \cup \{\bar{e}\}$ for all $i = 2, \dots, r_1$
4. $F = T_1^1 \cup T_2^i \cup \{\bar{e}\}$ for all $i = 2, \dots, r_2$
5. $F = T_1^1 \cup T_2^1 \cup \{e\}$ for all edges $e \in \delta(S_1)$ with $e \neq \bar{e}$
6. $F = T_1^1 \cup (T_2^1 \backslash \{\bar{h}_2\}) \cup \{\mathring{e}_1, \bar{e}\}$
7. $F = (T_1^1 \backslash \{\bar{h}_1\}) \cup T_2^1 \cup \{\mathring{e}_2, \bar{e}\}$
8. $F = (T_1^1 \backslash \{\bar{h}_1\}) \cup T_2^1 \cup \{\mathring{e}_1, \mathring{e}_2\}$

We obtain a total number of

$$2 + (r_1 - 1) + (r_2 - 1) + (|S_1||S_2| - 1) + 3 = |E(G[S_1])| + |E(G[S_2])| + |\delta(S_1)| + 2 = |E| + 2$$

affinely independent vectors in P_F^c and P_F^d, respectively, yielding $\dim(P_F^c), \dim(P_F^d) \geq |E| + 1$. By the number of variables we have $\dim(P_F^c), \dim(P_F^d) \leq |E| + 1$, and thus equality in both cases. $\square$

The following results introduce one class of facet defining inequalities for each of the polytopes P_F^c and P_F^d, respectively. Both strengthen the subtour elimination constraints (4.2); we call them **quadratic subtour elimination constraints** in the following.

Theorem 4.2.2.

Let $S_1 \subset V$ be a set of vertices with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v} \in V \backslash S_1$. Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + y \leq |S_1| - 1 \tag{4.9}$$

is valid and induces a facet of P_F^c.

Proof. If $y = 0$, inequality (4.9) is obviously valid as it agrees with a subtour elimination constraint (4.2). Validity in case $y = 1$ also follows from the subtour elimination constraints by rewriting

$$\sum_{e \in E(G[S_1])} x_e = \sum_{e \in E(G[S_1 \cup \{\mathring{v}\}])} x_e - \sum_{\substack{e=\{\mathring{v},s\} \\ s \in S_1}} x_e.$$

By (4.2) the middle sum is at most $|S_1 \cup \{\mathring{v}\}| - 1 = |S_1|$, while the right sum subtracts at least a value of 2 since $x_{\mathring{e}_1} = x_{\mathring{e}_2} = 1$ due to $y = 1$. Combined and with the addition of $y = 1$, we obtain a value of at most $|S_1| - 1$ for the left-hand side of (4.9). To generate an easily interpreted graphic image of the quadratic subtour elimination constraints, consider Figure 4.4. The y-variable can be set to one only if there is no spanning tree in S_1 since otherwise a cycle via vertex $\mathring{v}$ is generated.

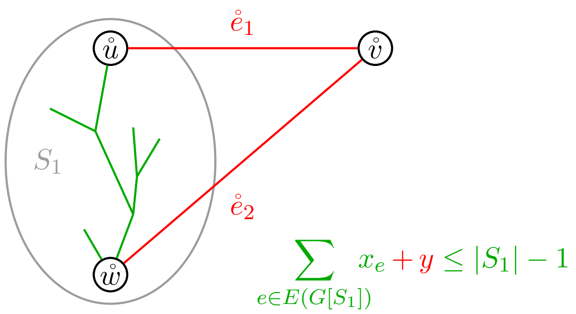


Figure 4.4: The quadratic subtour elimination constraints for the connected monomial corresponding to the edges $\mathring{e}_1 = \{\mathring{u}, \mathring{v}\}$ and $\mathring{e}_2 = \{\mathring{v}, \mathring{w}\}$: if the two edges $\mathring{e}_1$ and $\mathring{e}_2$ are in the solution, at least one edge from a spanning tree in S_1 has to be removed to keep the solution cycle-free.

Consider a fixed vertex set S_1 with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v} \in V \backslash S_1 =: S_2$. To prove the facet defining property, we show that the dimension of the face induced by inequality (4.9) equals $|E|$. Similar to the proof of Theorem 4.2.1 we construct $|E|+1$ valid and affinely independent vectors satisfying (4.9) with equality.

$|S_2| \geq 2:$ As in the proof of Theorem 4.2.1, define the trees T_1^i and T_2^i and the edges $\bar{e}, \bar{h}_1$ and $\bar{h}_2$. Then all $|E| + 1$ vectors defined in 1 to 6 and 8 satisfy $\sum_{e \in E(G[S_1])} x_e + y = |S_1| - 1$.

$|S_2| = 1:$ Define $\bar{f} := \{\bar{z}, \mathring{v}\}$ for a fixed vertex $\bar{z} \neq \mathring{u}, \mathring{v}, \mathring{w}$. Since $S_2 = \{\mathring{v}\}$, we have $\bar{f} \in \delta(S_1)$. Again, choose $r_1 := |E(G[S_1])| = |E| - (|V| - 1)$ trees $T_1^1, \ldots, T_1^{r_1}$ with affinely independent incidence vectors on the subgraph induced by $G[S_1]$ and let $\bar{h}_1$ be an edge in the cycle of $T_1^1 \cup \{\mathring{e}_1, \mathring{e}_2\}$. The reasoning for affine independence is as before, with $y = 1$ only in case 5:

1. $F = T_1^1$
2. $F = T_1^1 \cup \{\bar{f}\}$
3. $F = T_1^i \cup \{\bar{f}\}$ for $i = 2, \ldots, r_1$
4. $F = T_1^1 \cup \{f\}$ for all edges $f \in \delta(S_1)$ with $f \neq \bar{f}$
5. $F = (T_1^1 \backslash \{\bar{h}_1\}) \cup \{\mathring{e}_1, \mathring{e}_2\}$

We therefore have $2 + (r_1 - 1) + (|V| - 2) + 1 = |E| + 1$ affinely independent vectors being tight in (4.9).

In summary, for all cases of $S_1 \subset V$ with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v} \in V \backslash S_1$, the dimension of the induced face is $|E|$, showing that it is a facet of P_F^c. □

Theorem 4.2.3.

Let $S_1, S_2 \subset V$ be disjoint subsets of vertices such that both edges $\mathring{e}_1$ and $\mathring{e}_2$ have exactly one end vertex in S_1 and one end vertex in S_2. Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e + y \leq |S_1| + |S_2| - 2 \tag{4.10}$$

is valid and induces a facet of P_F^d.

Proof. In case of $y = 0$, the inequality is obviously valid since it is the sum of two subtour elimination constraints. In the case of $y = 1$, we rewrite

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e = \sum_{e \in E(G[S_1 \cup S_2])} x_e - \sum_{\substack{e = \{s_1, s_2\} \\ s_1 \in S_1,\, s_2 \in S_2}} x_e$$

and due to (4.2) and with the same arguments as in the proof for Theorem 4.2.2, inequality (4.10) follows. Figure 4.5 illustrates that the maximal number of edges in the subsets S_1 and S_2 is reduced by one if both monomial edges are in the solution since otherwise a cycle is closed.

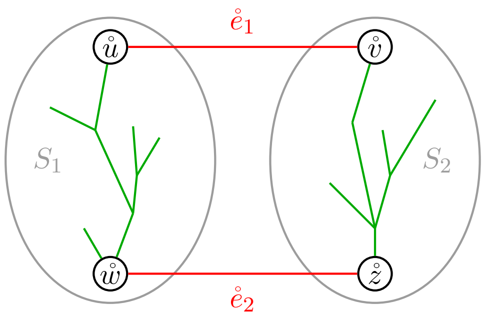


Figure 4.5: The quadratic subtour elimination constraints for the disconnected monomial corresponding to the edges $\mathring{e}_1 = \{\mathring{u}, \mathring{v}\}$ and $\mathring{e}_2 = \{\mathring{w}, \mathring{z}\}$: to prevent the solution from cycles either two spanning trees in the sets S_1 and S_2 are allowed or both monomial edges $\mathring{e}_1$ and $\mathring{e}_2$.

For the proof of the facet defining property, assume without loss of generality $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v}, \mathring{z} \in S_2$. We again construct $|E| + 1$ affinely independent vectors satisfying (4.10) with equality. We distinguish by the number of vertices in $S_3 := V \backslash (S_1 \cup S_2)$.

$|S_3| = 0:$ As in the proof of Theorem 4.2.1, define spanning trees T_1^i and T_2^i on the subgraphs induced by $G[S_1]$ and $G[S_2]$, respectively, and consider the edge $\bar{e} := \{\mathring{u}, \mathring{z}\}$. Let $\bar{h}_1 \in T_1^1$, $\bar{h}_2 \in T_2^1$ again be edges in the paths in T_1^1 from $\mathring{u}$ to $\mathring{w}$ and in T_2^1 from $\mathring{v}$ to $\mathring{z}$, respectively. Now the $|E|$ vectors 1 to 5 and 8 of the proof of Theorem 4.2.1 satisfy (4.10) with equality. The missing affinely independent vector can be chosen as the incidence vector corresponding to the forest $T_1^1 \cup (T_2^1 \backslash \bar{h}_2) \cup \{\mathring{e}_1, \mathring{e}_2\}$.

$|S_3| > 1:$ Let $\bar{a}, \bar{b} \in S_3$. Define the three edges $\bar{e} := \{\mathring{u}, \mathring{z}\}$, $\bar{f} := \{\mathring{u}, \bar{a}\}$ and $\bar{g} := \{\mathring{v}, \bar{b}\}$ connecting the vertex sets S_1, S_2 and S_1, S_3 and S_2, S_3, respectively. Again consider $r_j := |E(G[S_j])|$ affinely independent incidence vectors of spanning trees $T_j^1, \ldots, T_j^{r_j}$ on the subgraphs of $G[S_j]$, for $j = 1, 2, 3$. Furthermore let the edges $\bar{h}_1 \in T_1^1$ and $\bar{h}_2 \in T_2^1$ be in the cycle in $T_1^1 \cup T_2^1 \cup \{\mathring{e}_1, \mathring{e}_2\}$, and finally let $\bar{h}_3 \in T_3^1$ be an edge in the cycle in $T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{e}, \bar{f}, \bar{g}\}$, Figure 4.6 illustrates the fixings.

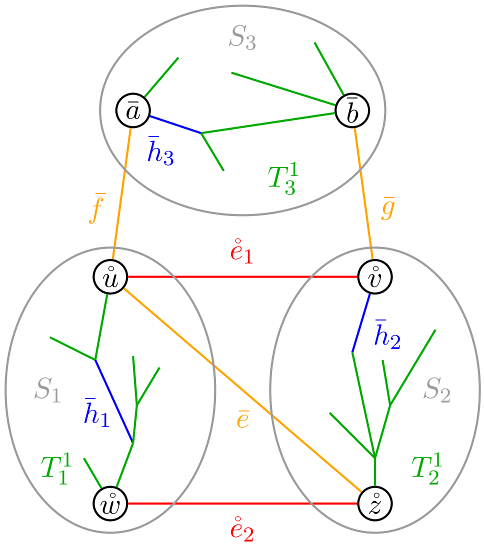


Figure 4.6: Illustration of the fixed trees and edges.

We again construct $|E| + 1$ affinely independent vectors with appropriate y-value, which are tight in inequality (4.10).

1. $F = T_1^1 \cup T_2^1$
2. $F = T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{e}, \bar{f}\}$
3. $F = T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{f}, \bar{g}\}$
4. $F = T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{g}, \bar{e}\}$
5. $F = T_1^i \cup T_2^1 \cup T_3^1 \cup \{\bar{e}, \bar{f}\}$ for $i = 2, \ldots, r_1$
6. $F = T_1^1 \cup T_2^i \cup T_3^1 \cup \{\bar{e}, \bar{f}\}$ for $i = 2, \ldots, r_2$
7. $F = T_1^1 \cup T_2^1 \cup T_3^i \cup \{\bar{e}, \bar{f}\}$ for $i = 2, \ldots, r_3$
8. $F = T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{e}, f\}$ for all edges $f \neq \bar{f}$ with exactly one end vertex in S_1 and one end vertex in S_3
9. $F = T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{f}, g\}$ for all edges $g \neq \bar{g}$ with exactly one end vertex in S_2 and one end vertex in S_3
10. $F = T_1^1 \cup T_2^1 \cup T_3^1 \cup \{\bar{g}, e\}$ for all edges $e \neq \bar{e}$ with exactly one end vertex in S_1 and one end vertex in S_2

11. $F = T_1^1 \cup T_2^1 \cup (T_3^1 \backslash \{\bar{h}_3\}) \cup \{\bar{e}, \bar{f}, \bar{g}\}$
12. $F = T_1^1 \cup (T_2^1 \backslash \{\bar{h}_2\}) \cup T_3^1 \cup \{\mathring{e}_1, \mathring{e}_2, \bar{f}\}$
13. $F = (T_1^1 \backslash \{\bar{h}_1\}) \cup T_2^1 \cup T_3^1 \cup \{\mathring{e}_1, \mathring{e}_2, \bar{f}\}$

Summing up, we obtain $|E| + 1$ affinely independent vectors being tight in (4.10).

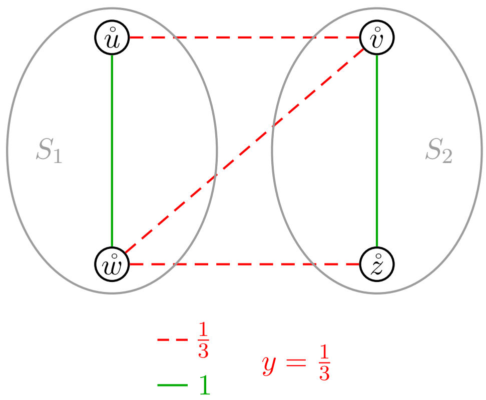
$|S_3| = 1$: The only forest in S_3 is the empty forest, therefore set $T_3^1 = \emptyset$ and consider the same forests as before except the ones in 7 and 9 which do not exist. In total they sum up to $|E| + 1$ forests again.

For each case of the disjoint vertex sets S_1 and S_2 with the required properties for the vertices $\mathring{u}, \mathring{v}, \mathring{w}$ and $\mathring{z}$, the face induced by inequality (4.10) has dimension $|E|$ and therefore is a facet of P_F^d. □

The two new classes of inequalities (4.9) and (4.10) take the influence of the product variable on the original side constraints into account and therefore improve the LP formulations (LQP_{QMSF}) to a better approximation of the polytopes P_F^c and P_F^d. Indeed they cut off parts of the polytopes P_F^{ql} and P_F^{ql}, respectively, as the following example on four vertices shows for both classes of inequalities.

Example 4.2.1.

Consider the fractional solution illustrated on the right-hand side, with non-zero values on the edge variables $x_{\mathring{u}\mathring{v}} = x_{\mathring{v}\mathring{w}} = x_{\mathring{w}\mathring{z}} = 1/3$ and $x_{\mathring{u}\mathring{w}} = x_{\mathring{v}\mathring{z}} = 1$, and the value $y = 1/3$ for the product variable.
This solution is feasible for the subtour elimination constraints (4.2) and satisfies (4.3) and (4.4), i. e., the inequalities of the standard linearization. However, the quadratic subtour elimination constraints (4.9) and (4.10) are both violated for the subset S_1 and the subsets S_1 and S_2, respectively.



Theorems 4.2.2 and 4.2.3 show that the quadratic subtour elimination contraints are needed in any complete polyhedral description of P_F^c and P_F^d, respectively. In the following, we show that they also suffice to describe these polyhedra completely, together with (4.2)–(4.4). However, we first consider the case of a nonnegative weight on the product variable, where it turns out that quadratic subtour elimination contraints are not needed, neither in the connected nor in the disconnected case.

Proposition 4.2.2.

If $q_{\mathring{e}_1\mathring{e}_2} \geq 0$, the linear program

$$(\text{LP}^{\geq 0}) \qquad \begin{aligned} \min \quad & \sum_{e\in E} c_e x_e + q_{\mathring{e}_1\mathring{e}_2} y \\ \text{s. t.} \quad & \sum_{e\in E(G[S])} x_e \leq |S| - 1 \qquad \forall \emptyset \neq S \subset V \\ & y \leq x_{\mathring{e}_1}, x_{\mathring{e}_2} \\ & y \geq x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1 \\ & x, y \geq 0 \end{aligned}$$

has an integer optimal solution.

Proof. Let (x^*, y^*) be a best possible integer solution of $(\mathrm{LP}^{\geq 0})$ with respect to the objective function, so that x^* is the incidence vector of a spanning forest F^* and $y^* = x^*_{\mathring{e}_1} x^*_{\mathring{e}_2}$. It suffices to exhibit a feasible solution z^* of the dual of $(\mathrm{LP}^{\geq 0})$ such that (x^*, y^*) and z^* satisfy the complementary slackness conditions 1.2.5 (c). Our construction uses the argumentative structure as given in the proof of Theorem 2.2.6.

As F^* is a minimal spanning forest, for each of its edges the optimality criterion

$$c_e \leq 0 \qquad \forall\, e \in E(F^*) \tag{4.11}$$

is satisfied, since edges with positive costs are not considered in an optimal solution, and for all edges not contained in the forest we have the optimality criteria

$$c_e \geq \begin{cases} c_f & \forall\, e \notin E(F^*) \text{ leading to a cycle } \mathcal{C}_e \text{ in } F^* \cup \{e\} \text{ and } \forall\, f \in \mathcal{C}_e \\ 0 & \forall\, e \notin E(F^*) \text{ otherwise} \end{cases} \tag{4.12}$$

as otherwise the insertion of e, eventually with a removal of f, would yield a better feasible solution.

In order to set up the dual problem, we introduce a dual variable z_S for each set $\emptyset \neq S \subseteq V$. Additionally, three variables z_1, z_2 and z_{12} are needed for the linearization inequalities. We obtain

$$\begin{array}{llll}
(\mathrm{DP}^{\geq 0}) & \max & -\sum\limits_{\emptyset \neq S \subseteq V} (|S|-1)\, z_S - z_{12} & \\
& \text{s.t.} & -\sum\limits_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S \leq c_e & \forall\, e \in E \backslash \{\mathring{e}_1, \mathring{e}_2\} \\
& & -\sum\limits_{\substack{S \subseteq V \\ \mathring{e}_1 \in E(G[S])}} z_S + z_1 - z_{12} \leq c_{\mathring{e}_1} & \\
& & -\sum\limits_{\substack{S \subseteq V \\ \mathring{e}_2 \in E(G[S])}} z_S + z_2 - z_{12} \leq c_{\mathring{e}_2} & \\
& & -z_1 - z_2 + z_{12} \leq q_{\mathring{e}_1 \mathring{e}_2} & \\
& & z_S, z_1, z_2, z_{12} \geq 0 & \forall\, \emptyset \neq S \subseteq V
\end{array}$$

We first assume that none of the edges $\mathring{e}_1$ and $\mathring{e}_2$ belongs to F^*, so that $y^* = 0$. Our construction of z^* starts as in Theorem 2.2.6: let the edges $E(F^*) = \{f_1, \ldots, f_{m-1}\}$ of the optimal spanning forest F^* be sorted by ascending costs, i. e. $c_{f_1} \leq \ldots \leq c_{f_{m-1}}$. For $k = 1, \ldots, m-1$, let $S_k \subseteq V$ be the connected component of the subgraph $(V, \{f_1, \ldots, f_k\})$ containing edge f_k. Now for each $k \leq m-2$, we assign $z^*_{S_k} := c_{f_l} - c_{f_k}$, where l is the first index greater than k for which $f_l \cap S_k \neq \emptyset$. Additionally, we set $z^*_{S_{m-1}} := -c_{f_{m-1}}$ and $z^*_S := 0$ for all $S \notin \{S_1, \ldots, S_{m-1}\}$. Note that by this construction we have $z^*_S \geq 0$ for all $S \subseteq V$ due to the ascending sorting and due to (4.11). Finally, we assign $z^*_1 := 0, z^*_2 := 0$ and $z^*_{12} := 0$. If the end vertices of an edge e are in the same connected component of F^*, this construction yields

$$-\sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S = c_{f_i},$$

where i is the smallest index with $e \subseteq S_i$. If otherwise the end vertices are in different connected components of F^*, we have

$$-\sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S = 0.$$

The solution z^* is thus dual feasible by (4.12). Moreover, the dual constraint corresponding to an edge e is satisfied with equality whenever $x^*_e > 0$, whereas $z^*_S > 0$ implies that the corresponding subtour elimination constraint is tight. In summary, the complementary slackness conditions are satisfied by (x^*, y^*) and z^*.

Now let only one of the product edges, say $\mathring{e}_1$, be contained in F^*, i.e. $x^*_{\mathring{e}_1} = 1, x^*_{\mathring{e}_2} = 0$ and thus $y^* = 0$. Then, the optimality criterion (4.11) still holds, but if insertion of $\mathring{e}_2$ leads to a cycle $\mathcal{C}_{\mathring{e}_2}$, the corresponding inequalities (4.12) are no longer valid for $\mathring{e}_2$ and $f \in \mathcal{C}_{\mathring{e}_2}$ but only the weaker optimality criterion

$$c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq c_f \qquad \forall\, f \in \mathcal{C}_{\mathring{e}_2} \backslash \{\mathring{e}_1\}. \tag{4.13}$$

We construct z^* analogously but define $z^*_1 := q_{\mathring{e}_1\mathring{e}_2}$ and $z^*_{12} := q_{\mathring{e}_1\mathring{e}_2}$; thus $z^*_1, z^*_{12} \geq 0$. For all edges $e \neq \mathring{e}_1, \mathring{e}_2$ the complementary slackness constraints are satisfied by (4.12) and the same arguments as before. For edge $\mathring{e}_1$ we have equality in the dual problem by $z^*_1 = z^*_{12}$ and $x^*_{\mathring{e}_1} > 0$; in particular, we obtain complementary slackness. Furthermore, if the insertion of $\mathring{e}_2$ leads to a cycle, the left-hand side of the inequality corresponding to $\mathring{e}_2$ equals $c_{f_i} - q_{\mathring{e}_1\mathring{e}_2}$ which in turn is not greater than $c_{\mathring{e}_2}$ due to optimality criterion (4.13). Otherwise, the left-hand side equals $-q_{\mathring{e}_1\mathring{e}_2} \leq 0$ such that complementary slackness is satisfied by optimality criterion (4.12). Finally, $-z^*_1 - z^*_2 + z^*_{12} = 0 \leq q_{\mathring{e}_1\mathring{e}_2}$ proves dual feasibility of z^*.

It thus remains to consider the case that F^* contains both $\mathring{e}_1$ and $\mathring{e}_2$. Then, the optimality criterion (4.11) does not hold for $\mathring{e}_1, \mathring{e}_2$ but we have

$$c_{\mathring{e}_1} + q_{\mathring{e}_1\mathring{e}_2} \leq 0 \;\text{ and }\; c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \leq 0, \tag{4.14}$$

since otherwise removing one of these edges would increase the solution value. In this case we change the entire construction of the dual solution by considering a modified objective function

$$\widetilde{c}_e := \begin{cases} c_e & \text{if } e \in E\backslash\{\mathring{e}_1, \mathring{e}_2\} \\ c_{\mathring{e}_1} + q_{\mathring{e}_1\mathring{e}_2} & \text{if } e = \mathring{e}_1 \\ c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} & \text{if } e = \mathring{e}_2 \end{cases}$$

and by recomputing the basic dual solution z^* according to this new cost function $\widetilde{c}$ instead of c. Note that $\widetilde{c}_{\mathring{e}_1}, \widetilde{c}_{\mathring{e}_2} \leq 0$ because of (4.14). Moreover, we set $z^*_{12} := q_{\mathring{e}_1\mathring{e}_2}$ in this case. Again, this solution turns out to be dual feasible and complementary slackness conditions corresponding to all $x^*_e > 0$ as well as to all $z^*_S > 0$ are satisfied. The additional complementary slackness condition resulting from $y^* > 0$ is $z^*_{12} = q_{\mathring{e}_1\mathring{e}_2}$ and hence satisfied by definition. □

The modified objective function $\widetilde{c}$, used in the last case of the preceding proof, is motivated by the following reasoning: if the optimal forest contains both edges $\mathring{e}_1$ and $\mathring{e}_2$, then removing one of these edges not only decreases the objective function by the linear weight $c_{\mathring{e}_1}$ or $c_{\mathring{e}_2}$, but also by the product weight $q_{\mathring{e}_1\mathring{e}_2}$, as the variable y switches to zero as well in this case. The linear optimality criterion (4.12) can thus be extended to $\widetilde{c}$, leading to (4.14).

Proposition 4.2.2 shows that quadratic subtour elimination constraints are not needed if the objective function coefficient of the single product term is nonnegative. Nevertheless, for general objective functions, Example 4.2.1 shows that the quadratic subtour elimination constraints lead to a tighter description of the corresponding polytope. In fact, we can show that they even yield a complete polyhedral description of P^c_F and P^d_F, respectively.

Theorem 4.2.4.

$$P^c_F = \left\{ (x, y) \in [0,1]^{|E|+1} \;\middle|\; (x, y) \text{ satisfies } (4.2), (4.3), (4.4) \text{ and } (4.9) \right\}.$$

Proof. All constraints (4.2), (4.3), (4.4), and (4.9) are valid for P_F^c, it thus remains to show that they yield a complete polyhedral description of P_F^c. As in the proof of Proposition 4.2.2, we use duality. The primal problem reads

$$
\begin{array}{llll}
\text{(LP)} & \min & \sum_{e\in E} c_e x_e + q_{\mathring{e}_1\mathring{e}_2} y & \\
& \text{s.t.} & \sum_{e\in E(G[S])} x_e + y \le |S|-1 & \text{for } \emptyset \ne S \subset V \text{ with } \mathring{u},\mathring{w}\in S,\ \mathring{v}\notin S \\
& & \sum_{e\in E(G[S])} x_e \le |S|-1 & \text{for } S\subseteq V \text{ else} \\
& & y \le x_{\mathring{e}_1}, x_{\mathring{e}_2} & \\
& & y \ge x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1 & \\
& & x, y \ge 0 &
\end{array}
$$

Again, we introduce a dual variable z_S for each $\emptyset \ne S \subseteq V$ and one variable each for the three linearization inequalities, denoted by z_1, z_2 and z_{12}. The dual then turns out to be

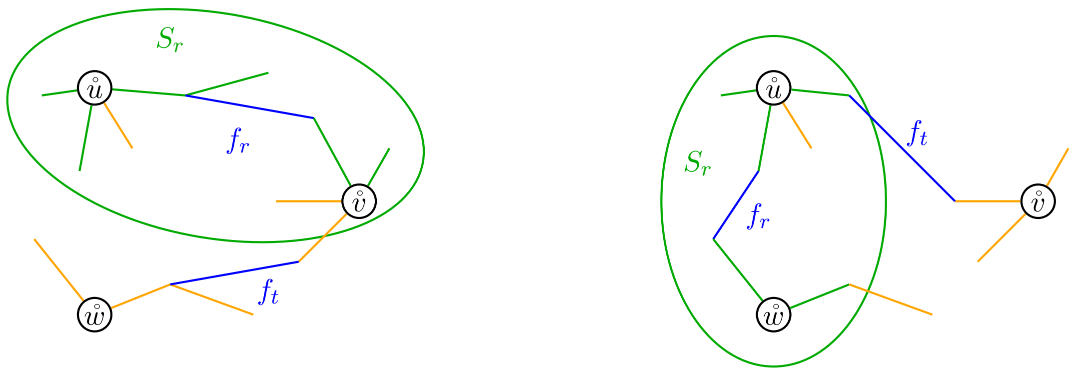
$$
\begin{array}{llll}
\text{(DP)} & \max & -\sum_{\emptyset\ne S\subseteq V} (|S|-1) z_S - z_{12} & \\
& \text{s.t.} & -\sum_{\substack{S\subseteq V\\ e\in E(G[S])}} z_S \le c_e & \text{for } e\in E\backslash\{\mathring{e}_1,\mathring{e}_2\} \quad \text{(d1)} \\
& & -\sum_{\substack{S\subseteq V\\ \mathring{e}_1\in E(G[S])}} z_S + z_1 - z_{12} \le c_{\mathring{e}_1} & \text{(d2)} \\
& & -\sum_{\substack{S\subseteq V\\ \mathring{e}_2\in E(G[S])}} z_S + z_2 - z_{12} \le c_{\mathring{e}_2} & \text{(d3)} \\
& & -\sum_{\substack{S\subseteq V\\ \mathring{u},\mathring{w}\in S,\ \mathring{v}\notin S}} z_S - z_1 - z_2 + z_{12} \le q_{\mathring{e}_1\mathring{e}_2} & \text{(d4)} \\
& & z_S, z_1, z_2, z_{12} \ge 0 & \text{for } \emptyset\ne S\subseteq V
\end{array}
$$

Let (x^*, y^*) be an optimal integer solution of (LP), so that x^* is the incidence vector of a spanning forest F^* and $y^* = x^*_{\mathring{e}_1} x^*_{\mathring{e}_2}$. As in the proof of Proposition 4.2.2, we sort the forest edges $E(F^*) = \{f_1, \dots, f_{m-1}\}$ by ascending costs, construct the connected components S_k and define the corresponding basic dual solution z^*, to be modified in the following. Note that again the optimality criteria (4.11) and (4.12) hold such that $z^*_S \ge 0$ and the dual constraint (d1) follows as in the linear case by construction. Moreover we can assume $q_{\mathring{e}_1\mathring{e}_2} < 0$ by Proposition 4.2.2.

As the spanning forest F^* can either contain or not contain the edges $\mathring{e}_1$ and $\mathring{e}_2$, we split up the construction of the dual solution into four cases two of which are symmetric.

$x^*_{\mathring{e}_1} = x^*_{\mathring{e}_2} = y^* = 0$, i.e. none of the edges $\mathring{e}_1$ and $\mathring{e}_2$ belong to F^*

Initially, consider the case that the three vertices $\mathring{u}, \mathring{v}$ and $\mathring{w}$ are connected in F^*. Let r be the smallest index with $|S_r \cap \{\mathring{u}, \mathring{v}, \mathring{w}\}| = 2$ and t the smallest index with $\{\mathring{u}, \mathring{v}, \mathring{w}\} \subseteq S_t$. In the following, we distinguish between two cases: either S_r contains $\mathring{u}$ and $\mathring{v}$ (*case I*), or it contains $\mathring{u}$ and $\mathring{w}$ (*case II*), see Figure 4.7. The case that S_r contains $\mathring{v}$ and $\mathring{w}$ is analogous to case I.



(a) case I: S_r contains the vertices $\mathring{u}$ and $\mathring{v}$.

(b) case II: S_r contains the vertices $\mathring{u}$ and $\mathring{w}$.

Figure 4.7: Illustration of the cases I and II with $x_{\mathring{e}_1} = x_{\mathring{e}_2} = 0$. The edges according to the subset S_r are colored in green. The yellow edges are inserted in the course of the algorithm until f_t is inserted, yielding the subset S_t.

In both cases, $\mathring{e}_1, \mathring{e}_2 \notin F^*$ yields the optimality criterion

$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq c_{f_r} + c_{f_t} \tag{4.15}$$

as otherwise replacing f_r and f_t by $\mathring{e}_1$ and $\mathring{e}_2$ in $E(F^*)$ would yield a strictly better solution than (x^*, y^*).

case I: We extend the basic dual solution by setting

$$z_1^* := c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := c_{\mathring{e}_2} - c_{f_t}, \qquad z_{12}^* := 0.$$

This solution is valid due to $c_{\mathring{e}_1} \geq c_{f_r}$ and $c_{\mathring{e}_2} \geq c_{f_t}$ since both monomial edges are not contained in F^*. Furthermore, z^* satisfies (d2) with equality, as

$$-\sum_{\substack{S \subseteq V \\ \mathring{e}_1 \in E(G[S])}} z_S^* + z_1^* - z_{12}^* = c_{f_r} + c_{\mathring{e}_1} - c_{f_r} = c_{\mathring{e}_1},$$

and equality in (d3) follows analogously. To show (d4), we use the optimality criterion (4.15) and the fact that $z_S^* = 0$ for all $S \subset V$ with $\mathring{u}, \mathring{w} \in S, \mathring{v} \notin S$. This leads to

$$-\sum_{\substack{S \subseteq V \\ \mathring{u},\mathring{w} \in S,\, \mathring{v} \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* = c_{f_r} - c_{\mathring{e}_1} + c_{f_t} - c_{\mathring{e}_2} \leq q_{\mathring{e}_1\mathring{e}_2}.$$

case II: As t is both minimal with $\mathring{u}, \mathring{v} \in S_t$ and with $\mathring{v}, \mathring{w} \in S_t$, the first sums on the left-hand sides of (d2) and (d3) both equal c_{f_t}. Moreover, $c_{\mathring{e}_1} \geq c_{f_t}$ and $c_{\mathring{e}_2} \geq c_{f_t}$ since otherwise one of the monomial edges would have been inserted in F^* instead of f_t. Adding

$$z_1^* := c_{\mathring{e}_1} - c_{f_t}, \qquad z_2^* := c_{\mathring{e}_2} - c_{f_t}, \qquad z_{12}^* := 0$$

to the basic dual solution, we obtain equality in both (d2) and (d3). Inequality (d4) is satisfied since

$$-\sum_{\substack{S \subseteq V \\ \mathring{u},\mathring{w} \in S,\, \mathring{v} \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* = c_{f_r} - c_{f_t} - z_1^* - z_2^* = c_{f_r} - c_{\mathring{e}_1} + c_{f_t} - c_{\mathring{e}_2},$$

which by optimality criterion (4.15) is bounded by $q_{\mathring{e}_1\mathring{e}_2}$.

Now consider the case that only two of the three vertices $\mathring{u}, \mathring{v}$ and $\mathring{w}$ are connected. Then again, let r be the index with $|S_r \cap \{\mathring{u}, \mathring{v}, \mathring{w}\}| = 2$ such that we have the optimality criterion

$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq c_{f_r}. \tag{4.16}$$

As before we distinguish the two cases where $\mathring{u}, \mathring{v} \in S_r$ (*case I*) and where $\mathring{u}, \mathring{w} \in S_r$ (*case II*), since the case where $\mathring{v}, \mathring{w} \in S_r$ is analogous to case I. Ignoring the yellow edges and f_t, Figure 4.7 also illustrates these cases.

case I: $\mathring{u}, \mathring{v} \in S_r$ results in $c_{\mathring{e}_2} \geq 0$ by optimality criterion (4.12). We extend z^* by

$$z_1^* := c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := c_{\mathring{e}_2}, \qquad z_{12}^* := 0,$$

accounting that $c_{\mathring{e}_1} \geq c_{f_r}$. Then, (d2) is satisfied with equality by the same arguments as before. As there is no edge in F^* connecting $\mathring{u}$ or $\mathring{v}$ with $\mathring{w}$, we have

$$-\sum_{\substack{S \subseteq V \\ \mathring{e}_1 \in E(G[S])}} z_S^* = 0 \qquad \text{and} \qquad -\sum_{\substack{S \subseteq V \\ \mathring{u}, \mathring{w} \in S,\, \mathring{v} \notin S}} z_S^* = 0,$$

such that the left-hand sides of (d3) and (d4) sum up to $c_{f_r} - c_{\mathring{e}_1} - c_{\mathring{e}_2}$. By (4.16), this is not greater than $q_{\mathring{e}_1\mathring{e}_2} \leq 0 \leq c_{\mathring{e}_2}$, such that we have feasibility in both (d3) and (d4).

case II: $\mathring{u}, \mathring{w} \in S_r$ and (4.12) lead to $c_{\mathring{e}_1}, c_{\mathring{e}_2} \geq 0$. We set

$$z_1^* := c_{\mathring{e}_1}, \qquad z_2^* := c_{\mathring{e}_2}, \qquad z_{12}^* := 0.$$

Then, we obtain

$$-\sum_{\substack{S \subseteq V \\ \mathring{e}_1 \in E(G[S])}} z_S^* - z_1^* = -c_{\mathring{e}_1} \leq 0 \leq c_{\mathring{e}_1}, \qquad -\sum_{\substack{S \subseteq V \\ \mathring{e}_2 \in E(G[S])}} z_S^* - z_2^* = -c_{\mathring{e}_2} \leq 0 \leq c_{\mathring{e}_2},$$

and with $\mathring{u}, \mathring{w} \in S_r$

$$-\sum_{\substack{S \subseteq V \\ \mathring{u}, \mathring{w} \in S,\, \mathring{v} \notin S}} z_S^* = c_{f_r} - c_{\mathring{e}_1} - c_{\mathring{e}_2} \leq q_{\mathring{e}_1\mathring{e}_2}.$$

Finally, if $\mathring{u}, \mathring{v}$ and $\mathring{w}$ are in pairwise different components of F^*, we have $c_{\mathring{e}_1}, c_{\mathring{e}_2} \geq 0$ by (4.12) and the optimality criterion

$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq 0. \tag{4.17}$$

We again extend z^* by

$$z_1^* := c_{\mathring{e}_1}, \qquad z_2^* := c_{\mathring{e}_2}, \qquad z_{12}^* := 0$$

such that (d2) and (d3) are satisfied as in case II directly above and we have

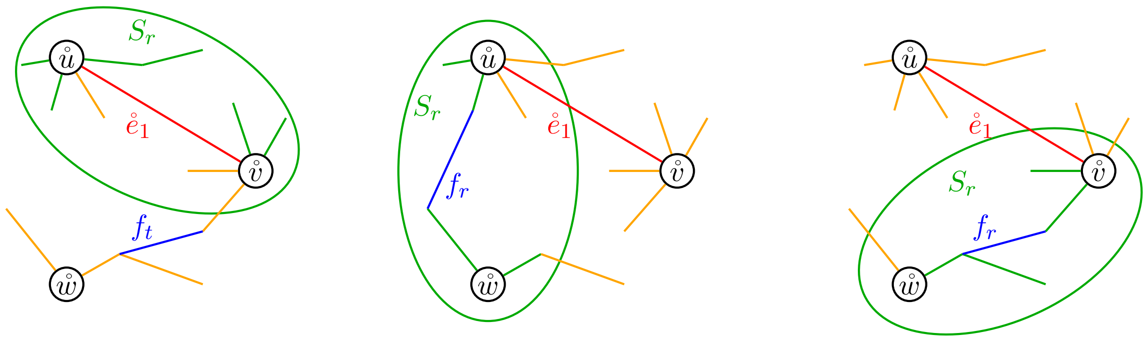
$$-\sum_{\substack{S \subseteq V \\ \mathring{u}, \mathring{w} \in S,\, \mathring{v} \notin S}} z_S^* = 0 - c_{\mathring{e}_1} - c_{\mathring{e}_2} \leq q_{\mathring{e}_1\mathring{e}_2}$$

due to (4.17).

We have thus constructed a dual feasible solution in all cases of $\mathring{e}_1, \mathring{e}_2 \notin F^*$. The complementary slackness conditions for $x_e^* > 0$ and $z_S^* > 0$ are satisfied as in the linear case, while the remaining ones are satisfied by the construction of z_1^*, z_2^* and z_{12}^*.

$x^*_{\mathring{e}_1} = 1, x^*_{\mathring{e}_2} = 0, y^* = 0$ (the case $x^*_{\mathring{e}_1} = 0, x^*_{\mathring{e}_2} = 1, y^* = 0$ is analogous).

In this case we again make use of the optimality criteria (4.11), (4.12) and (4.13) and first of all we consider the case where the vertices $\mathring{u}, \mathring{v}$ and $\mathring{w}$ are connected in F^*. Let again r be the smallest index with $|S_r \cap \{\mathring{u}, \mathring{v}, \mathring{w}\}| = 2$ and t be the smallest index with $\{\mathring{u}, \mathring{v}, \mathring{w}\} \subseteq S_t$. Here, we distinguish between the cases where either $\mathring{u}, \mathring{v} \in S_r$ (*case I*) or $\mathring{u}, \mathring{w} \in S_r$ (*case II*) or $\mathring{v}, \mathring{w} \in S_r$ (*case III*). Note that $f_r = \mathring{e}_1$ in case I and $f_t = \mathring{e}_1$ in case II and III, see Figure 4.8.



(a) case I: $\mathring{u}, \mathring{v} \in S_r$. (b) case II: $\mathring{u}, \mathring{w} \in S_r$. (c) case III: $\mathring{v}, \mathring{w} \in S_r$.

Figure 4.8: Illustration of the cases I, II and III with $x_{\mathring{e}_1} = 1$ and $x_{\mathring{e}_2} = 0$. The edges according to the subset S_r are colored in green. The yellow edges are inserted in the course of the algorithm until f_t is inserted, yielding the subset S_t.

case I: We set

$$z^*_1 := 0, \qquad z^*_2 := -q_{\mathring{e}_1\mathring{e}_2}, \qquad z^*_{12} := 0.$$

Note that $q_{\mathring{e}_1\mathring{e}_2} < 0$ implies $z^*_2 > 0$. Inequality (d2) is satisfied as in the linear case. Furthermore, from (4.13), in particular $c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq c_{f_t}$ as the insertion of $\mathring{e}_2$ to F^* closes a cycle containing f_t, we derive

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_2\in E(G[S])}} z^*_S + z^*_2 = c_{f_t} - q_{\mathring{e}_1\mathring{e}_2} \leq c_{\mathring{e}_2};$$

this shows (d3). Constraint (d4) is trivially satisfied in case I, since $z^*_S = 0$ for all sets S with $\mathring{u}, \mathring{w} \in S$, $\mathring{v} \notin S$.

case II: We set

$$z^*_1 := 0, \qquad z^*_2 := c_{\mathring{e}_2} - c_{\mathring{e}_1}, \qquad z^*_{12} := 0.$$

Note that (4.11) and (4.12) guarantee $z^*_2 \geq 0$ since otherwise an exchange of $\mathring{e}_1$ and $\mathring{e}_2$ would lead to a solution with less costs. Inequality (d2) is satisfied as in the linear case. Being in case II, we have $f_t = \mathring{e}_1$, so that we obtain equality in (d3)

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_2\in E(G[S])}} z^*_S + z^*_2 = c_{f_t} + c_{\mathring{e}_2} - c_{\mathring{e}_1} = c_{\mathring{e}_2}.$$

By optimality criterion (4.13), in particular $c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq c_{f_r}$ as $f_r \in \mathcal{C}_{\mathring{e}_2}$, we obtain feasibility in (d4):

$$-\sum_{\substack{S\subseteq V\\ \mathring{u},\mathring{w}\in S,\, \mathring{v}\notin S}} z^*_S - z^*_1 - z^*_2 + z^*_{12} = c_{f_r} - c_{f_t} - c_{\mathring{e}_2} + c_{\mathring{e}_1} = c_{f_r} - c_{\mathring{e}_2} \leq q_{\mathring{e}_1\mathring{e}_2}.$$

case III: Analogous to case I we set

$$z_1^* := 0, \qquad z_2^* := -q_{\mathring{e}_1\mathring{e}_2}, \qquad z_{12}^* := 0.$$

In case III the optimality criterion (4.13) holds for $f_r \in \mathcal{C}_{\mathring{e}_2}$, such that (d3) is satisfied:

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_2\in E(G[S])}} z_S^* + z_2^* = c_{f_r} - q_{\mathring{e}_1\mathring{e}_2} \leq c_{\mathring{e}_2}.$$

Constraints (d1), (d2) and (d4) are satisfied by the same arguments as in case I.

Now consider the case that $\mathring{w}$ is not connected with $\mathring{u}$ and $\mathring{v}$. Then we obtain the additional optimality criterion

$$c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq 0 \tag{4.18}$$

and set

$$z_1^* := 0, \qquad z_2^* := -q_{\mathring{e}_1\mathring{e}_2}, \qquad z_{12}^* := 0.$$

By the same arguments as in case I we obtain feasibility in (d1), (d2) and (d4), furthermore, the left-hand side of (d3) equals $-q_{\mathring{e}_1\mathring{e}_2}$ which is not greater than $c_{\mathring{e}_2}$ due to (4.18).

In all cases, the complementary slackness conditions for $x_e^* > 0$ and $z_S^* > 0$ are satisfied as in the linear case, observing $z_1^* = 0$ and $z_{12}^* = 0$ for equality in (d2). The remaining complementary slackness conditions are satisfied by construction.

$x_{\mathring{e}_1}^* = x_{\mathring{e}_2}^* = y^* = 1$**,** i.e. both $\mathring{e}_1, \mathring{e}_2 \in F^*$.

Let F' be a minimal *linear* spanning forest subject to the cost function c. We may assume $E(F^*)\backslash E(F') \subseteq \{\mathring{e}_1, \mathring{e}_2\}$ since a minimal linear forest can be constructed by applying Kruskal's algorithm to the forest $(V, E(F^*)\backslash\{\mathring{e}_1, \mathring{e}_2\})$. Optimality follows, since the optimality criteria (4.11) and (4.12) are satisfied for all newly inserted edges by construction, and for the existing edges $E(F^*)\backslash\{\mathring{e}_1, \mathring{e}_2\}$ by optimality of F^*. For the construction of a dual solution define the sets S_k and the basic solution z^* as before, but based on the forest F' instead of F^*.

Initially assume that $\mathring{u}, \mathring{v}$ and $\mathring{w}$ are connected in F'. Let again r be the smallest index with $|S_r \cap \{\mathring{u}, \mathring{v}, \mathring{w}\}| = 2$ and let t be the smallest index with $\{\mathring{u}, \mathring{v}, \mathring{w}\} \subseteq S_t$. We again distinguish between the two cases that either S_r contains $\mathring{u}$ and $\mathring{v}$ (*case I*), or it contains $\mathring{u}$ and $\mathring{w}$ (*case II*). The case that S_r contains $\mathring{v}$ and $\mathring{w}$ is analogous to case I.

In both cases, we obtain (d1) as in the linear case. Moreover, we can derive

$$c_{f_r} + c_{f_t} \geq c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \tag{4.19}$$

from the optimality of F^*, as otherwise the forest F' would yield a better solution of (LP) than F^*. Note that we do not exclude that $\mathring{e}_1$ or $\mathring{e}_2$ agree with f_r or f_t.

case I: We extend z^* by setting

$$z_1^* := c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := c_{\mathring{e}_2} - c_{f_t}, \qquad z_{12}^* := 0, \qquad z_{\{\mathring{u},\mathring{w}\}}^* := -q_{\mathring{e}_1\mathring{e}_2} - z_1^* - z_2^*\,.$$

Optimality of F' yields $z_1^* \geq 0$ and $z_2^* \geq 0$, while $z_{\{\mathring{u},\mathring{w}\}}^* \geq 0$ follows from (4.19). We now obtain equality in both (d2) and (d3), as

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_1\in E(G[S])}} z_S^* + z_1^* - z_{12}^* = c_{f_r} + c_{\mathring{e}_1} - c_{f_r} = c_{\mathring{e}_1}$$

and

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_2\in E(G[S])}} z^*_S + z^*_2 - z^*_{12} = c_{f_t} + c_{\mathring{e}_2} - c_{f_t} = c_{\mathring{e}_2}.$$

Equality in (d4) also follows, since

$$\sum_{\substack{S\subseteq V\\ \mathring{u},\mathring{w}\in S,\,\mathring{v}\notin S}} z^*_S = z^*_{\{\mathring{u},\mathring{w}\}}$$

in case I and hence

$$-\sum_{\substack{S\subseteq V\\ \mathring{u},\mathring{w}\in S,\,\mathring{v}\notin S}} z^*_S - z^*_1 - z^*_2 + z^*_{12} = q_{\mathring{e}_1\mathring{e}_2} + z^*_1 + z^*_2 - z^*_1 - z^*_2 = q_{\mathring{e}_1\mathring{e}_2}.$$

case II: We extend z^* by setting

$$z^*_1 := c_{\mathring{e}_1} - c_{f_t}, \qquad z^*_2 := c_{\mathring{e}_2} - c_{f_t}, \qquad z^*_{12} := 0, \qquad z^*_{\{\mathring{u},\mathring{w}\}} := -q_{\mathring{e}_1\mathring{e}_2} - z^*_1 - z^*_2.$$

Note that $z^*_1 \geq 0$, as we are in case II. Moreover, we have $z^*_2 \geq 0$ by optimality of F', and $z^*_{\{\mathring{u},\mathring{w}\}} \geq 0$ as

$$-q_{\mathring{e}_1\mathring{e}_2} - c_{\mathring{e}_1} + c_{f_t} - c_{\mathring{e}_2} + c_{f_t} \geq -q_{\mathring{e}_1\mathring{e}_2} - c_{\mathring{e}_1} + c_{f_r} - c_{\mathring{e}_2} + c_{f_t} \geq 0$$

by $c_{f_t} \geq c_{f_r}$ and (4.19). Insertion into (d2)–(d4) yields equality:

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_1\in E(G[S])}} z^*_S + z^*_1 - z^*_{12} = c_{f_t} + c_{\mathring{e}_1} - c_{f_t} = c_{\mathring{e}_1},$$

$$-\sum_{\substack{S\subseteq V\\ \mathring{e}_2\in E(G[S])}} z^*_S + z^*_2 - z^*_{12} = c_{f_t} + c_{\mathring{e}_2} - c_{f_t} = c_{\mathring{e}_2},$$

$$-\sum_{\substack{S\subseteq V\\ \mathring{u},\mathring{w}\in S,\,\mathring{v}\notin S}} z^*_S - z^*_1 - z^*_2 + z^*_{12} = q_{\mathring{e}_1\mathring{e}_2} + z^*_1 + z^*_2 - z^*_1 - z^*_2 = q_{\mathring{e}_1\mathring{e}_2}.$$

In both cases, the complementary slackness conditions are satisfied, noting that equality in (d2)–(d4) holds as required by $x^*_{\mathring{e}_1} = x^*_{\mathring{e}_2} = y^* = 1$, and that setting $z^*_{\{\mathring{u},\mathring{w}\}} > 0$ does not violate the complementary slackness conditions, since the subtour elimination constraint for $S = \{\mathring{u}, \mathring{w}\}$ is satisfied with equality. Moreover, setting $z^*_{\{\mathring{u},\mathring{w}\}} > 0$ increases the slack only in (d1) and only for edge $\{\mathring{u}, \mathring{w}\}$, in which case equality is not required.

If F' is not connected and no indices r or t exist with $|S_r \cap \{\mathring{u}, \mathring{v}, \mathring{w}\}| = 2$ and $\{\mathring{u}, \mathring{v}, \mathring{w}\} \subseteq S_t$, the same construction as above can be used with $c_{f_r} = 0$ or $c_{f_t} = 0$. □

The above proof shows that the constraint $y \geq x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1$, corresponding to the dual variable z^*_{12}, is only needed in the case $q_{\mathring{e}_1\mathring{e}_2} \geq 0$, which was addressed in Proposition 4.2.2.

The following theorem considers the disconnected case. For this, define the set of pairs of vertex subsets which are connected by the monomial edges $\mathring{e}_1$ and $\mathring{e}_2$ as

$$\mathcal{S} := \Big\{ \{S_1, S_2\} \;\Big|\; S_1, S_2 \subseteq V, S_1 \cap S_2 = \emptyset, \text{ and } \mathring{e}_1 \text{ and } \mathring{e}_2 \text{ have exactly one vertex in } S_1 \text{ and one vertex in } S_2 \Big\}.$$

Theorem 4.2.5.

$$P_F^d = \Big\{ (x,y) \in [0,1]^{|E|+1} \;\Big|\; (x,y) \text{ satisfies } (4.2), (4.3), (4.4) \text{ and } (4.10) \Big\}.$$

Proof. Analogous to the proof of Theorem 4.2.4 we dualize the primal problem

$$\begin{array}{llll}
\text{(LP)} & \min & \sum_{e \in E} c_e x_e + q_{\mathring{e}_1\mathring{e}_2} y & \\
& \text{s. t.} & \sum_{e \in E(G[S])} x_e \leq |S| - 1 & \text{for } \emptyset \neq S \subseteq V \\
& \multicolumn{2}{l}{\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e + y \leq |S_1| + |S_2| - 2} & \text{for } \{S_1, S_2\} \in \mathcal{S} \\
& & y \leq x_{\mathring{e}_1}, x_{\mathring{e}_2} & \\
& & y \geq x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1 & \\
& & x, y \geq 0 &
\end{array}$$

yielding the dual problem

$$\begin{array}{llll}
\text{(DP)} & \max & -\sum_{\emptyset \neq S \subseteq V} (|S|-1) z_S - \sum_{\{S_1,S_2\} \in \mathcal{S}} (|S_1|+|S_2|-2) z_{S_1S_2} - z_{12} & \\
& \text{s. t.} & -\sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S - \sum_{\substack{\{S_1,S_2\} \in \mathcal{S}: \\ e \in E(G[S_1]) \cup E(G[S_2])}} z_{S_1S_2} \leq c_e & \text{for } e \in E \backslash \{\mathring{e}_1, \mathring{e}_2\} \quad \text{(d1)} \\
& & -\sum_{\substack{S \subseteq V \\ \mathring{e}_1 \in E(G[S])}} z_S + z_1 - z_{12} \leq c_{\mathring{e}_1} & \text{(d2)} \\
& & -\sum_{\substack{S \subseteq V \\ \mathring{e}_2 \in E(G[S])}} z_S + z_2 - z_{12} \leq c_{\mathring{e}_2} & \text{(d3)} \\
& & -\sum_{\{S_1,S_2\} \in \mathcal{S}} z_{S_1S_2} - z_1 - z_2 + z_{12} \leq q_{\mathring{e}_1\mathring{e}_2} & \text{(d4)} \\
& & z_S, z_{S_1S_2}, z_1, z_2, z_{12} \geq 0 & \text{for } \emptyset \neq S \subseteq V \\
& & & \text{and } \{S_1, S_2\} \in \mathcal{S}
\end{array}$$

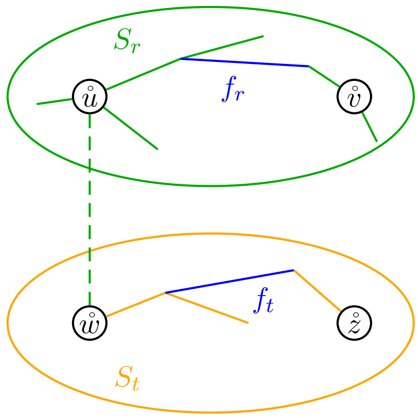
Let again (x^*, y^*) be an optimal integer solution of (LP) with x^* incidence vector of a spanning forest F^* and $y^* = x^*_{\mathring{e}_1} x^*_{\mathring{e}_2}$. As in the proof of Theorem 4.2.4, we construct the basic dual solution z^* and modify it accordingly. In each case we present the corresponding optimality criteria which are needed in addition to the criteria (4.11) and (4.12) and consequently write the modifications of the dual solution. We again assume $q_{\mathring{e}_1\mathring{e}_2} < 0$ by Proposition 4.2.2 and set $z^*_{12} = 0$ in each case as this variable is only needed in the case $q_{\mathring{e}_1\mathring{e}_2} \geq 0$.

$x^*_{\mathring{e}_1} = x^*_{\mathring{e}_2} = y^* = 0$.

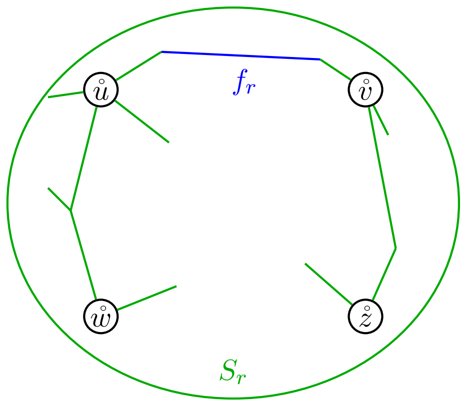
Initially, assume that there exist paths in F^* connecting $\mathring{u}$ with $\mathring{v}$ and $\mathring{w}$ with $\mathring{z}$ respectively. Let r, t be the minimal indices with $\mathring{u}, \mathring{v} \in S_r$ and $\mathring{w}, \mathring{z} \in S_t$. Distinguish between $r \neq t$ (*case I*) and $r = t$ (*case II*), see Figure 4.9.

case I: We obtain the optimality criterion

$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq c_{f_r} + c_{f_t}$$



(a) case I: both $\mathring{u}, \mathring{v} \in S_r$ but not both $\mathring{w}, \mathring{z} \in S_r$.



(b) case II: f_r connects the pairs $\mathring{u}, \mathring{w}$ and $\mathring{v}, \mathring{z}$.

Figure 4.9: Distinction of the cases I and II with $x_{\mathring{e}_1} = x_{\mathring{e}_2} = 0$. In case I it is also possible that one of the vertices $\mathring{w}$ or $\mathring{z}$ is in the subset S_r, as indicated by the green dashed edge. In case II both pairs $\mathring{u}, \mathring{v}$ and $\mathring{w}, \mathring{z}$ (or $\mathring{u}, \mathring{z}$ and $\mathring{v}, \mathring{w}$) have to be connected before edge f_r connects the four of them.

as otherwise a replacement of the edges f_r, f_t by $\mathring{e}_1, \mathring{e}_2$ yields a better solution. A dual solution is given by the same extension as in the corresponding case in the proof of Theorem 4.2.4,

$$z_1^* := c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := c_{\mathring{e}_2} - c_{f_t}, \qquad z_{S_1 S_2}^* := 0 \ \ \forall \{S_1, S_2\} \in \mathcal{S},$$

such that positiveness, feasibility and complementary slackness follow by the same arguments.

case II: Since $r = t$, the vertices $\mathring{u}$ and $\mathring{v}$ and the vertices $\mathring{w}$ and $\mathring{z}$ are connected by the insertion of one single edge. Thus, there exist two disjoint subsets S_p, S_q with p, q minimal such that either $\mathring{u}, \mathring{w} \in S_p$ and $\mathring{v}, \mathring{z} \in S_q$ or $\mathring{u}, \mathring{z} \in S_p$ and $\mathring{v}, \mathring{w} \in S_q$, such that these subsets are connected by f_r. We consider the first of the two cases, the other case runs analogously. Let without loss of generality $p < q$. Let furthermore $p' < q' < r$ be the indices of the maximal subsets which contain exactly two of the four monomial vertices, without loss of generality let $\mathring{u}, \mathring{w} \in S_{p'}$ and $\mathring{v}, \mathring{z} \in S_{q'}$. For a visualization see Figure 4.10.

By this, the optimality criterion (4.15) reads

$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1 \mathring{e}_2} \geq c_{f_q} + c_{f_r} \tag{4.20}$$

since otherwise the edges f_q and f_r could be replaced by the monomial edges improving the solution. A dual solution is constructed as follows. Set

$$z_1^* := c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := c_{\mathring{e}_2} - c_{f_r},$$

which both are nonnegative due to (4.12). By this, constraints (d1), (d2) and (d3) are satisfied by the same arguments as in the respective case in the proof of Theorem 4.2.4, but not constraint (d4) since

$$-\sum_{\{S_1 S_2\} \in \mathcal{S}} z_{S_1 S_2}^* - z_1^* - z_2^* + z_{12}^* = 0 - (c_{\mathring{e}_1} - c_{f_r}) - (c_{\mathring{e}_2} - c_{f_r}) + 0$$

which is not greater than $q_{\mathring{e}_1 \mathring{e}_2} + c_{f_r} - c_{f_q}$ by optimality criterion (4.20). To gain a value not greater than $q_{\mathring{e}_1 \mathring{e}_2}$, i.e. to satisfy (d4), the value $d := c_{f_r} - c_{f_q}$, which is

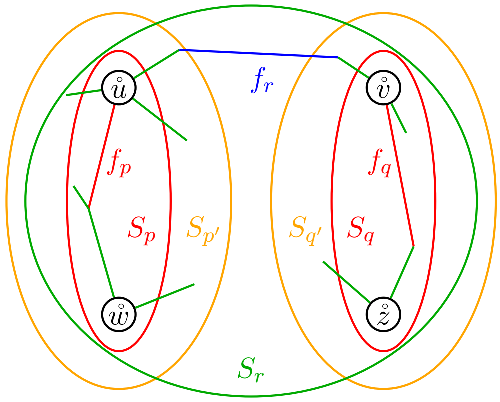


Figure 4.10: The red edge on the left, f_p, connects $\mathring{u}$ and $\mathring{w}$ and yields the subset S_p, $\mathring{v}$ and $\mathring{z}$ are connected by the red edge f_q on the right, yielding subset S_q. The maximal subsets containing exactly two of the monomial vertices are the yellow subsets $S_{p'}$ and $S_{q'}$, which finally are connected by the blue edge f_r.

nonnegative by construction ($r > q$), has to be transferred to the variables $z^*_{S_iS_j}$. For this, let I be the set of indices of the chain $S_{p'} \supset \ldots \supset S_p$ and let J be the set of indices of the chain $S_{q'} \supset \ldots \supset S_q$. For all $i \in I$ and $j \in J$ in decreasing order with respect to the corresponding values c_{f_i} and c_{f_j} set

$$z^*_{S_iS_j} := \min\left\{ z^*_{S_i} - \sum_{\substack{l \in J\\ l > j}} z^*_{S_iS_l},\ z^*_{S_j} - \sum_{\substack{k \in I\\ k > i}} z^*_{S_kS_j},\ d - \sum_{\substack{k \in I\\ k \geq i}} \sum_{\substack{l \in J\\ l \geq j}} z^*_{S_kS_l} \right\} \tag{4.21}$$

and subtract $\sum_{l \in J} z^*_{S_iS_l}$ from $z^*_{S_i}$ and $\sum_{k \in I} z^*_{S_kS_j}$ from $z^*_{S_j}$. The distinction in the minimization braces is due to the fact that the transferred value must come up to d in total but to guarantee nonnegativity it must never exceed the original values of $z^*_{S_i}$ and $z^*_{S_j}$. By construction we have $\sum_{i \in I} z^*_{S_i} = c_{f_r} - c_{f_p}$, which is greater than or equal to d due to (4.12), and also $\sum_{j \in J} z^*_{S_j} = c_{f_r} - c_{f_p} = d$. This guarantees that in sum the value d is reached.

This construction does not change the feasibility of the dual solution concerning constraints (d1): in each case where a value of $-\sum_{\{S_1S_2\} \in \mathcal{S}} z^*_{S_1S_2}$ is added to the left-hand side of the inequality, the corresponding values $z^*_{S_k}$ are decreased in total by the same value such that the total value of left-hand side does not change. Note that the complementary slackness is not violated by positive values for the respective variables $z^*_{S_iS_j}$ as the subsets S_i and S_j are chosen such that the corresponding primal inequalities are satisfied with equality. For constraints (d2) and (d3) the construction is not changed such that we have

$$-\sum_{\substack{S \subseteq V,\\ \mathring{e}_i \in E(G[S])}} z^*_S + z^*_i - z^*_{12} = c_{f_r} + c_{\mathring{e}_i} - c_{f_r} - 0 = c_{\mathring{e}_i}$$

for $i \in \{1, 2\}$. Finally this construction yields validity in (d4) by

$$-\sum_{\{S_1S_2\} \in \mathcal{S}} z^*_{S_1S_2} - z^*_1 - z^*_2 + z^*_{12} = (c_{f_q} - c_{f_r}) - (c_{\mathring{e}_1} - c_{f_r}) - (c_{\mathring{e}_2} - c_{f_r}) + 0 \leq q_{\mathring{e}_1\mathring{e}_2}$$

due to (4.20).

Now assume that only two of the vertex pairs $\mathring{u}, \mathring{v}$ and $\mathring{w}, \mathring{z}$ are connected in F^*, say $\mathring{u}$ and $\mathring{v}$ but not $\mathring{w}$ and $\mathring{z}$. Let r be the smallest index with $\mathring{u}, \mathring{v} \in S_r$. This leads to the optimality criterion

$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1 \mathring{e}_2} \geq c_{f_r}$$

and a dual solution is given by the extension

$$z_1^* := c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := c_{\mathring{e}_2}, \qquad z_{S_1 S_2}^* := 0 \;\; \forall \{S_1, S_2\} \in \mathcal{S}.$$

Note that again $z_2^* \geq 0$ by (4.12). Furthermore, the variables $z_{S_i S_j}^*$ can remain zero since (d4) is satisfied due to (4.20):

$$-\sum_{\{S_1 S_2\} \in \mathcal{S}} z_{S_1 S_2}^* - z_1^* - z_2^* + z_{12}^* = 0 - (c_{\mathring{e}_1} - c_{f_r}) - c_{\mathring{e}_2} + 0 \leq q_{\mathring{e}_1 \mathring{e}_2}.$$

Finally, let neither $\mathring{u}$ and $\mathring{v}$ nor $\mathring{w}$ and $\mathring{z}$ be connected in F^*. Then we have

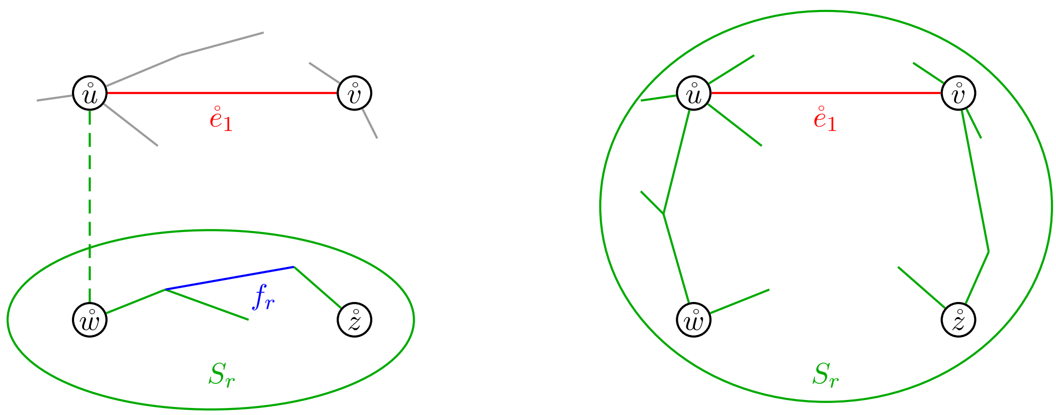
$$c_{\mathring{e}_1} + c_{\mathring{e}_2} + q_{\mathring{e}_1 \mathring{e}_2} \geq 0$$

and extend z^* by

$$z_1^* := c_{\mathring{e}_1}, \qquad z_2^* := c_{\mathring{e}_2}, \qquad z_{S_1 S_2}^* := 0 \;\; \forall \{S_1, S_2\} \in \mathcal{S}.$$

$x_{\mathring{e}_1}^* = 1, x_{\mathring{e}_2}^* = 0, y^* = 0$ (the case $x_{\mathring{e}_1}^* = 0, x_{\mathring{e}_2}^* = 1, y^* = 0$ is analogous).

Firstly, consider the case where $\mathring{w}$ and $\mathring{z}$ are connected in F^*. Let r be the minimal index with $\mathring{w}, \mathring{z} \in S_r$. Either we have $f_r \neq \mathring{e}_1$ (*case I*) or $f_r = \mathring{e}_1$ (*case II*), see Figure 4.11.



(a) case I: the vertices $\mathring{w}$ and $\mathring{z}$ are connected by edge f_r. (b) case II: $\mathring{e}_1$ connects the pairs $\mathring{u}, \mathring{w}$ and $\mathring{v}, \mathring{z}$.

Figure 4.11: Distinction of the cases I and II with $x_{\mathring{e}_1} = 1$ and $x_{\mathring{e}_2} = 0$. In case I it is also possible that one of the vertices $\mathring{u}$ or $\mathring{v}$ is in the subset S_r, as indicated by the green dashed edge. In case II both pairs $\mathring{u}, \mathring{v}$ and $\mathring{w}, \mathring{z}$ (or $\mathring{u}, \mathring{z}$ and $\mathring{v}, \mathring{w}$) are connected before the red edge $\mathring{e}_1$ connects the four of them.

case I: We have optimality criterion (4.13), in particular $c_{\mathring{e}_2} + q_{\mathring{e}_1 \mathring{e}_2} \geq c_{f_r}$, since otherwise the replacement of f_r by $\mathring{e}_2$ yields a better solution. A feasible dual solution is obtained by setting

$$z_1^* := 0, \qquad z_2^* := -q_{\mathring{e}_1 \mathring{e}_2}, \qquad z_{S_1 S_2}^* := 0 \;\; \forall \{S_1, S_2\} \in \mathcal{S}.$$

Constraints (d1) and (d3) are satisfied as in the linear case. Constraint (d2) is satisfied since a positive value is subtracted from the left-hand side and thus, the value still is not greater than $c_{\mathring{e}_2}$. Constraint (d4) follows directly since all values on the left-hand side equal zero except $z_2^* = -q_{\mathring{e}_1 \mathring{e}_2}$, such that we obtain equality in (d4).

case II: By setting $f_r = \mathring{e}_1$ the construction given in case II directly above can be easily adapted to this case.

Now let $\mathring{w}$ and $\mathring{z}$ be disconnected in F^*. Optimality criterion (4.18) holds, i. e. $c_{\mathring{e}_2} + q_{\mathring{e}_1\mathring{e}_2} \geq 0$, and we set

$$z_1^* := 0, \qquad z_2^* := c_{\mathring{e}_2}, \qquad z_{S_1S_2}^* := 0 \;\; \forall \{S_1, S_2\} \in \mathcal{S}.$$

Note that $z_2^* > 0$ since (4.18) leads to $c_{\mathring{e}_2} \geq -q_{\mathring{e}_1\mathring{e}_2} > 0$ by initial assumption. Constraints (d1) and (d3) are valid as in the linear case and (d2) and (d4) are satisfied with equality by construction.

$x_{\mathring{e}_1}^* = x_{\mathring{e}_2}^* = y^* = 1$.

Let again F' be the optimal *linear* spanning forest subject to c with $F^* \backslash F' \subseteq \{\mathring{e}_1, \mathring{e}_2\}$. Define the sets S_k and the basic dual solution z^* with respect to F'. Initially, assume that $\mathring{u}$ and $\mathring{v}$ are connected in F' and so are $\mathring{w}$ and $\mathring{z}$. Let r, t be the minimal indices with $\mathring{u}, \mathring{v} \in S_r$ and $\mathring{w}, \mathring{z} \in S_t$. Note that we neither exclude $f_r = \mathring{e}_1$ or $f_t = \mathring{e}_2$ nor $r = t$. We extend the basic dual solution by

$$z_1^* := -\frac{1}{2} q_{\mathring{e}_1\mathring{e}_2} + c_{\mathring{e}_1} - c_{f_r}, \qquad z_2^* := -\frac{1}{2} q_{\mathring{e}_1\mathring{e}_2} + c_{\mathring{e}_2} - c_{f_t}, \qquad z_{S_1S_2}^* := 0 \;\; \forall \{S_1, S_2\} \in \mathcal{S}.$$

and increase the original values of $z_{\{\mathring{u},\mathring{v}\}}^*$ and $z_{\{\mathring{w},\mathring{z}\}}^*$ by $-\frac{1}{2} q_{\mathring{e}_1\mathring{e}_2}$. Note that this is possible concerning the complementary slackness since the primal constraints corresponding to the subsets $\{\mathring{u}, \mathring{v}\}$ and $\{\mathring{w}, \mathring{z}\}$ are satisfied with equality. Furthermore, all dual variables are nonnegative due to $q_{\mathring{e}_1\mathring{e}_2} < 0$ and the optimality criterion (4.12) with respect to F'. Constraint (d1) is satisfied as in the linear case. The left-hand side of constraint (d2) reads $c_{f_r} - (-\frac{1}{2} q_{\mathring{e}_1\mathring{e}_2}) + (-\frac{1}{2} q_{\mathring{e}_1\mathring{e}_2} + c_{\mathring{e}_1} - c_{f_r}) = c_{\mathring{e}_1}$ and (d3) is satisfied by the same arguments. The left-hand side of (d4) sums to $q_{\mathring{e}_1\mathring{e}_2} - (c_{\mathring{e}_1} - c_{f_r}) - (c_{\mathring{e}_2} - c_{f_t})$ which is not greater than $q_{\mathring{e}_1\mathring{e}_2}$ due to (4.12) with respect to F'.

If there exist no index r or no index t, i. e. $\mathring{u}$ and $\mathring{v}$ or $\mathring{w}$ and $\mathring{z}$ are disconnected in F', set $c_{f_r} = 0$ or $c_{f_t} = 0$ in the settings above. With optimality criterion (4.11) with respect to F', validity of (d4) follows.

Note that in all cases the complementary slackness conditions are satisfied. If one of the variables x_1^*, x_2^* or x_{12}^* is set to a value greater than zero, the corresponding primal condition, i. e. the linearization constraint, is satisfied with equality. In all other cases, e. g. if variables z_S^* or $z_{S_iS_j}^*$ are changed, the corresponding subsets are chosen such that the primal constraints are satisfied with equality. □

To conclude this section, we remark that these results cannot easily be generalized to the case of matroid polytopes, as one might be tempted to believe, considering that the forests in G form the independent sets of the graphic matroid of G. One example is the uniform matroid, for which one can show that the convex hull of the linearized problem with one quadratic term has an exponential number of facets, while the corresponding polytope in the linear case has a compact polyhedral description. Nevertheless it is possible to obtain a more complex complete polyhedral description of the one-product case than just adding y to the left-hand side of facets of the linear case. This is shown in the very recent work of Fischer et al. [68], where matroids with one single monomial, here of arbitrary degree, are investigated. A complete description of the corresponding polytope and a complete characterization of the facets are presented which consist of linearization constraints and extended rank inequalities. These extensions are more complex than the extension of the subtour elimination constraints presented in this chapter.

4.3 Spanning trees with one quadratic term

In a similar vein to the QMSF problem we now consider the polyhedral properties of the QMST problem with one single product term. We analogously define the polytopes corresponding to QMST^c and QMST^d, i. e., the spanning tree polytopes with one linearized connected, respectively disconnected monomial:

$$P_T^c := \text{conv}\left\{(x,y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (4.2), (4.5) \text{ and } y = x_{\mathring{u}\mathring{v}} x_{\mathring{v}\mathring{w}}\right\}$$
$$P_T^d := \text{conv}\left\{(x,y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (4.2), (4.5) \text{ and } y = x_{\mathring{u}\mathring{v}} x_{\mathring{w}\mathring{z}}\right\}$$

By definition, we have $P_T^c \subseteq P_F^c$ and $P_T^d \subseteq P_F^d$.

It is well-known that a complete polyhedral description of the spanning tree problem in the linear case is given by nonnegativity and the constraints (4.2) and (4.5), i. e., by adding the cardinality constraint (4.5) to the complete description of the spanning forest polytope. In fact, we will show that even our polyhedral results obtained for the spanning forest problem with one quadratic term can be carried over to the spanning tree problem with one quadratic term.

First of all, we can derive the dimension of the polytopes in the spanning tree case from Theorem 4.2.1, since all incidence vectors constructed in the corresponding proof remain feasible, except for the first one.

Corollary 4.3.1.
$$\dim(P_T^c) = \dim(P_T^d) = |E|.$$

Furthermore, the quadratic subtour elimination constraints remain facet defining in both cases.

Corollary 4.3.2.

a) Let $S_1 \subset V$ be a set of vertices with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v} \in V \backslash S_1$. Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + y \leq |S_1| - 1$$

is valid and induces a facet of P_T^c.

b) Let $S_1, S_2 \subset V$ be disjoint subsets of vertices such that both edges $\{\mathring{u}, \mathring{v}\}$ and $\{\mathring{w}, \mathring{z}\}$ have exactly one end vertex in S_1 and one end vertex in S_2. Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e + y \leq |S_1| + |S_2| - 2$$

is valid and induces a facet of P_T^d.

Proof. Validity of (4.9) follows by $P_T^c \subset P_F^c$ and $P_T^d \subset P_F^d$, i. e., each valid inequality for the quadratic spanning forest polytope remains valid for the quadratic spanning tree polytope. For the facet-inducing property, consider the incidence vectors of Theorem 4.2.2 in case a) and of Theorem 4.2.3 in case b). All these vectors except the first one of each case also satisfy the cardinality constraint (4.5). Without these first vectors we result in $|E|$ feasible and affinely independent vectors in each case. □

In the spanning forest case, the main result of Section 4.2 states that the quadratic subtour elimination constraints yield a complete description of the spanning forest polytope with one quadratic term, when added to the well-known polyhedral description of the linear case and the standard linearization constraints. The same statement remains true for spanning trees, which is a direct consequence of the following observation.

Lemma 4.3.3.

a) P_T^c *is a face of* P_F^c.

b) P_T^d *is a face of* P_F^d.

Proof. By the subtour elimination constraints (4.2), one direction of the cardinality constraint (4.5) is valid for both polytopes P_F^c and P_F^d, so that (4.5) induces a face in both polytopes. In particular, the intersection of both P_F^c and P_F^d with (4.5) is an integer polytope and hence by definition agrees with P_T^c and P_T^d, respectively. □

Using Lemma 4.3.3, we derive the following results from Proposition 4.2.2 and Theorems 4.2.4 and 4.2.5, respectively.

Corollary 4.3.4.
Let $q_{\mathring{e}_1\mathring{e}_2} \geq 0$. *Then the linear program*

$$\begin{aligned}
\min \quad & \sum_{e\in E} c_e x_e + q_{\mathring{e}_1\mathring{e}_2} y \\
\text{s.t.} \quad & \sum_{e\in E} x_e = |V| - 1 \\
& \sum_{e\in E(G[S])} x_e \leq |S| - 1 \qquad \forall \emptyset \neq S \subset V \\
& y \leq x_{\mathring{e}_1}, x_{\mathring{e}_2} \\
& y \geq x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1 \\
& x, y \geq 0
\end{aligned}$$

has an integer optimal solution.

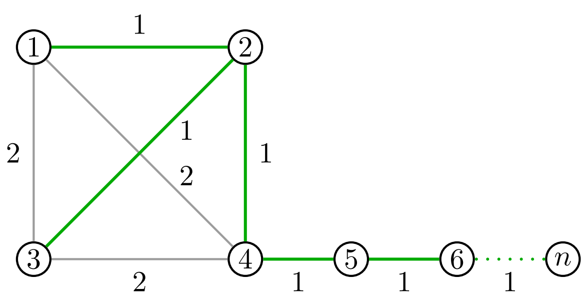
Corollary 4.3.5.

a) $$P_T^c = \left\{ (x,y) \in [0,1]^{|E|+1} \;\middle|\; (x,y) \text{ satisfies } (4.2), (4.3), (4.4), (4.5), \text{ and } (4.9) \right\}$$

b) $$P_T^d = \left\{ (x,y) \in [0,1]^{|E|+1} \;\middle|\; (x,y) \text{ satisfies } (4.2), (4.3), (4.4), (4.5), \text{ and } (4.10) \right\}$$

One might wonder whether the result of Corollary 4.3.4 also holds in the case of more than one quadratic term. The following example shows that for the spanning tree case this is not true in general even in the case of a fixed number of quadratic terms, even if the corresponding optimization problem is still tractable in this case.

Example 4.3.6.
Consider the graph $K_n = (V, E)$. *The costs of single edges are indicated in the illustration on the right; the omitted edges are assigned a cost value large enough to ensure that they never appear in any optimal solution. Quadratic costs* q_{ef} *are only given for the products of edges in the subgraph induced by* $T := \{1, 2, 3, 4\}$*; they are set to 2.*



The optimal integral solution of

$$\begin{aligned}
\min \quad & \sum_{e\in E} c_e x_e + \sum_{\{e,f\}\in E(G[T])} q_{ef} y_{ef} \\
\text{s. t.} \quad & \sum_{e\in E} x_e = |V| - 1 \\
& \sum_{e\in E(G[S])} x_e \le |S| - 1 && \text{for } \emptyset \neq S \subset V \\
& y_{ef} \le x_{e_1}, x_{e_2} \\
& y_{ef} \ge x_{e_1} + x_{e_2} - 1 \\
& x, y \ge 0
\end{aligned}$$

is the vector (x^*, y^*) *with* x^* *being the incidence vector of the spanning tree given by the green colored edge set* $\{\{1,2\},\{2,3\},\{2,4\},\{4,5\},\{5,6\},\dots,\{n-1,n\}\}$ *and* y^* *being the corresponding linearization vector, with an objective value of* $n+5$. *However,* (x^*, y^*) *is not optimal for the LP relaxation stated above, as there exists a feasible solution with lower objective value* $n + \frac{7}{3}$, *given as follows:*

- $x_{\{1,2\}} = x_{\{1,3\}} = x_{\{1,4\}} = \frac{1}{3}$,
- $x_{\{2,3\}} = x_{\{2,4\}} = x_{\{3,4\}} = \frac{2}{3}$,
- $x_{\{4,5\}} = x_{\{5,6\}} = \ldots = x_{\{n-1,n\}} = 1$,
- $y_{\{2,3\}\{2,4\}} = y_{\{2,3\}\{3,4\}} = y_{\{2,4\}\{3,4\}} = \frac{1}{3}$,
- $x_e = 0$ *and* $y_{ef} = 0$ *otherwise.*

4.4 Separation routines

All three classes of subtour elimination constraints (4.2), (4.9) and (4.10) are of exponential size, so that these inequalities cannot be separated by enumeration. Therefore, to use these inequalities within a cutting plane approach, a polynomial time separation routine is required. For the linear subtour elimination constraints (4.2), the separation algorithm is described in 2.2.3. For the separation of constraints (4.9) and (4.10) we propose highly analogous algorithms.

Connected case:

As in the separation of the linear subtour elimination constraints (4.2), the values

$$d_i = 2 - \sum_{e\in\delta(i)} x_e^*$$

and the network are defined and, with appropriate fixings, a maximal s-t-flow is calculated. There are only two differences to consider. The first one is the additional y-term, i. e., a vector $(x^*, y^*) \in [0,1]^{|E|+1}$ violates an inequality of type (4.9) if there exists a set S_1 with

$$\sum_{e\in E(G[S_1])} x_e^* - |S_1| > -1 - y^*. \tag{4.22}$$

Second, only those subsets S_1 including the vertices $\mathring{u}$ and $\mathring{w}$ but excluding vertex v are feasible. Therefore, we set infinite capacities on the edges $\{\mathring{u}, t\}, \{\mathring{w}, t\}$ and $\{s, \mathring{v}\}$, see Figure 4.12. As a result, only a single maximal s-t-flow has to be computed, since the cut cannot be empty in this context. Afterwards, it has to be checked whether the subset S_1 on the t-side of the corresponding cut satisfies inequality (4.22).

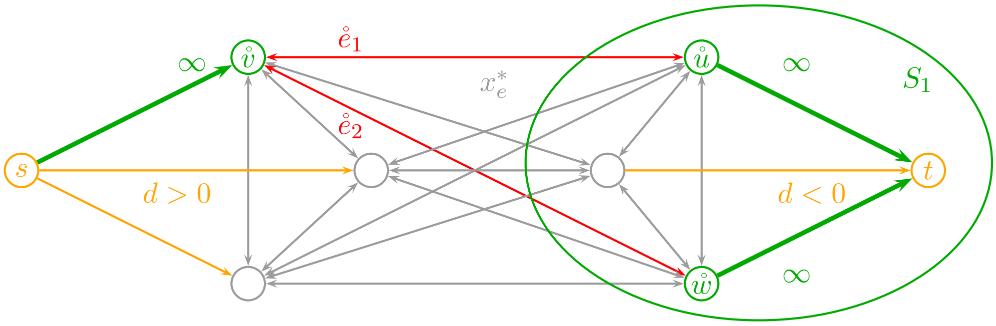


Figure 4.12: The vertices $\mathring{u}$ and $\mathring{w}$ are fixed to t and vertex $\mathring{v}$ is fixed to s. If inequality (4.22) is violated, (x^*, y^*) is valid for the quadratic subtour elimination constraint (4.9).

Disconnected case:

The separation of the quadratic subtour elimination constraints for the disconnected case, i. e. Constraints (4.10), is slightly more complicated. We can rewrite (4.10) as

$$\sum_{e \in E(G[S_1])} x_e^* - |S_1| + \sum_{e \in E(G[S_2])} x_e^* - |S_2| \leq -2 - y^*.$$

This in turn is equivalent to

$$4 + 2y^* + 2\kappa \leq \sum_{e \in \delta_{E'}^{in}(S_1 \cup \{t\})} c_e + \sum_{e \in \delta_{E'}^{in}(S_2 \cup \{t\})} c_e.$$

The requirement that $\mathring{e}_1$ and $\mathring{e}_2$ have to connect S_1 and S_2 leads to four cases out of which we describe the case $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v}, \mathring{z} \in S_2$; the other cases can be handled analogously. As in the former separation routines, we define d_i and the network with capacities, set infinite costs on the edges $\{\mathring{u}, t\}, \{\mathring{w}, t\}, \{s, \mathring{v}\}$ and $\{s, \mathring{z}\}$ and calculate the minimal cut set S_1 containing t, see Figure 4.13.

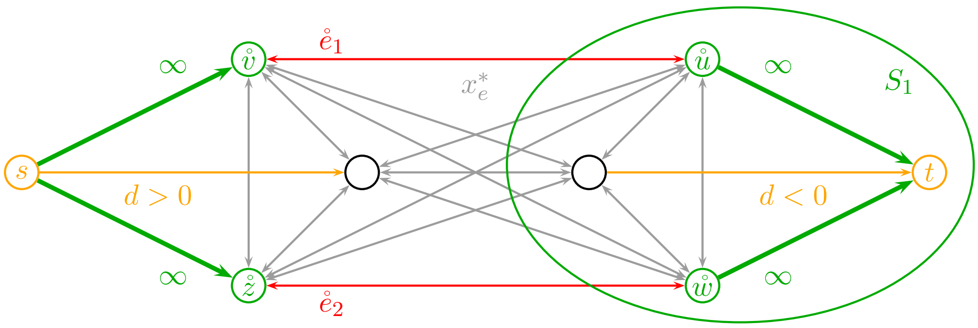


Figure 4.13: The vertices $\mathring{u}$ and $\mathring{w}$ are fixed to t and the vertices $\mathring{v}$ and $\mathring{z}$ are fixed to s such that $\mathring{e}_1$ and $\mathring{e}_2$ are in the cut $\delta(S_1)$.

In a second step, we go for the same but invert the linkings to s and t and calculate the minimal cut set S_2 containing t. The combination of S_1 and S_2 is used to check inequality (4.10) for violation. Although this approach does not necessarily lead to disjoint sets S_1 and S_2, the separation routine is correct, as the inequality remains valid for non-disjoint sets S_1 and S_2.

In all cases, the proposed separation algorithms can be implemented to run in polynomial time, as at most eight maximum s-t-flows have to be calculated.

4.5 Summary

The intention of this chapter is the investigation of the polytopes corresponding to the quadratic minimimum spanning forest problem with one quadratic term and its relative, the quadratic minimum spanning tree problem with one quadratic term. In general, two cases concerning the correlation of the edges which correspond to the quadratic term have to be considered. On the one hand this is the connected case if the two monomial edges share a common edge, on the other hand the disconnected case if the monomial edges are disjoint.

For both of the polytopes which result from a linearization of the quadratic term we could classify new facet defining inequalities, the quadratic subtour elimination constraints, which in both cases are highly related to their linear counterparts. In the connected case, an additional y-term strengthens the respective linear subtour elimination constraint, in the disconnected case the y-term strengthens the sum of two of them.

The main result in this chapter is the derivation of a complete description of the two polytopes. We could show that one single quadratic term does not change the polyhedral structures significantly. In addition to the constraints needed for the linear spanning forest polytope and the linear spanning tree polytope respectively, the linearization constraints and the quadratic subtour elimination constraints indeed suffice to obtain a complete polyhedral descriptions.

Furthermore, based on the separation algorithm of the linear subtour elimination constraints we could derive two polynomial time separation routines for the two new quadratic constraints. Even though the existence of such polynomial time separation algorithms is clear by reasons of complexity, these concrete algorithms are useful for an application in practice, which is shown by the computational results presented in Chapter 8.

Chapter 5

Quadratic Branchings and Arborescences

The directed relatives of QMSF and QMST are the **quadratic branching** (QBra) and the **quadratic arborescence** (QArb) problem. They combine the linear versions of the branching and the arborescence problem with additional quadratic costs q_{ef} for pairs of different edges in the objective function.

The combination of a branching or an arborescence problem and a quadratic cost function is fairly new such that there exists very few literature. The first problem formulation of quadratic arborescences is presented by Galbiati in [75]. Here the quadratic cost function is based only on adjacent edges, such as in the AQMST problem, and is given by an edge coloring, i. e., if two adjacent edges in the arborescence are of colors a and b, the costs they contribute to the objective function are given by q_{ab}. The so-called **changeover costs** of an arborescence A at a vertex v, different from the root node, is then given by the sum of q_{ab} for all edges $b \in E(A)$ which leave v, where a is the unique edge entering v. This problem definition is motivated by a real network problem, where devices to support the changes of carrier need to be installed in each node, and it is proven to be NP-complete [75]. To the best of our knowledge there is no literature about the general QArb or QBra problems with arbitrary quadratic terms.

The quadratic branching and the quadratic arborescence problem can be formulated as integer programs with the same constraints as in the linear case but with an objective function containing quadratic terms. We again consider only edge pairs with nonzero quadratic costs and denote the corresponding index set with $\mathcal{Q}$. After linearization we obtain

$$
\begin{aligned}
(\mathrm{LQP}_{\mathrm{QBra}}) \qquad \min \ & \sum_{e \in E} c_e x_e + \sum_{\{e,f\} \in \mathcal{Q}} q_{ef} y_{ef} & & \\
\text{s. t.} \ & \sum_{e \in E(G[S])} x_e \le |S| - 1 & \forall\, \emptyset \neq S \subseteq V & \qquad (5.1)\\
& \sum_{e \in \delta^{in}(v)} x_e \le 1 & \forall\, v \in V & \qquad (5.2)\\
& y_{ef} \le x_e, x_f & \forall\, \{e,f\} \in \mathcal{Q} & \qquad (5.3)\\
& y_{ef} \ge x_e + x_f - 1 & \forall\, \{e,f\} \in \mathcal{Q} & \qquad (5.4)\\
& x \in \{0,1\}^{|E|} & & \\
& y \in \{0,1\}^{|\mathcal{Q}|} & &
\end{aligned}
$$

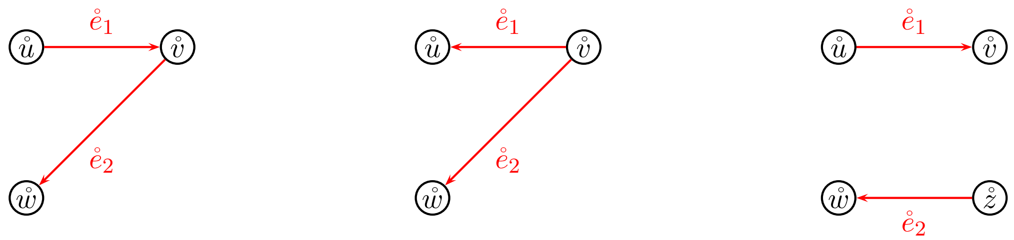
for the quadratic branching problem. Analogously, the quadratic arborescence problem can be set up by replacing (5.1) for $S = V$ by the cardinality constraint

$$\sum_{e \in E} x_e = |V| - 1. \tag{5.5}$$

5.1 Branchings and arborescences with one quadratic term

In the undirected case of spanning forests with one quadratic term it is sufficient to distinguish the two cases of a connected and of a disconnected monomial. Considering directed graphs also the direction of the arcs have to be considered such that it is necessary to distinguish between three cases in the following.

We again denote the edges forming the quadratic term with $\mathring{e}_1$ and $\mathring{e}_2$ and consider the connected case first. Either the arrow head of one arc points into the arrow tail of the other, such that we have the **head-tail** (ht) case with $\mathring{e}_1 = (\mathring{u}, \mathring{v})$ and $\mathring{e}_2 = (\mathring{v}, \mathring{w})$, or the two arrow tails meet in the shared vertex, which results in the **tail-tail** (tt) case with $\mathring{e}_1 = (\mathring{v}, \mathring{u})$ and $\mathring{e}_2 = (\mathring{v}, \mathring{w})$. The case where the monomial edges do not share any vertex we again call **disconnected** (d) case with $\mathring{e}_1 = (\mathring{u}, \mathring{v})$ and $\mathring{e}_2 = (\mathring{z}, \mathring{w})$. The three cases are visualized in Figure 5.1.



(a) ht: $\mathring{e}_1 = (\mathring{u}, \mathring{v}), \mathring{e}_2 = (\mathring{v}, \mathring{w})$ (b) tt: $\mathring{e}_1 = (\mathring{v}, \mathring{u}), \mathring{e}_2 = (\mathring{v}, \mathring{w})$ (c) d: $\mathring{e}_1 = (\mathring{u}, \mathring{v}), \mathring{e}_2 = (\mathring{z}, \mathring{w})$

Figure 5.1: Illustration of the three cases of monomial edges.

Analogously to the undirected case we investigate the three polytopes corresponding to minimal branching problems with one quadratic term

$$P^{ht}_{Bra} := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (5.1), (5.2) \text{ and } y = x_{(\mathring{u},\mathring{v})} x_{(\mathring{v},\mathring{w})}\right\},$$
$$P^{tt}_{Bra} := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (5.1), (5.2) \text{ and } y = x_{(\mathring{u},\mathring{v})} x_{(\mathring{u},\mathring{w})}\right\},$$
$$P^{d}_{Bra} := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (5.1), (5.2) \text{ and } y = x_{(\mathring{u},\mathring{v})} x_{(\mathring{z},\mathring{w})}\right\},$$

and the three polytopes corresponding to minimal arborescence problems with one quadratic term

$$P^{ht}_{Arb} := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (5.5), (5.1), (5.2) \text{ and } y = x_{(\mathring{u},\mathring{v})} x_{(\mathring{v},\mathring{w})}\right\},$$
$$P^{tt}_{Arb} := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (5.5), (5.1), (5.2) \text{ and } y = x_{(\mathring{u},\mathring{v})} x_{(\mathring{u},\mathring{w})}\right\},$$
$$P^{d}_{Arb} := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (5.5), (5.1), (5.2) \text{ and } y = x_{(\mathring{u},\mathring{v})} x_{(\mathring{z},\mathring{w})}\right\}.$$

By definition, $P^{ht}_{Arb} \subseteq P^{ht}_{Bra}$, $P^{tt}_{Arb} \subseteq P^{tt}_{Bra}$ and $P^{d}_{Arb} \subseteq P^{d}_{Bra}$.

In the following we show that several results concerning P^c_F and P^d_F, in particular the facet defining properties of the quadratic subtour elimination constraints (4.9) and (4.10), can be transferred to the branching polytopes P^{ht}_{Bra}, P^{tt}_{Bra} and P^{d}_{Bra}. On the other hand we also show that constraints (4.9) and (4.10) do not suffice to yield a complete description of the corresponding polytopes, since more inequalities containing the product variable are needed.

We assume $|V| \geq 4$. The following theorems can be proven analogously to Theorems 4.2.1, 4.2.2 and 4.2.3, under the restriction of the additional degree constraint (2.7). For this it is necessary to ensure that each time an arborescence is combined with an ingoing edge $e = (v_i, v_j)$, the root node of the arborescence equals v_j. The existence of such arborescences is guaranteed by Lemma 2.3.2.

The first elementary theorem provides the dimensions of the three branching and the three arborescence polytopes, which indeed rise in each case by one compared to the linear problems due to the additional linearization variable.

Theorem 5.1.1.

$$\dim(P^{ht}_{Bra}) = \dim(P^{tt}_{Bra}) = \dim(P^{d}_{Bra}) = \dim(P_{Bra}) + 1 = |E| + 1.$$

and

$$\dim(P^{ht}_{Arb}) = \dim(P^{tt}_{Arb}) = \dim(P^{d}_{Arb}) = \dim(P_{Arb}) + 1 = |E|.$$

Proof. The proof runs analogously to the proof of Theorem 4.2.1, except that the degree constraint has to be satisfied for each branching and each arborescence. Let $\bar{z} \in V \backslash \{\mathring{u}, \mathring{v}, \mathring{w}\}$ in the head-tail and the tail-tail case and $\bar{z} = \mathring{z}$ in the disconnected case.

First, we consider the branching polytopes. For this, let S_1, S_2 partition V into two subsets with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v}, \bar{z} \in S_2$, such that $\mathring{e}_1, \mathring{e}_2 \in \delta(S_1)$. Define the edges $\bar{h}_1 := (\mathring{u}, \mathring{w})$, $\bar{h}_2 := (\bar{z}, \mathring{v})$, and $\bar{g}_1 := (\bar{z}, \mathring{u})$, $\bar{g}_2 := (\mathring{u}, \bar{z})$. As in the proof of Theorem 4.2.1 we choose $r_1 = |E(G[S_1])$ arborescences $A_1^1, \dots, A_1^{r_1}$ on the subgraphs induced by $G[S_1]$ and $r_2 = |E(G[S_2])$ arborescences $A_2^1, \dots, A_2^{r_2}$ on the subgraphs induced by $G[S_2]$, such that their incidence vectors are pairwise affinely independent. We assume without loss of generality that $\mathring{u}$ is root node of A_1^1 and that $\bar{h}_1 \in A_1^1$, further that $\bar{z}$ is root node of A_2^1 and that $\bar{h}_2 \in A_2^1$. For a visualization see Figure 5.2.

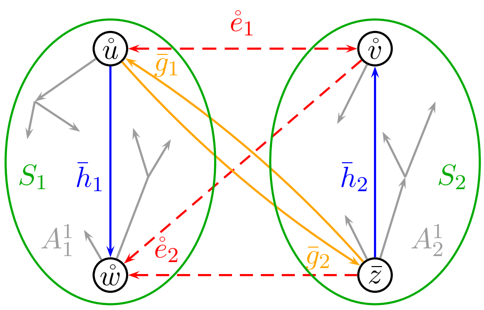


Figure 5.2: Illustration of the subsets S_1 and S_2 and the fixings in the different cases. The dashed lines represent the different monomial edges, i. e. $\mathring{e}_1 = (\mathring{u}, \mathring{v}), \mathring{e}_2 = (\mathring{v}, \mathring{w})$ in the head-tail case, $\mathring{e}_1 = (\mathring{v}, \mathring{u}), \mathring{e}_2 = (\mathring{v}, \mathring{w})$ in the tail-tail case and $\mathring{e}_1 = (\mathring{u}, \mathring{v}), \mathring{e}_2 = (\bar{z}, \mathring{w})$ in the disconnected case.

We list $|E|+2$ branchings whose incidence vectors with appropriate y-value are pairwise affinely independent.

1. $B = A_1^1 \cup A_2^1$
2. $B = A_1^1 \cup A_2^1 \cup \{\bar{g}_1\}$

3. $B = A_1^1 \cup A_2^1 \cup \{\bar{g}_2\}$
4. $B = A_1^i \cup A_2^1 \cup \{\bar{g}_2\}$ for all $i = 2, \ldots, r_1$
5. $B = A_1^1 \cup A_2^i \cup \{\bar{g}_1\}$ for all $i = 2, \ldots, r_2$
6. $B = A_1^i \cup A_2^1 \cup \{e\}$ for all edges $e \in \delta^{in}(S_1)\backslash\{\bar{g}_1\}$
   where for each edge $e = (a, b)$ the arborescence A_1^i is chosen with root node b
7. $B = A_1^1 \cup A_2^i \cup \{e\}$ for all edges $e \in \delta^{out}(S_1)\backslash\{\bar{g}_2\}$
   where for each edge $e = (a, b)$ the arborescence A_2^i is chosen with root node b
8. $B = A_1^1 \cup (A_2^1\backslash\{\bar{h}_2\}) \cup \{\bar{g}_1, (\mathring{w}, \mathring{v})\}$
9. $B = (A_1^1\backslash\{\bar{h}_1\}) \cup A_2^1 \cup \{\bar{g}_2, (\mathring{v}, \mathring{w})\}$
10. $B = (A_1^1\backslash\{\bar{h}_1\}) \cup A_2^i \cup \{\mathring{e}_1, \mathring{e}_2\}$
   where the arborescence A_2^i is chosen with root node $\mathring{v}$

We obtain a total number of

$$3 + (r_1 - 1) + (r_2 - 1) + 2(|S_1||S_2| - 1) + 3 = |E| + 2$$

affinely independent vectors in P_B^{ht} and P_B^d, respectively such that $\dim(P_F^c), \dim(P_F^d) \geq |E| + 1$ By the number of variables we have $\dim(P_F^c), \dim(P_F^d) \leq |E| + 1$, and thus equality in both cases. Note that the choice of the arborescences with a certain root node is always possible due to Lemma 2.3.2.

Since the branchings defined in 2 to 10 are arborescences, they directly lead to a dimension of $|E|$ for the arborescence polytopes. □

Regarding the facets of the polytopes it turns out that the different variants of the quadratic subtour elimination constraints also appear in the case of branchings and arborescences.

Theorem 5.1.2.
Let $S_1 \subset V$ be a set of vertices with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v} \in V\backslash S_1$. Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + y \leq |S_1| - 1 \tag{5.6}$$

is valid and induces a facet of P_{Bra}^{ht} and of P_{Bra}^{tt}, and also of P_{Arb}^{ht} and of P_{Arb}^{tt}.

Proof. Validity follows analogously to the undirected case. The facet defining property for the branching polytopes is shown by listing $|E|+1$ pairwise affinely independent incidence vectors of branchings which satisfy (5.6) with equality. Let S_1 be an arbitrary subset of V with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v} \notin S_1$ and let $S_2 := V\backslash S_1$. We distinguish between the case where $|S_2|$ consists of at least two vertices and the case where $S_2 = \{\mathring{v}\}$.

$|S_2| \geq 2$: In this case all definitions and notations of the proof of Theorem 5.1.1 can be reused. Since the vectors corresponding to the branchings defined in 1 to 8 and 10 satisfy the inequality (5.6) with equation, the inequality is facet inducing for P_{Bra}^{ht} and for P_{Bra}^{tt}. The facet property for P_{Arb}^{ht} and for P_{Arb}^{tt} follows directly by excluding the branching defined in 1.

$|S_2| = 1$: Since we assume $|V| \geq 4$ there exists another vertex $\bar{t} \in S_1\backslash\{\mathring{u}, \mathring{w}\}$ such that we can define $\bar{g} := (t, \mathring{v})$. Furthermore, we define the arborescences $A_1^1, \ldots, A_1^{r_1}$ and the edge $\bar{h}_1$ as before, see Figure 5.3.

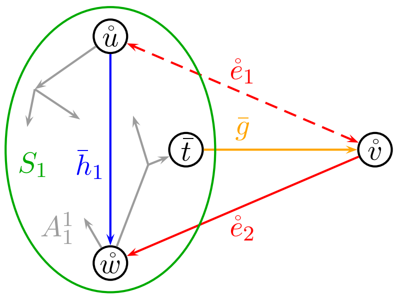


Figure 5.3: The subset S_1, the vertex t and the fixed edges $\bar{h}_1$ and $\bar{g}$. The dashed edge represents the different monomial edges $\mathring{e}_1$ in the head-tail case, where $\mathring{e}_1 = (\mathring{u}, \mathring{v})$, and in the tail-tail case, where $\mathring{e}_1 = (\mathring{u}, \mathring{v})$.

Then, the $|E| + 1$ incidence vectors of the branchings

1. $B = A_1^1$
2. $B = A_1^1 \cup \{\bar{g}\}$
3. $B = A_1^i \cup \{\bar{g}\}$ for all $i = 2, \ldots, r_1$
4. $B = A_1^i \cup \{e\}$ for all edges $e \in \delta(S_1) \backslash \{\bar{g}\}$
   where for each edge $e = (a, b)$ the arborescence A_1^i is chosen with root node b
5. $B = (A_1^1 \backslash \{\bar{h}_1\}) \cup \{\mathring{e}_1, \mathring{e}_2\}$
   where the arborescence A_2^i is chosen with root node $\mathring{v}$,

combined with appropriate y-value, are pairwise affinely independent and they all satisfy $\sum_{e \in E(G[S_1])} x_e + y = |S_1| - 1$, which proves that (5.6) is a facet of P_{Bra}^{ht} and P_{Bra}^{tt}.

For the arborescence polytopes P_{Arb}^{ht} and P_{Arb}^{tt} consider the same incident vectors as before, except the first one in each of the cases, yielding $|E|$ pairwise affinely independent incidence vectors of arborescences which satisfy (5.6) with equality. □

Theorem 5.1.3.
Let $S_1, S_2 \subset V$ be disjoint subsets of vertices with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v}, \mathring{z} \in S_2$. Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e + y \le |S_1| + |S_2| - 2 \tag{5.7}$$

is valid and induces a facet of P_{Bra}^d and of P_{Arb}^d.

Proof. Validity is given as in the undirected case. For the facet inducing property let S_1, S_2 be disjoint subsets with $\mathring{u}, \mathring{w} \in S_1$ and $\mathring{v}, \mathring{z} \in S_2$. As in the proof of Theorem 4.2.3 we introduce a third subset $S_3 := V \backslash (S_1 \cup S_2)$ and distinguish by the number of vertices in S_3.

$|S_3| = 0$: We reuse all definitions given in the proof of Theorem 5.1.1 and with the vectors given in 1 to 7 and 10 plus the incidence vector of the additional branching

11. $B = A_1^i \cup A_2^1 \backslash \{\bar{h}_2\} \cup \{\mathring{e}_1, \mathring{e}_2\}$
    where the arborescence A_1^i is chosen with root node $\mathring{w}$

we obtain $|E| + 1$ affinely independent vectors with appropriate y-variable, which satisfy (5.7) with equation, yielding its facet property for P_{Bra}^d. Excluding the branching defined in 1, the proof holds for the arborescence polytope P_{Arb}^d.

$|S_3| \geq 2$: Let $\bar{a}, \bar{b} \in S_3$ and $A_3^1, \ldots, A_3^{r_3}$ be arborescences in S_3 with pairwise affinely independent incidence vectors. Denote the edges $\bar{h}_1, \bar{h}_2$ and $\bar{g}_1, \bar{g}_2$ as in the proof of Theorem 5.1.1, furthermore denote $\bar{g}_3 := (\bar{a}, \mathring{u}), \bar{g}_4 := (\mathring{v}, \bar{b})$ and $\bar{h}_3 := (\bar{b}, \bar{a})$. Also define the arborescences A_1^i and A_2^i as in the proof of Theorem 5.1.1 and let without loss of generality $\bar{h}_1 \in A_1^1, \bar{h}_2 \in A_2^1$ and $\bar{h}_3 \in A_3^1$, and $\mathring{u}, \mathring{z}$ and $\bar{b}$ be the root nodes of A_1^1, A_2^1 and A_3^1 respectively, see Figure 5.4.

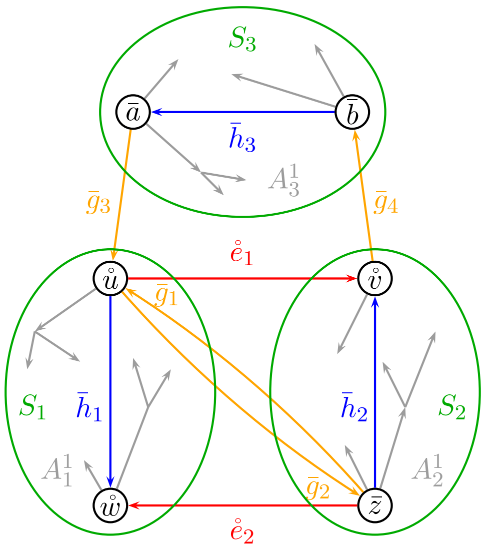


Figure 5.4: Illustration of the subsets, vertices and edges.

We again construct $|E|+1$ branchings with pairwise affinely independent incidence vectors and appropriate y-value such that they all satisfy inequality (4.10) with equality.

1. $B = A_1^1 \cup A_2^1$
2. $B = A_1^1 \cup A_2^1 \cup A_3^1 \cup \{\bar{g}_1, \bar{g}_4\}$
3. $B = A_1^1 \cup A_2^1 \cup A_3^1 \cup \{\bar{g}_2, \bar{g}_4\}$
4. $B = A_1^1 \cup A_2^1 \cup A_3^1 \cup \{\bar{g}_3, \bar{g}_4\}$
5. $B = A_1^i \cup A_2^1 \cup A_3^1 \cup \{\bar{g}_2, \bar{g}_4\}$ for $i = 2, \ldots, r_1$
6. $B = A_1^1 \cup A_2^i \cup A_3^1 \cup \{\bar{g}_1, \bar{g}_4\}$ for $i = 2, \ldots, r_2$
7. $B = A_1^1 \cup A_2^1 \cup A_3^i \cup \{\bar{g}_2, \bar{g}_3\}$ for $i = 2, \ldots, r_3$
8. $B = A_1^i \cup A_2^1 \cup A_3^1 \cup \{\bar{g}_4, e\}$ for all edges $e = (a, b), e \in \delta^{in}(S_1) \backslash \{\bar{g}_1, \bar{g}_3\}$
   where the arborescence A_1^i is chosen with root node b
9. $B = A_1^1 \cup A_2^i \cup A_3^1 \cup \{\bar{g}_3, e\}$ for all edges $e = (a, b), e \in \delta^{in}(S_2) \backslash \{\bar{g}_2\}$
   where the arborescence A_2^i is chosen with root node b
10. $B = A_1^1 \cup A_2^1 \cup A_3^i \cup \{\bar{g}_1, e\}$ for all edges $e = (a, b), e \in \delta^{in}(S_1) \backslash \{\bar{g}_4\}$
    where the arborescence A_3^i is chosen with root node b
11. $B = A_1^1 \cup A_2^1 \cup (A_3^1 \backslash \{\bar{h}_3\}) \cup \{\bar{g}_2, \bar{g}_3, \bar{g}_4\}$
12. $B = A_1^i \cup (A_2^1 \backslash \{\bar{h}_2\}) \cup A_3^1 \cup \{\mathring{e}_1, \mathring{e}_2, (\bar{b}, \bar{z})\}$
    where the arborescence A_1^i is chosen with root node $\mathring{w}$
13. $B = (A_1^1 \backslash \{\bar{h}_1\}) \cup A_2^1 \cup A_3^1 \cup \{\mathring{e}_1, \mathring{e}_2, (\bar{a}, \mathring{u})\}$
    where the arborescence A_2^i is chosen with root node $\mathring{v}$

Summing up, we obtain $|E| + 1$ (or $|E|$) affinely independent vectors of branchings (arborescences) being tight in (4.10).

$|S_3| = 1$: Let $S_3 = \{\bar{a}\}$. We define the arborescences A_1^i and A_2^i and the edges $\bar{h}_1, \bar{h}_2$ and $\bar{g}_1, \bar{g}_2$ as before. Since there is no arborescence in S_3, we define $A_3^1 = \emptyset$ with $r_3 = 0$, and the edges $\bar{g}_3 := (\bar{a}, \mathring{u})$ and $\bar{g}_4 = (\mathring{v}, \bar{a})$, see Figure 5.5.

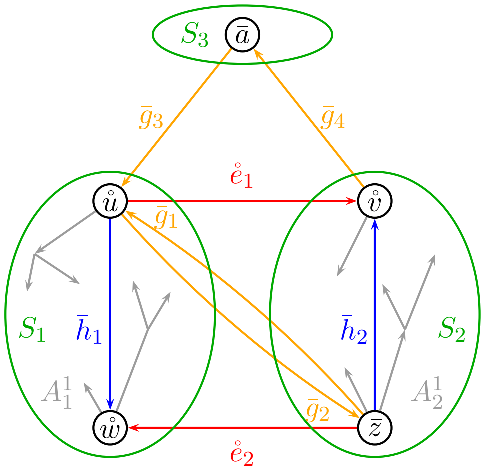


Figure 5.5: In this case the subset S_3 consists of only one vertex $\bar{a}$.

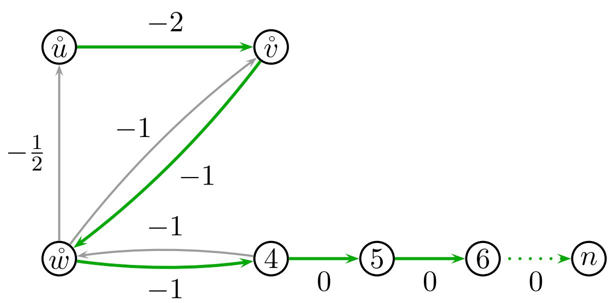
The $|E| + 1$ incidence vectors of the branchings defined in 1 to 6, 8, 9, 12 and 13 in the former case all satisfy (5.7) with equality. As a matter of fact the same holds for the $|E|$ arborescences defined in 2 to 6, 8, 9, 12 and 13. Thus the quadratic subtour elimination constraints (5.7) are facet-inducing for P^d_{Bra} and P^d_{Arb}. □

A separation algorithm for these directed quadratic subtour elimination constraints can be constructed completely analogously to the separation of the undirected versions, only d_i is defined by the ingoing cuts $d_i := 2 - \sum_{e \in \delta^{in}(i)} x_e^*$ for $i \in V$.

As the directed and the undirected case are quite similar, a natural conjecture is that also in the branching and arborescence case the optimal solution of a problem with $c_y \geq 0$ can be found by only considering the linear branching or arborescence constraints combined with the constraints of the standard linearization (5.3) and (5.4). However, the following example shows for the head-tail case that this is not true as there exists a fractional solution satisfying all these constraints having a better value than the integral optimum.

Example 5.1.1.

Consider the graph $K_n = (V, E)$. The costs of single edges are indicated in the illustration on the right; the omitted edges have positive cost such that they never appear in any optimal solution. The quadratic costs are $q_{\mathring{e}_1 \mathring{e}_2} = 1 > 0$ for the edges $\mathring{e}_1 = (\mathring{u}, \mathring{v})$ and $\mathring{e}_2 = (\mathring{v}, \mathring{w})$.



One optimal integral solution of

$$\begin{aligned}
\min \quad & \sum_{e \in E} c_e x_e + q_{\mathring{e}_1\mathring{e}_2} y_{\mathring{e}_1\mathring{e}_2} \\
\text{s.t.} \quad & \sum_{e \in E(G[S])} x_e \leq |S| - 1 && \forall\, \emptyset \neq S \subset V \\
& \sum_{e \in \delta^{in}(v)} x_e \leq 1 && \forall\, v \in V \\
& y_{\mathring{e}_1\mathring{e}_2} \leq x_{\mathring{e}_1}, x_{\mathring{e}_2} \\
& y_{\mathring{e}_1\mathring{e}_2} \geq x_{\mathring{e}_1} + x_{\mathring{e}_2} - 1 \\
& x_e, y_{\mathring{e}_1\mathring{e}_2} \geq 0 && \forall\, e \in E,
\end{aligned}$$

combined with $\sum_{e \in E} x_e = |V| - 1$ in the arborescence case, is given by the highlighted set with an objective value of -3. However, there exists a better fractional solution with a value of $-\frac{17}{5}$ given as follows:

- $x_{(\mathring{u},\mathring{v})} = \frac{4}{5}$, $x_{(\mathring{v},\mathring{w})} = \frac{1}{5}$, $y = 0$,
- $x_{(\mathring{w},\mathring{v})} = x_{(\mathring{w},4)} = \frac{1}{5}$,
- $x_{(\mathring{w},\mathring{u})} = x_{(4,\mathring{w})} = \frac{4}{5}$,
- $x_{(i,i+1)} = 1$ *for all* $i \in \{4, \ldots, n-1\}$,
- $x_e = 0$ *otherwise.*

Examples for the tail-tail and the disconnected cases can be constructed in the same way. Note that the fractional solution of the example is valid for the quadratic subtour elimination constraint (5.6) (and for (5.7) in the respective disconnected case). Therefore we have to assert that the directed problems in the quadratic case have a more complicated structure and that the Theorems 4.2.4 and 4.2.5 cannot be transferred analogously to the quadratic branching or arborescences problems.

However, this motivates further research on facet defining inequalities for a better description of the polytopes. An additional facet class for each of the monomial cases is presented in the following theorem. It is a very small class since it depends on only six edges connecting four vertices, which are the monomial vertices and, in the connected cases, a fourth vertex $\bar{z}$. The edges which contribute a value to the inequalities are the ingoing edges of the two tail-vertices, i. e. the vertices to which the monomial edges do not point to. Thus we call the inequalities **tail-in constraints** in the following.

Theorem 5.1.4.

Let $\bar{z} \in V \backslash \{\mathring{u}, \mathring{v}, \mathring{w}\}$ in the head-tail and the tail-tail case and let $\bar{z} = \mathring{z}$ in the disconnected case. Then the inequality

$$x_{(\mathring{v},\mathring{u})} + x_{(\mathring{w},\mathring{u})} + x_{(\bar{z},\mathring{u})} + x_{(\mathring{u},\bar{z})} + x_{(\mathring{v},\bar{z})} + x_{(\mathring{w},\bar{z})} + y \leq 2 \tag{5.8}$$

is valid and induces a facet of $P^{ht}_{Bra}, P^{d}_{Bra}$ and $P^{ht}_{Arb}, P^{d}_{Arb}$, and the inequality

$$x_{(\mathring{u},\mathring{v})} + x_{(\mathring{w},\mathring{v})} + x_{(\bar{z},\mathring{v})} + x_{(\mathring{u},\bar{z})} + x_{(\mathring{v},\bar{z})} + x_{(\mathring{w},\bar{z})} + y \leq 2 \tag{5.9}$$

is valid and induces a facet of P^{tt}_{Bra} and P^{tt}_{Arb}.

Proof. To prove validity of the tail-in constraint (5.8) let $S = \{\mathring{u}, \mathring{v}, \mathring{w}, \bar{z}\}$. The left hand side of (5.8) is equivalent to

$$\sum_{\substack{e \in \delta^{in}(\mathring{u}) \\ e \in E(G[S])}} x_e + \sum_{\substack{e \in \delta^{in}(\bar{z}) \\ e \in E(G[S])}} x_e + y.$$

By the degree constraints (5.2) for the vertices $\mathring{u}$ and $\bar{z}$ both sums are not greater than one and in combination not greater than 2. If $y = 0$, we are done. If $y = 1$, consider the subtour elimination constraint (5.1) for S, which is $\sum_{e \in E(G[S])} x_e \leq 3$. Since $x_{\mathring{e}_1} = x_{\mathring{e}_2} = 1$ due to $y = 1$, at most one other edge in S can be chosen such that

$$\sum_{\substack{e \in \delta^{in}(\mathring{u}) \\ e \in E(G[S])}} x_e + \sum_{\substack{e \in \delta^{in}(\bar{z}) \\ e \in E(G[S])}} x_e \leq 1.$$

The same arguments hold for the tail-in constraint (5.9). Figure 5.6 visualizes the two facet classes, where the corresponding tail-vertices are colored in blue.

(a) head-tail case with $y = x_{\mathring{u}\mathring{v}} x_{\mathring{v}\mathring{w}}$ and disconnected case with $y = x_{\mathring{u}\mathring{v}} x_{\mathring{z}\mathring{w}}$.

(b) tail-tail case with $y = x_{\mathring{v}\mathring{u}} x_{\mathring{v}\mathring{w}}$

Figure 5.6: The subgraph corresponding to (5.8) is visualized on the left-hand side, where the monomial edge $\mathring{e}_2$ is dotted since it either points from $\mathring{v}$ to $\mathring{w}$ in the head-tail case or from $\mathring{z}$ to $\mathring{w}$ in the disconnected case. The subgraph corresponding to (5.9) is given on the right-hand side. If $y = 1$, the gray monomial edges belong to the branching, and thus at most one of the green ones.

The facet inducing property again follows by a construction of $|E| + 1$ affinely independent incidence vectors of branchings and of $|E|$ affinely independent incidence vectors of arborescences, respectively, which all satisfy the constraints (5.8) and (5.9), respectively, with equality. □

Note that the tail-in constraints are not contained in the set of the quadratic subtour elimination constraints (5.6) and (5.6). Since they are facet defining, their additional consideration indeed improves the polyhedral description of the corresponding polytopes. Note further that the number of tail-in constraints is linear in the number of vertices of the underlying graph in the connected cases and actually is made of exactly one inequality in the disconnected case. Thus, their validity can be tested in the direct way such that no extra separation routine is needed.

Inserting the constructed fractional solution of Example 5.1.1 one can easily see that this solution satisfies the tail-in constraint of the head-tail case. Thus we have to assert that even these additional inequalities do not yield a complete polyhedral description of P^{ht}_{Bra} and P^{ht}_{Arb}. In fact, further studies show that in all connected and disconnected cases there exist various other facets, some of which are even described by inequalities with variable coefficients greater than one. Thus, further intensive studies of the facets are necessary to possibly develop a complete polyhedral description.

5.2 Summary

Branchings and arborescences are strongly related to spanning forests and spanning trees since they only differ in the directedness of the edges. This suggests a similar polyhedral structure, too, which in the linear case is given to a large extent, as the polyhedra only differ by the additional degree constraints. When considering the polytopes of the problems with one quadratic term we have to assert that the similarity is conserved only partially. The quadratic subtour elimination constraints can be carried over to the directed cases, however the polyhedral description becomes much more complicated as the polytopes are not completely described by the constraints of the linear cases, the linearization and the quadratic subtour elimination constraints. The main difficulty seems to lie in the additional degree constraints such that inequalities as the tail-in constraints become necessary. Nevertheless, by reasons of complexity, an optimization of the problems is possible, such that it seems promising that further studies on this topic yield complete descriptions of the different branching and arborescence polytopes.

Chapter 6

Quadratic Assignments

In this chapter we investigate the **quadratic assignment problem** (QAP) which requires an assignment minimizing an objective function containing linear and quadratic terms c_e and q_{ef} for (pairs of) edges in the underlying graph. The QAP is NP-hard [156] and still one of the hardest optimization problems as even instances with $n > 30$ exceed reasonable computational times.

The problem was introduced by Koopmans and Beckmann in 1957 [116] as a model for a facility location problem. Here n facilities need to be allocated to n locations, and a combination of distances and flow between two facilities and the construction costs for each facility have to be minimized. Each facility has to be assigned to exactly one location and vice versa, which leads to a quadratic assignment problem. Further applications for the QAP come from registration problems, where two objects of nearly similar shape have to be matched automatically [115], computer backboard design, where the wiring of the backboard is optimized [25,162], and others; for a survey see [45].

The QAP is well studied and there exist various works on complexity, polyhedral and algorithmic studies. In the following we present a selection of results concerning this problem which is not supposed to be exhaustive but only shall give an overview about research related to the scope of this thesis. We refer to literature considering advanced studies at the appropriate location, but already refer to a comprehensive book about theory and algorithms of the QAP by Çela [40] and a very recent QAP survey by Burkard et al. [34]. In 1991 Burkard et al. installed a library **QAPLIB** for test instances for QAP [35, 36]. The state-of-the-art concerning exact solutions, lower bounds and other current information, is collected on the web page [94].

6.1 Properties and algorithms

6.1.1 Formulations

The original problem formulation introduced by Koopmans and Beckmann [116] is based on three input matrices $F, D, C \in \mathbb{R}^{n\times n}$, where elements f_{ij} of F model the flow between facility i and facility j, the elements d_{kl} of D represent the distances between locations k and l, and where the elements c_{ik} of C model the costs for placing facility i at location k. With $N := \{1, \dots, n\}$ let $\mathcal{S}_n$ be the set of all permutations $\sigma : N \to N$. The **Koopmans-Beckmann formulation** of QAP reads

$$\min_{\sigma\in\mathcal{S}_n} \sum_{i,j\in N} f_{ij} d_{\sigma(i)\sigma(j)} + \sum_{i\in N} c_{i\sigma(i)}. \tag{6.1}$$

To generalize the formulation, Lawler [121] replaced the flow and the distance matrices F and D and introduced a four-dimensional cost matrix Q with coefficients q_{ijkl} instead and reformulated the problem as

$$\min_{\sigma \in \mathcal{S}_n} \sum_{i,j \in N} q_{i\sigma(i)j\sigma(j)} + \sum_{i \in N} c_{i\sigma(i)}, \tag{6.2}$$

where setting $q_{ijkl} := f_{ik}d_{jl}$ for all i, j, k, l with $i \neq k$ or $j \neq l$ and $q_{ijij} := f_{ii}d_{jj} + c_{ij}$ yields the original Koopmans-Beckmann formulation. Furthermore he reformulated the permutation constraint by the use of a **permutation matrix** X with elements

$$x_{ij} = \begin{cases} 1 & \text{if } \sigma(i) = j \\ 0 & \text{otherwise.} \end{cases}$$

With the constraints

$$\sum_{i \in N} x_{ij} = 1 \qquad \forall\, j \in N \qquad \text{and} \qquad \sum_{j \in N} x_{ij} = 1 \qquad \forall\, i \in N \tag{6.3}$$

for binary variables x_{ij}, the matrix X characterizes a permutation on the numbers $1, \ldots, n$ and, due to Birkhoff's Theorem 2.4.4 and analogously to the ILP formulation of the linear assignment problem AP in Section 2.4, this yields an equivalent IP formulation with quadratic objective function.

$$\begin{array}{llll} \text{(QAP)} & \min & \displaystyle\sum_{i,j,k,l \in N} q_{ijkl} x_{ij} x_{kl} + \sum_{i,j \in N} c_{ij} x_{ij}. & \\ & \text{s. t.} & \displaystyle\sum_{i \in N} x_{ij} = 1 & \forall\, j \in N \\ & & \displaystyle\sum_{j \in N} x_{ij} = 1 & \forall\, i \in N \\ & & x_{ij} \in \{0, 1\} & \forall\, i, j \in N \end{array}$$

Replacing the product terms $x_{ij}x_{kl}$ by new variables y_{ijkl} and adding the constraint $y_{ijkl} = x_{ij}x_{kl}$ then leads to an equivalent program with linear objective function, and the convex hull of all feasible points is called the **quadratic assignment polytope**, or briefly **QAP polytope**

$$P_A^{ql} := \operatorname{conv} \left\{ (x, y) \in \{0, 1\}^{n^2 + n^2(n^2-1)/2} \;\middle|\; x \text{ satisfies (6.3) and } y_{ijkl} = x_{ij}x_{kl} \;\; \forall\, i, j, k, l \in N \right\}.$$

There exist various other formulations for the QAP, such as a concave quadratic formulation introduced by Bazaraa and Sherali [16], a trace formulation given by Edwards [62, 63], a formulation based on the Kronecker product [121] or the very recent discrete linear reformulations of Nyberg and Westerlund, which allowed to solve some instances of the QAPLIB to optimality that have been unsolved before [136, 137].

6.1.2 Linearizations

Analogous to the previous chapters 4 and 5, the here considered linearization for the QAP is the standard linearization, which we apply to (QAP). As usual, denote with $\mathcal{Q}$ the set of index tuples (i, j, k, l) with nonzero costs $q_{ijkl} \neq 0$, and replace each product term $x_{ij}x_{kl}$ with $\{i, j, k, l\} \in \mathcal{Q}$ by a new variable $y_{ijkl} \geq 0$ and add the connecting constraints (4.3) and (4.4).

The equivalent ILP formulation then reads

$$
\begin{aligned}
(\mathrm{LQP_{QAP}}) \qquad & \min \sum_{i,j\in N} c_{ij}x_{ij} + \sum_{(i,j,k,l)\in\mathcal{Q}} q_{ijkl}y_{ijkl} & & \\
& \text{s.t.} \quad \sum_{i\in N} x_{ij} = 1 & \forall\, j \in N \qquad & (6.4)\\
& \qquad \sum_{j\in N} x_{ij} = 1 & \forall\, i \in N \qquad & (6.5)\\
& \qquad y_{ijkl} \le x_{ij}, x_{kl} & \forall\,(i,j,k,l) \in \mathcal{Q} \qquad & (6.6)\\
& \qquad y_{ijkl} \ge x_{ij} + x_{kl} - 1 & \forall\,(i,j,k,l) \in \mathcal{Q} \qquad & (6.7)\\
& \qquad x \in \{0,1\}^{n^2} & & \\
& \qquad y \in \{0,1\}^{|\mathcal{Q}|}. & &
\end{aligned}
$$

Besides the standard linearization and the alternatives discussed in Section 3.1 there exist several different custom-built approaches to get rid of the quadratic terms in the objective function.

Lawler modeled the quadratic dependency $y_{ijkl} = x_{ij}x_{kl}$ by $1 + n^4$ additional linear constraints

$$\sum_{i,j,k,l\in N} y_{ijkl} = n^2 \qquad \text{and} \qquad x_{ij} + x_{kl} \ge 2y_{ijkl} \qquad \forall\, i,j,k,l \in N \tag{6.8}$$

for n^4 additional binary variables y_{ijkl} [121]. The set of inequalities guarantees $y_{ijkl} = 0$ whenever one or both of the corresponding linear variables are zero. Combined with the linear degree constraints (6.4) and (6.5), which force $x_{ij} = 1$ for exactly n linear variables, this yields the fact that at most n^2 y-variables can obtain a value of one. The equality of (6.8) guarantees that this cardinality of n^2 is indeed obtained and thus $y_{ijkl} = 1$ when $x_{ij} = x_{kl} = 1$. Thus, $y_{ijkl} = x_{ij}x_{kl}$ for all $i, j, k, l \in N$.

Assuming without loss of generality nonnegative coefficients q_{ijkl}, Kaufmann and Broeckx rearranged the quadratic part of the objective function

$$\sum_{i,j,k,l\in N} q_{ijkl}x_{ij}x_{kl} = \sum_{i,j\in N} x_{ij} \sum_{k,l\in N} q_{ijkl}x_{kl}$$

and replaced the latter part of the right-hand side by a set of n^2 new real and nonnegative variables $w_{ij} := x_{ij}\sum_{k,l\in N} q_{ijkl}x_{kl}$ for all $i, j \in N$. Then, they minimize the mixed integer linear minimization problem with objective function $\sum_{i,j\in N} c_{ij}x_{ij} + \sum_{i,j\in N} w_{ij}$, the degree constraints (6.4) and (6.5) and the n^2 additional constraints

$$a_{ij}x_{ij} + \sum_{k,l\in N} q_{ijkl}x_{kl} - w_{ij} \le a_{ij} \qquad \forall\, i,j \in N$$

for constants $a_{ij} := \sum_{k,l\in N} q_{ijkl}$ [113]. The additional constraints yield

$$w_{ij} \ge \sum_{k,l\in N} (x_{ij} + x_{kl} - 1) = \begin{cases} 0 & \text{if } x_{ij} = 0 \\ \displaystyle\sum_{k,l\in N} q_{ijkl}x_{kl} & \text{if } x_{ij} = 1 \end{cases}$$

for all $i, j \in N$ and equality emanates from the fact that the objective function minimizes the nonnegative w-variables.

An extensive linearization in terms of variables and constraints is the one of Frieze and Yadegar. They consider n^4 continuous variables $y_{ijkl} \in [0,1]$ and add $4n^3 + n^2$ constraints

$$\sum_{i \in N} y_{ijkl} = x_{kl} \qquad \forall\, j,k,l \in N, \qquad \sum_{j \in N} y_{ijkl} = x_{kl} \qquad \forall\, i,k,l \in N, \tag{6.9}$$

$$\sum_{k \in N} y_{ijkl} = x_{ij} \qquad \forall\, i,j,l \in N, \qquad \sum_{l \in N} y_{ijkl} = x_{ij} \qquad \forall\, i,j,k \in N, \tag{6.10}$$

$$\text{and} \quad y_{ijij} = x_{ij} \qquad \forall\, i,j \in N, \tag{6.11}$$

obtaining a mixed integer linear programming formulation being equivalent to (QAP) [73]. The equivalence follows since the constraints model $y_{ijkl} = x_{ij}x_{kl}$ for all $i,j,k,l \in N$: if on the one hand for one linear variable $x_{ij} = 0$, the equalities (6.10) and the nonnegativity of y yield $y_{ijkl} = 0$ for all $k,l \in N$, analogously for $x_{kl} = 0$ and $y_{ijkl} = 0$ for all $i,j \in N$. On the other hand, if two linear variables $x_{ij} = x_{kl} = 1$, constraints (6.9) yield $\sum_{t \in N} y_{tjkl} = 1$. Assume that there exist two variables $y_{t_1jkl}, y_{t_2jkl} > 0$. Then, by the previous arguments, the corresponding linear variables $x_{t_1j} = 1$ and $x_{t_2j} = 1$, leading to $t_1 = t_2 = i$ due to the degree constraints (6.5), analogously for the other indices j,k,l.

The formulation of Frieze and Yadegard is larger but also stronger than the others when regarding the lower bounds obtained by Lagrangean relaxation, which leads to the bounds FY1 and FY2 which are better than all bounds obtained by the reduction techniques on the Gilmore-Lawler bound, see Section 6.1.4.

The linearization of Adams and Johnson resembles the one of Frieze and Yadegar but here the inequalities (6.10) and (6.11) are replaced by the constraints

$$y_{ijkl} = y_{klij} \qquad \forall\, i,j,k,l \in N.$$

Note that this formulation with n^4 new variables and n^4+2n^3 new constraints can be obtained by applying the Sherali-Adams linearization on the IP formulation (QAP). Furthermore, relaxing the integrality constraints in all mentioned linearizations, all constraints of the other relaxations can be expressed as linear combinations of the constraints of the relaxed Adams and Johnson linearization, and, moreover, are less tight [3, 105].

6.1.3 Complexity

As already mentioned, Sahni and Gonzales proved that QAP is NP-hard. Moreover, they showed that even the problem of finding an ϵ-approximation, i. e. a solution $\bar{x}$ with

$$\left| \frac{z(\bar{x}) - z(x^*)}{z(x^*)} \right| \leq \epsilon$$

for any fixed $\epsilon > 0$ and an optimal solution x^* with respect to a quadratic objective function z, is not polynomially solvable unless P=NP [156]. Both statements have been shown by a reduction from the NP-complete Hamiltonian cycle problem. Furthermore the quadratic assignment problem is related to the NP-hard **traveling salesman problem** (TSP). Namely, the TSP can be modeled as a QAP where a facility (position number in the tour) needs to be assigned to each location (city), regarding the distances (costs for traveling between the cities) and with zero construction costs. Other special cases of the QAP such as the linear ordering problem are surveyed in [40]. Further results on the hardness of the quadratic assignment problem concerning different types of approximations can be found in [108]. Some easy special cases of the QAP based on anti-Monge and benevolent Toeplitz matrices are analyzed by Burkard and Çela et al. [33, 41].

6.1.4 Lower bounds

To reduce the set of feasible solutions and therefore the search domain of optimal QAP solutions, such as in branch-and-bound algorithms or related methods, good lower bounds are necessary to cut off as many non-optimal solutions as possible. In the past 15 years, great effort was put into bound improvements. In fact, Loiola et al. state that there exist more than a hundred papers about the development and improvement of heuristics and bounds since 1999 [128].

A natural way of obtaining lower bounds are relaxations of (mixed) integer linear programming formulations. Especially the formulation of Frieze and Yadegar and the one of Adams and Johnson, c. f. Section 6.1.2, both result in fairly good results improving the gaps of the Gilmore-Lawler bound [3, 73].

Reformulations using other coefficients c' and q', which provide the original objective value for each feasible QAP solution, are also popular methods for the calculation of lower bounds. An iterative process, where an appropriate reformulation rule models the next reformulation by adapting the last, yields different Gilmore-Lawler bounds, out of which the best is chosen [8,38].

Another approach, called reduction method, reduces the contribution of the quadratic term by decomposing and moving quadratic costs to the linear term [46, 73]. A combination of the reduction method and the GLB yield the Hahn-Grant bound (HGB) with promising results for B&B approaches [95, 96].

Further methods are eigenvalue bound functions, which are based on the relationship between the objective function value and the eigenvalues of the flow and distance matrices F and D [67,93,155], semidefinite relaxations [109,172,173] and an approach based on a continuous convex quadratic optimization problem [6]. The current best solutions with respect to instances of the QAPLIB are based on SDP relaxations, such as matrix-splitting [147, 148] or the exploitation of group symmetry [54].

All these approaches yield lower bounds which are different in their complexity and efficiency in the branch-and-bound tree and in the gap quality. Therefore a comparison turns out to be difficult, but concerning the asymptotic behavior of the QAP, a small gap seems to be the most important factor for a succesful solution of larger QAP instances. Loiola et al. give more details on the different lower bounds and discuss their qualities [128].

6.1.5 Exact algorithms

The high complexity of the QAP is also reflected in practice. Great effort is put in speeding up existing QAP algorithms or in the development of new ones, but in fact only few instances of QAPLIB of a size greater than 30 were solved to optimality so far. The most common methods for determining an exact solution are branch-and-bound and branch-and-cut algorithms.

Besides the branching strategy, the branch-and-bound algorithm depends on good lower bounds, as mentioned in the previous section. For smaller instances the most popular and successful bound is the Gilmore-Lawler bound, which combines simplicity and low computational time. However, the corresponding gap grows very quickly with increased problem size such that the GLB becomes weak and inefficient. Due to this, other bounds begin to attract more interest, e. g. the Hahn-Grant bound or a variance reduction bound, and recently yield promising results [95, 96, 146]. Out of the different types of branching strategies the single assignment branching rule, which assigns a facility to a location in each step, appears to be the most efficient [32, 82, 121, 131]. For larger or more challenging QAP instances, parallel implementations of B&B schemes more and more establish [26, 44, 145] and recently led to the exact solution of a to date unsolved QAPLIB instance of size $n = 30$ [97].

Since there is not much knowledge about the polyhedral structure of the QAP polytope and since the time needed to generate upper and lower bounds during the procedure is very large, only very small instances can be solved to optimality. However, branch-and-cut algorithms yield promising results [108, 142] which leads to the expectation that a better polyhedral description could achieve even better results within a B&C approach.

6.1.6 The QAP polytope

Although QAP has been addressed long before, Barvinok in 1992 was the first presenting polyhedral results on the QAP polytope P_A^{ql}, which was defined by the convex hull of all vectors (x, y) which are feasible solutions of the MILP linearization by Frieze and Yadegar [15].

By considering the affine hull of the QAP polytope, which is given by the following equations

$$\sum_{i=1}^{n} x_{ij} = 1 \qquad \forall\, j \in \{1,\dots,n-1\} \tag{6.12}$$

$$\sum_{j=1}^{n} x_{ij} = 1 \qquad \forall\, i \in \{1,\dots,n\} \tag{6.13}$$

$$-x_{kl} + \sum_{i=1}^{k-1} y_{ijkl} + \sum_{i=k+1}^{n} y_{klij} = 0 \qquad \begin{array}{l}\forall\, j \neq l \in \{1,\dots,n\}, k \in \{1,\dots,n-1\} \text{ or}\\ \forall\, l \leq j \in \{1,\dots,n\}, k = n\end{array} \tag{6.14}$$

$$-x_{ij} + \sum_{l=1}^{j-1} y_{ijkl} + \sum_{l=j+1}^{n} y_{ijkl} = 0 \qquad \begin{array}{l}\forall\, j \in \{1,\dots,n\}, i \in \{1,\dots,n-3\},\\ \quad k \in \{\, i,\dots,n-1\} \text{ or}\\ \forall\, j \in \{1,\dots,n-1\}, i = n-2, k = n-1\end{array} \tag{6.15}$$

$$-x_{kj} + \sum_{l=1}^{j-1} y_{ilkj} + \sum_{l=j+1}^{n} y_{ilkj} = 0 \qquad \begin{array}{l}\forall\, j \in \{1,\dots,n-1\}, i \in \{1,\dots,n-3\},\\ \quad k \in \{\, i,\dots,n-1\},\end{array} \tag{6.16}$$

Barvinok [15], Padberg and Rijal [142] and Jünger and Kaibel [106] independently determined the dimension of P_A^{ql}, leading to the following theorem.

Theorem 6.1.1 (Barvinok, Jünger and Kaibel, Padberg and Rijal)**.**

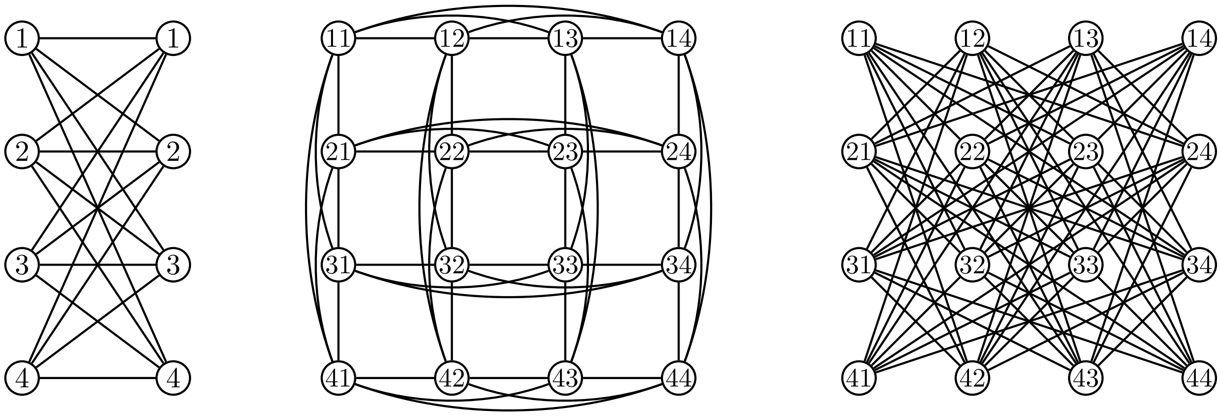
(a) *The affine hull of the QAP polytope P_A^{ql} is given by the linear equations* (6.12)–(6.16)*. These equations are pairwise linearly independent and the rank of the system is $2n(n-1)^2 - (n-1)(n-2)$, for $n \geq 3$.*

(b) *The dimension of P_A^{ql} is equal to $1 + (n-1)^2 + n(n-1)(n-2)(n-3)/2$ for $n \geq 3$.*

(c) *The inequalities $y_{ijkl} \geq 0, i < k, j \neq l$, define facets of P_A^{ql}.*

The search for other than the trivial facets in (c) however turns out to be very complicated. Jünger and Kaibel approached the QAP polytope with a formulation based on cliques [106]. For this, consider the graph $G_n = (V_n, E_n)$ with vertex set $V_n = \{(i,j) \mid i,j \in N\}$ and edge set $E_n = \{\{(i,j),(k,l)\} \mid i \neq k,\ j \neq l\}$, which can be seen as the complement of the line graph of a complete bipartite graph with n vertices on each side, see Figure 6.1 for an example with $n = 4$.

Apparently, each maximal clique in G_n contains n edges and can be reduced to a feasible assignment in the bipartite graph. Considering the linear costs c_{ij} of a QAP instance in the Lawler form as vertex weights in G_n and the quadratic costs q_{ijkl} as weights on the edges, a maximal clique with minimal total vertex and edge cost results in an optimal solution of the



(a) Bipartite graph (b) Corresponding line graph (c) Complement graph G_n

Figure 6.1: The complement graph G_n of a complete bipartite graph contains all edges except the "horizontal" and "vertical" ones.

QAP instance. Then, the QAP polytope equivalently can be formulated as the convex hull of all incidence vectors (x^C, y^C) of n-cliques C in $\mathbb{R}^n$, i. e. by

$$P_A^{ql} = \text{conv}\left\{(x^C, y^C) \;\middle|\; C \text{ is a clique with } n \text{ vertices in } G_n\right\}.$$

Using the construction of the complement graph, Padberg and Rijal presented two classes of valid inequalities for P_A^{ql}.

Lemma 6.1.2 (Padberg and Rijal)**.**
Let $G_n = (V_n, E_n)$ be the complement graph as defined above.

(a) *For any subset $S \subseteq V_n$ and any integer α the* **clique inequality**

$$\alpha \sum_{(i,j)\in S} x_{ij} \;-\; \sum_{((i,j),(k,l))\in E(G_n[S])} y_{ijkl} \le \frac{\alpha(\alpha+1)}{2}$$

is a valid inequality for P_A^{ql}.

(b) *For any subset $S \subseteq V_n$ with $|S| \ge 1$ and any subset $T \subseteq V_n \backslash S$ with $|T| \ge 2$ the* **cut inequality**

$$\sum_{(i,j)\in S} x_e \;+\; \sum_{((i,j),(k,l))\in E(G_n[S])} y_{ijkl} \;\ge\; \sum_{(i,j)\in S,(k,l)\in T} y_{ijkl} \;-\; \sum_{((i,j),(k,l))\in E(G_n[S])} y_{ijkl}$$

is a valid inequality for P_A^{ql}.

Note that these inequalities are related to the inequalities (4.6) and (4.7) which are presented for the boolean quadric forest polytope in Section 4.1.4. Validity can be shown analogously. For the cut inequalities, Padberg and Rijal presented a set of cases in which they are implied by other facets and conjecture for the other cases that they indeed are facet defining [142]. For a more comprehensive analysis of the previous inequalities, Jünger and Kaibel proposed an isomorphic transformation of the polytope, called **star transformation**, generalized and combined the previous facet classes to the class of **box inequalities** and, for the 1-box and the 2-box inequalities, they either proved the facet defining property or presented a counter-argument, e. g., a dominating facet [106, 107].

6.2 Assignments with one quadratic term

In this section we investigate the polyhedral structure of the QAP with one single quadratic term in the objective function. Again, the idea is to find classes of valid inequalities for the reduced problem since they remain valid for the general problem as a matter of fact.

By the problem definition and the equations (6.4) and (6.5) an assignment never contains two edges which share a common vertex. This directly leads to the fact that quadratic costs of two adjacent edges never contribute a value to the objective function since a product $x_e x_f$ with edges $e = \{u, v\}$ and $f = \{v, w\}$ equals zero in any feasible solution. Therefore, a natural reduced formulation of the problem omits those quadratic terms from the outset and restricts $\mathcal{Q}$, the set of edge pairs with $q_{ef} \neq 0$, to only contain non-adjacent edge pairs $e, f \in E$, $e \neq f$ with $q_{ef} \neq 0$. On account of this, we do not need to distinguish between different positions of edges as we did in the previous chapters.

In the following let $G = (V_a \dot\cup V_b, E)$ be a bipartite graph with vertex sets $V_a = \{a_1, \dots, a_n\}$ and $V_b = \{b_1, \dots, b_n\}$. For the ease of notation we abbreviate $\{a_i, b_j\}$ by writing (i, j) with the convention that vertices in V_a are named first. For edge variables we shortly write x_{ij} instead of $x_{(a_i,b_j)}$.

Pursuing the investigation of problems with one quadratic term we consider two fixed non-adjacent edges. Without loss of generality we consider the monomial edges $\mathring{e}_1 = \{\mathring{a}_1, \mathring{b}_1\} = (\mathring{1}, \mathring{1})$ and $\mathring{e}_2 = \{\mathring{a}_2, \mathring{b}_2\} = (\mathring{2}, \mathring{2})$. We investigate the assignment polytope with respect to the (disconnected) monomial $x_{\mathring{e}_1} x_{\mathring{e}_2}$, i. e.

$$P_A^d := \operatorname{conv}\left\{(x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies } (6.4), (6.5) \text{ and } y = x_{\mathring{1}\mathring{1}} x_{\mathring{2}\mathring{2}}\right\}.$$

We assume $|V_a|, |V_b| \geq 2$ in the following. Before analyzing the facets of the polytope P_A^d, we first have a look at its dimension. In fact, the linearization variable increases the dimension of the linear assignment polytope by exactly one such that we have

Theorem 6.2.1.

$$\dim(P_A^d) = \dim(P_A) + 1 = n^2 - 2n + 2.$$

Proof. Clearly, $\dim(P_A^d) \leq \dim(P_A) + 1$. To show equality we list $n^2 - 2n + 3$ affinely independent vectors $(x, y) \in P_A^d$. More precisely, we list the assignments and define x as the corresponding incidence vector and $y = x_{\mathring{1}\mathring{1}} x_{\mathring{2}\mathring{2}}$. First note that $\dim(P_A) = n^2 - 2n + 1$, thus there exist $d := (n-1)^2 - 2(n-1) + 2$ affinely independent incidence vectors of assignments A_i on the subgraph $G[V_a \backslash \{\mathring{a}_1\} \dot\cup V_b \backslash \{\mathring{b}_2\}]$.

1. $A = A_i \cup \{(\mathring{1}, \mathring{2})\}$ $\qquad \forall\, i \in \{1, \dots, d\}$
2. $A = \{(\mathring{1}, \mathring{1}), (\mathring{2}, i), (i, \mathring{2})\} \cup \{(j, j) \mid j \in \{4, \dots, n\},\ j \neq i\}$ $\qquad \forall\, i \in \{3, \dots, n\}$
3. $A = \{(\mathring{1}, 3), (\mathring{2}, \mathring{1}), (3, \mathring{2})\} \cup \{(j, j) \mid j \in \{4, \dots, n\}\}$
4. $A = \{(\mathring{1}, i), (i, \mathring{1}), (\mathring{2}, 3), (3, \mathring{2})\} \cup \{(j, j) \mid j \in \{4, \dots, n\},\ j \neq i\}$ $\qquad \forall\, i \in \{4, \dots, n\}$
5. $A = \{(\mathring{1}, 3), (3, \mathring{1}), (\mathring{2}, \mathring{2})\} \cup \{(j, j) \mid j \in \{4, \dots, n\}\}$
6. $A = \{(\mathring{1}, \mathring{1}), (\mathring{2}, \mathring{2})\} \cup \{(j, j) \mid j \in \{3, \dots, n\}\}$

We obtain $d + (n-2) + (n-3) + 3 = n^2 - 2n + 3$ vectors which by Lemma 1.4.1 are pairwise affinely independent since in each of the steps 2–6 one edge is assigned which does not belong to any of the previous assignments. □

Next we regard the facets of P_A^d. It turns out that at least two new classes of inequalities are necessary for a description of the polytope. For this, define

$$\begin{aligned}\mathcal{S} &:= \{ (S_a, S_b) \mid S_a \subseteq V_a,\ S_b \subseteq V_b,\ \mathring{a}_1, \mathring{a}_2 \notin S_a,\ \mathring{b}_1, \mathring{b}_2 \in S_b,\ |S_b| = |S_a| + 1\} \\ \mathcal{T} &:= \{ (T_a, T_b) \mid T_a \subseteq V_a,\ T_b \subseteq V_b,\ \mathring{a}_1 \in T_a, \mathring{a}_2 \notin T_a,\ \mathring{b}_1 \notin T_b, \mathring{b}_2 \in T_b,\ |T_b| = |T_a|\}.\end{aligned}$$

Theorem 6.2.2.
Let $(S_a, S_b) \in \mathcal{S}$. Then the **$\wedge$-clique inequality**

$$\sum_{\substack{a \in S_a \\ b \in S_b}} x_{ab} + y \leq |S_a| \tag{6.17}$$

is valid and induces a facet of P_A^d.

Proof. If not both of the monomial edges belong to the assignment, $y = 0$ and validity follows directly from the degree constraints (6.4) and (6.5) and the bipartiteness of the graph since

$$\sum_{\substack{a \in S_a \\ b \in S_b}} x_{ab} \leq \min \{ |S_a|, |S_b| \},$$

which equals $|S_a| < |S_b|$. If $y = 1$, the vertices $\mathring{b}_1, \mathring{b}_2 \in S_b$ are connected with $\mathring{a}_1, \mathring{a}_2 \notin S_a$ such that they cannot be connected with any vertex in S_a, which is illustrated in Figure 6.2. Therefore, we have

$$\sum_{\substack{a \in S_a \\ b \in S_b}} x_{ab} + y = \sum_{\substack{a \in S_a \\ b \in S_b \setminus \{\mathring{b}_1, \mathring{b}_2\}}} x_{ab} + 1 \leq \min \{ |S_a|, |S_b \setminus \{\mathring{b}_1, \mathring{b}_2\}| \} + 1 = \min \{ |S_a|, |S_a| - 1 \} + 1 = |S_a|.$$

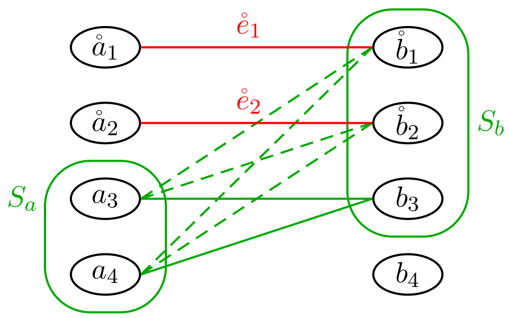


Figure 6.2: Inequality (6.17) states that at most $|S_a| - 1$ vertices in S_a can be matched with vertices in S_b if both monomial edges are in the assignment. Otherwise it can be at most $|S_a|$.

To prove the facet inducing property, we list $\dim(P_A^d)$ many affinely independent incidence vectors of assignments with corresponding product variable $y = x_{\mathring{1}\mathring{1}} x_{\mathring{2}\mathring{2}}$. For this, let $(S_a, S_b) \in \mathcal{S}$ and define $T_a := V_a \setminus S_a$ and $T_b := V_b \setminus S_b$. Denote $k := |S_a|$, and let the subsets be ordered such that $S_a = \{\alpha_1, \ldots, \alpha_k\}$ and $S_b = \{\beta_1, \ldots, \beta_{k+1}\}$ for suitable permutations α and β with $\beta_1 = \mathring{b}_1$ and $\beta_2 = \mathring{b}_2$. Denote analogously $l := |T_a| = n - k$, and let the subsets be ordered such that $T_a = \{\alpha'_1, \ldots, \alpha'_l\}$ and $T_b = \{\beta'_1, \ldots, \beta'_{l-1}\}$ for suitable permutations α' and β' with $\alpha'_1 = \mathring{a}_1$ and $\alpha'_2 = \mathring{a}_2$.

By the dimension of the linear assignment polytope there exist $r_1 := k^2 - 2k + 2$ many affinely independent incidence vectors of assignments in the subgraph $G[S_a \dot\cup (S_b \setminus \{\beta_k\})]$ and analogously $r_2 := (l-1)^2 - 2(l-1) + 2$ many affinely independent incidence vectors of assignments in the subgraph $G[(T_a \setminus \{\alpha'_l\}) \dot\cup T_b]$. Denote these assignments with $A_1^1, \ldots, A_1^{r_1}$ and $A_2^1, \ldots, A_2^{r_2}$, respectively. Without loss of generality let A_1^1 contain exactly the edges $(\alpha_1, \mathring{b}_1), (\alpha_2, \mathring{b}_2)$ and (α_i, β_i) for $i \in \{3, \dots, k\}$, and let A_2^1 contain exactly the edges $(\mathring{a}_1, \beta_1'), (\mathring{a}_2, \beta_2')$ and (α_i', β_i') for $i \in \{3, \dots, l-1\}$. Furthermore, define the edge $\bar{e} := (\alpha_l', \beta_{k+1})$. The construction is visualized in Figure 6.3.

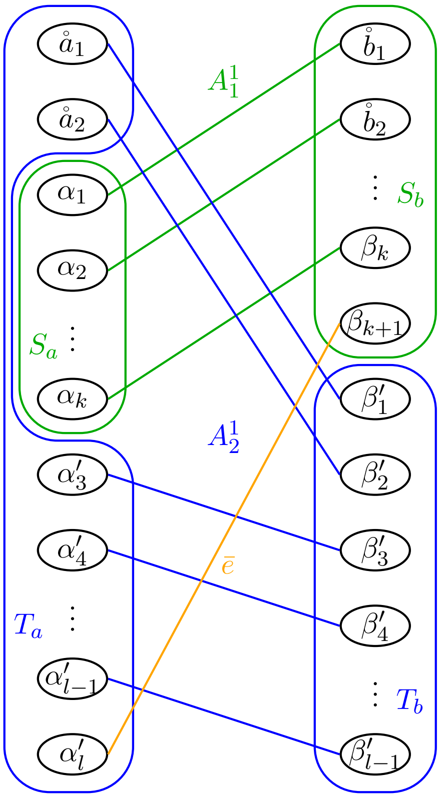


Figure 6.3: Visualization of the subsets S_a, S_b and T_a, T_b. The yellow edge $\bar{e}$ connects the partial assignments A_1^1 and A_2^1 in green and blue.

First of all we consider assignments in the subsets $S_a \cup (S_b \backslash \{\beta_k\})$ and $(T_a \backslash \{\alpha_l'\}) \cup T_b$ and combine them with the edge $\bar{e}$. Then, we vary the edge which combines the assignments in the corresponding subsets. Finally, we consider the assignments containing both monomial edges $\mathring{e}_1, \mathring{e}_2$ such that $y = 1$. All in all, we obtain the following $n^2 - 2n + 2$ assignments which yield pairwise affinely independent vectors (x, y), where x is the incidence vector of the assignment and $y = x_{\mathring{1}\mathring{1}} x_{\mathring{2}\mathring{2}}$.

1. $A = A_1^1 \cup A_2^1 \cup \{\bar{e}\}$
2. $A = A_1^i \cup A_2^1 \cup \{\bar{e}\}$ for all $i \in \{2, \dots, r_1\}$
3. $A = A_1^1 \cup A_2^i \cup \{\bar{e}\}$ for all $i \in \{2, \dots, r_2\}$
4. $A = A^j \cup A_2^1 \cup \{(\alpha_l', \mathring{b}_1)\}$ for all $j \in \{1, \dots, k\}$ with A^j assignment on $G[S_a \cup (S_b \backslash \{\mathring{b}_1\})]$ containing (α_j, β_{k+1})
5. $A = A_1^1 \cup A^j \cup \{(\mathring{a}_1, \beta_{k+1})\}$ for all $j \in \{1, \dots, l-1\}$ with A^j assignment on $G[T_a \cup (T_b \backslash \{\mathring{a}_1\})]$ containing (α_l', β_j')
6. $A = A_1^s \cup A_2^t \cup \{e\}$ for all $e = (t, s)$ with $s \in S_b, t \in T_a$, $e \notin \{\bar{e}, (\alpha_l', \mathring{b}_1), (\mathring{a}_1, \beta_{k+1})\}$ with A_1^s assignment on $G[S_a \cup (S_b \backslash \{s\})]$ and A_2^t assignment on $G[(T_a \backslash \{t\}) \cup T_b]$

7. $A = A_1^s \cup A_2^t \cup \{e, \mathring{e}_1, \mathring{e}_2\}$ for all $e = (s,t)$ with $s \in S_a, t \in T_b$
with A_1^s assignment on $G[(S_a \backslash \{s\}) \cup (S_b \backslash \{\mathring{b}_1, \mathring{b}_2\})]$
and A_2^t assignment on $G[(T_a \backslash \{\mathring{a}_1, \mathring{a}_2\}) \cup (T_b \backslash \{t\})]$

The incidence vectors of the assignments defined in 4–7 are affinely independent from all previous ones since in each case the corresponding edge $(\alpha_l', \mathring{b}_1)$, $(\mathring{a}_1, \beta_{k+1})$ and e respectively are not contained in any of the previous assignments. The incidence vector of the last assignment is affinely independent from the previous ones since it is the only one with $y = 1$. We obtain

$$1 + (r_1 - 1) + (r_2 - 1) + k + (l - 1) + (|S_b||T_a| - 3) + (|S_a||T_b|) = n^2 - 2n + 2$$

affinely independent vectors in P_A^d which all satisfy (6.17) with equality. □

Theorem 6.2.3.
Let $(T_a, T_b) \in \mathcal{T}$. *Then the* $\vee$**-clique inequality**

$$\sum_{\substack{a \in T_a \\ b \in T_b}} x_{ab} + x_{\mathring{e}_1} + x_{\mathring{e}_2} - y \leq |T_a| \tag{6.18}$$

is valid and induces a facet of P_A^d.

Proof. Let A be an assignment in G. If none of the edges $\mathring{e}_1, \mathring{e}_2$ are in A, the inequality is valid due to the degree constraints (6.4) and (6.5). If exactly one of the monomial edges, say e_1, belongs to A, the vertex $\mathring{a}_1$ is already matched to a vertex in $V \backslash T_a$ and thus the degree constraints (6.4) and (6.5) yield

$$\sum_{\substack{a \in T_a \backslash \{\mathring{a}_1\} \\ b \in T_b}} x_{ab} \leq |T_a| - 1.$$

With $x_{\mathring{1}\mathring{1}} = 1$ and $x_{\mathring{2}\mathring{2}} = 0$ inequality (6.18) follows. If both edges $\mathring{e}_1, \mathring{e}_2 \in A$, we obtain

$$\sum_{\substack{a \in T_a \backslash \{\mathring{a}_1\} \\ b \in T_b \backslash \{\mathring{b}_2\}}} x_{ab} \leq |T_a| - 1,$$

yielding (6.18) due to $x_{\mathring{1}\mathring{1}} + x_{\mathring{2}\mathring{2}} - y = 1$. A visualization of constraint (6.18) is given in Figure 6.4.

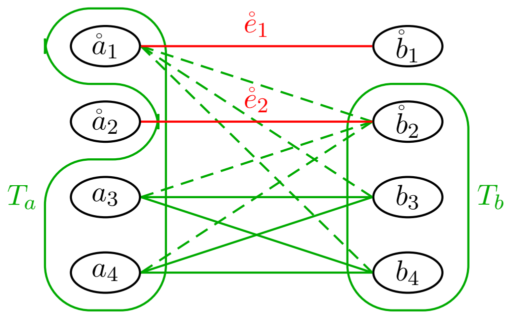


Figure 6.4: If one or both edges $\mathring{e}_1$ and $\mathring{e}_2$ belong to the assignment, not more than $|S_a| - 1$ vertices in S_a can be matched with vertices in S_b. Only if none of the monomial edges are in the assignment, at most $|S_1|$ edges are matchable between the two subsets.

We again show the facet inducing property by listing $n^2 - 2n + 2$ pairwise affinely independent vectors of assignments which all satisfy (6.18) with equality. Let $(T_a, T_b) \in \mathcal{T}$, $S_a := V_a \backslash T_a$ and $S_b := V_b \backslash T_b$. Define $k := |T_a|$, $l := |S_a| = n - k$ and r_1, r_2 as in the proof above. Again, let $A_1^1, \dots, A_1^{r_1}$ be affinely independent incidence vectors of assignments in $G[T_a \dot{\cup} T_b]$ and $A_2^1, \dots, A_2^{r_2}$ be affinely independent incidence vectors of assignments in $G[S_a \dot{\cup} S_b]$. Then, the incidence vectors with appropriate y-entry of the following assignments are affinely independent.

1. $A = A_1^i \cup A_2^1$ for all $i \in \{1, \dots, r_1\}$
2. $A = A_1^1 \cup A_2^i$ for all $i \in \{2, \dots, r_2\}$
3. $A = A^j \cup A^i \cup \{\mathring{e}_1, (\alpha'_i, \beta_j)\}$ for all $j \in \{1, \dots, k\}$ and all $i \in \{1, \dots, l\}$ with A^j assignment on $G[T_a \backslash \{\mathring{a}_1\} \cup (T_b \backslash \{\beta_j\})]$ and A^i assignment on $G[S_a \backslash \{\alpha'_i\} \cup (S_b \backslash \{\mathring{b}_1\})]$
4. $A = A^i \cup A^j \cup \{\mathring{e}_2, (\alpha_i, \beta'_j)\}$ for all $i \in \{1, \dots, k\}$ and all $j \in \{1, \dots, l\}$, $(i, j) \neq (\mathring{1}, \mathring{1})$ with A^i assignment on $G[T_a \backslash \{\alpha_i\} \cup (T_b \backslash \{\mathring{b}_2\})]$ and A^j assignment on $G[S_a \backslash \{\mathring{a}_2\} \cup (S_b \backslash \{\beta'_j\})]$

The incidence vectors of the assignments defined in 3 and 4 are affinely independent from all previous ones since the edges (α'_i, β_j) and (α_i, β'_j) respectively are not contained in any of the previous assignments. This yields a total number of

$$r_1 + (r_2 - 1) + 2kl - 1 = n^2 - 2n + 2$$

affinely independent vectors in P_A^d which all satisfy (6.18) with equality. □

Note that for the subsets $T_a = \{\mathring{a}_1\}$ and $T_b = \{\mathring{b}_2\}$ the $\vee$-clique inequality equals the second linearization constraint (6.7).

In experimental studies we generated the affine hull and all facets of the polytopes P_A^d with the software tool PORTA [42] up to instance sizes of $n = 6$. Due to the generated results we conjecture that the addition of the $\wedge$-clique and the $\vee$-clique facets to the linear degree constraints and the standard linearization indeed suffice to describe P_A^d completely.

Conjecture 6.2.4.

$$P_A^d = \left\{ (x, y) \in [0, 1]^{|E|+1} \;\middle|\; (x, y) \text{ satisfies } (6.4), (6.5), (6.6), (6.17) \text{ and } (6.18) \right\}.$$

One very interesting result of this section concerns the number of facets of the polytope P_A^d. In contrast to the spanning forest and the spanning tree problem, we can state that the number of facets rises significantly when only adding one single product term to the linear version. More precisely, the linear assignment polytope is described by its affine hull and the nonnegativity constraints $x_e \geq 0$, i.e. only polynomially many constraints are needed. On the other hand, for the polyhedral description of the assignment problem with one quadratic term not only the linearization constraints need to be added but also two new facet defining inequality classes, which are of exponential size since they depend on the subsets $S_a, S_b \subset V$ and $T_a, T_b \subset V$, respectively. Nevertheless it is clear from the complexity of the assignment problem with one quadratic term that it is possible to separate P_A^d in polynomial time. According to our conjecture we present two polynomial time separation algorithms for the exponentially sized $\wedge$-clique and $\vee$-clique inequalities.

6.3 Separation routines

The exponential size of the $\wedge$-clique and the $\vee$-clique inequalities (6.17) and (6.18) makes a separation by enumeration inefficient. Nevertheless the two facet classes are useful in a cutting plane approach, as they can be separated in polynomial time by the separation routines which we present in the following. Both can be reduced to a blossom separation problem, which was discussed in Section 2.4.3.

Separation of the $\wedge$-clique inequalities:

First we consider the separation of the $\wedge$-clique inequalities (6.17). For this, let (x^*, y^*) be a nonnegative fractional solution which satisfies the degree constraints (6.4) and (6.5) and the linearization constraints (6.6) and (6.7). Given the bipartite graph $G = (V_a \dot\cup V_b, E)$ we construct a complete weighted graph $G' = (V', E', w)$ with vertices $V' := (V_a \backslash \{\mathring{a}_1, \mathring{a}_2\}) \dot\cup V_b$. To abbreviate the notation we define $V'_a := V_a \backslash \{\mathring{a}_1, \mathring{a}_2\}$. For G' we define the weights

$$\begin{aligned} w_{ij} &:= x^*_{ij} && \text{for all } (i,j) \in E \setminus \delta(\{\mathring{a}_1, \mathring{a}_2\}), \\ w_{\mathring{b}_1 \mathring{b}_2} &:= y^* && \text{and} \\ w_{ij} &:= 0 && \text{else,} \end{aligned}$$

and visualize the construction in Figure 6.5.

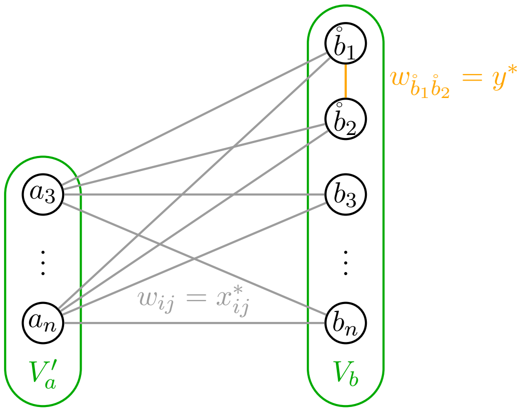


Figure 6.5: G' is constructed from G by omitting the vertices $\mathring{a}_1, \mathring{a}_2$. The weights are given by the fractional solution (x^*, y^*).

Let $\mathcal{U} := \{U \subseteq V' \mid \mathring{b}_1, \mathring{b}_2 \in U, |U \cap V'_a| = |U \cap V_b| - 1\}$. Given a subset $U \in \mathcal{U}$ define $k_U := |U \cap V'_a|$ and the two subsets $S_a := U \cap V_a$ and $S_b := U \cap V_b$. Then, $(S_a, S_b) \in \mathcal{S}$ and

$$w(U) := \sum_{\{i,j\} \in E(G'[U])} w_{ij} = \sum_{\substack{a \in S_a \\ b \in S_b}} x^*_{ab} + y^*.$$

Note that $|S_a| = k_U = \lfloor \frac{|U|}{2} \rfloor$. By this construction, the $\wedge$-clique inequality (6.17) for (S_a, S_b) is violated if $w(U) > k_U$, i. e., if the **blossom inequality**

$$\sum_{\{i,j\} \in E(G'[U])} w_{ij} \le \left\lfloor \frac{|U|}{2} \right\rfloor \tag{6.19}$$

is violated.

Conversely, let U' be an arbitrary odd subset of V' which violates the blossom inequality (6.19). We show that $U' \in \mathcal{U}$. For this, note that the degree constraints $\sum_{e\in\delta(v)} w_e \leq 1$ are satisfied for all $v \in V'$. This is obvious for all vertices $v \in V' \backslash \{\mathring{b}_1, \mathring{b}_2\}$ by definition of the weight function. For vertex $\mathring{b}_1$ we have

$$1 \;\geq \sum_{e\in\delta_G(\mathring{b}_1)} x^*_e \;=\; x^*_{\mathring{1}\mathring{1}} + x^*_{\mathring{2}\mathring{1}} + \sum_{e\in\delta_{G'}(\mathring{b}_1)} x^*_e \geq y^* + \sum_{\substack{e\in\delta_{G'}(\mathring{b}_1)\\ e\neq(\mathring{b}_1,\mathring{b}_2)}} x^*_e \;=\; \sum_{e\in\delta_{G'}(\mathring{b}_1)} w_e,$$

since $x^*_{\mathring{1}\mathring{1}} \geq y^*$, and the same holds for vertex $\mathring{b}_2$.

Let $\bar{U} \notin \mathcal{U}$ and let the weights w_{ij} be defined by the fractional solution (x^*, y^*) as discussed above. Then, by the degree constraints we have

$$w(\bar{U}) = \sum_{\substack{i\in\bar{U}\cap V'_a\\ j\in\bar{U}\cap V_b}} w_{ij} + w_{\mathring{b}_1\mathring{b}_2} \leq |\bar{U}\cap V'_a| + 1 \leq \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor$$

$$\text{if } \mathring{b}_1, \mathring{b}_2 \in \bar{U} \text{ and } |\bar{U}\cap V'_a| \leq |\bar{U}\cap V_b| - 2,$$

$$w(\bar{U}) = \sum_{\substack{i\in\bar{U}\cap V'_a\\ j\in\bar{U}\cap V_b\backslash\{\mathring{b}_1,\mathring{b}_2\}}} w_{ij} + \sum_{e\in\delta_{G'}(\{\mathring{b}_1,\mathring{b}_2\})} w_e \leq (|\bar{U}\cap V_b| - 2) + 2 \leq \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor$$

$$\text{if } \mathring{b}_1, \mathring{b}_2 \in \bar{U} \text{ and } |\bar{U}\cap V'_a| \geq |\bar{U}\cap V_b| + 1,$$

$$w(\bar{U}) = \sum_{\substack{i\in\bar{U}\cap V'_a\\ j\in\bar{U}\cap V_b}} w_{ij} \leq \min\{|S_a|, |S_b|\} \leq \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor \quad \text{if } \mathring{b}_1 \notin \bar{U} \text{ or } \mathring{b}_2 \notin \bar{U}.$$

All in all, the blossom inequality (6.19) is always satisfied for odd sets $U \notin \mathcal{U}$, or, vice versa, can only be violated by sets $U \in \mathcal{U}$. A violating set U in turn directly yields $(S_a, S_b) \in \mathcal{S}$ which violates (6.17). Thus, the separation of (6.17) is reducable to a polynomial time solvable blossom separation problem in a graph G' with weights w which are constructed from a fractional solution of the quadratic assignment problem in G.

Separation of the ∨-clique inequalities:

Now we consider the ∨-clique inequalities (6.18). Again, let (x^*, y^*) be a nonnegative fractional solution which satisfies the degree constraints (6.4) and (6.5) and the linearization constraints (6.6) and (6.7). We construct another complete weighted graph $G'' = (V'', E'', w)$ with vertices $V'' := V_a\backslash\{\mathring{a}_2\} \cup V_b\backslash\{\mathring{b}_1\} \cup \{z\}$ for a new vertex z, and we define the vertex sets $V''_a := V_a\backslash\{\mathring{a}_2\}$ and $V''_b := V_b\backslash\{\mathring{b}_1\}$. Finally we define the edge weights of G''

$$\begin{aligned} w_{ij} &:= x^*_{ij} && \text{for all } (i,j) \in E \setminus \delta(\{\mathring{a}_2, \mathring{b}_1\}),\\ w_{\mathring{a}_1 z} &:= x^*_{\mathring{e}_1} && \text{and}\\ w_{z\mathring{b}_2} &:= x^*_{\mathring{e}_2} - y^*, && \end{aligned}$$

and set $w_{ij} = 0$ in all other cases. Note that $w \geq 0$ by nonnegativity of x^* and due to the standard linearization (6.6). The construction is illustrated in Figure 6.6.

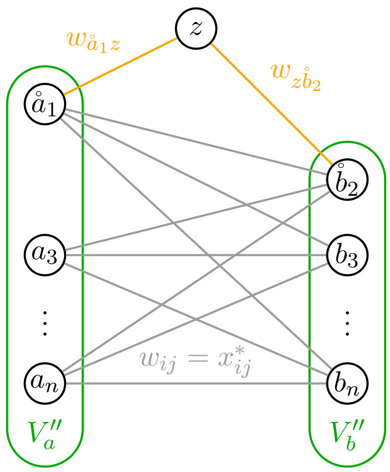


Figure 6.6: G'' is constructed from G by omitting the vertices $\mathring{a}_2, \mathring{b}_1$ and adding a new vertex z. Nonzero weights are only given on the original edges of G and the two edges $\{\mathring{a}_1, z\}$ and $\{z, \mathring{b}_2\}$.

Analogous to the construction for the separation of the $\wedge$-clique inequalities (6.17) we consider another set of subsets $\mathcal{U} := \{U \subseteq V'' \mid \mathring{a}_1, \mathring{b}_2, z \in U,\ |U \cap V'_a| = |U \cap V_b|\}$ and, for a given subset $U \in \mathcal{U}$, we define $k_U := |U \cap V'_a|$ and the two sets $T_a := U \cap V_a$ and $T_b := U \cap V_b$. Then, $(T_a, T_b) \in \mathcal{T}$ and

$$w(U) := \sum_{\{i,j\} \in E(G''[U])} w_{ij} = \sum_{\substack{a \in T_a \\ b \in T_b}} x^*_{ab} + x^*_{\mathring{e}_1} + x^*_{\mathring{e}_2} - y^*.$$

Since $|T_a| = k_U = \lfloor \frac{|U|}{2} \rfloor$, this construction leads to the fact that the $\vee$-clique inequality (6.18) is violated with respect to (T_a, T_b) if the blossom inequality

$$\sum_{\{i,j\} \in E(G''[U])} w_{ij} \le \left\lfloor \frac{|U|}{2} \right\rfloor \tag{6.20}$$

is violated for the corresponding $U \in \mathcal{U}$.

Also in G'' the degree constraints are satisfied for all vertices $v \in V''$. This is obvious for all $v \in V'' \setminus \{\mathring{a}_1, \mathring{b}_2, z\}$ since the vertex degree is not changed compared to the original graph G. For vertices $\mathring{a}_1$ and $\mathring{b}_2$ the construction leads to

$$\sum_{e \in \delta_{G''}(\mathring{a}_1)} w_e = \sum_{\substack{e \in \delta_{G''}(\mathring{a}_1) \\ e \neq \{\mathring{a}_1, z\}}} w_e + w_{\mathring{a}_1 z} = \sum_{\substack{e \in \delta_G(\mathring{a}_1) \\ e \neq \{\mathring{a}_1, \mathring{b}_1\}}} x^*_e + x^*_{\mathring{e}_1} = \sum_{e \in \delta_G(\mathring{a}_1)} x^*_e \le 1,$$

and

$$\sum_{e \in \delta_{G''}(\mathring{b}_2)} w_e = \sum_{\substack{e \in \delta_{G''}(\mathring{b}_2) \\ e \neq \{z, \mathring{b}_2\}}} w_e + w_{z\mathring{b}_2} = \sum_{\substack{e \in \delta_G(\mathring{b}_2) \\ e \neq \{\mathring{a}_2, \mathring{b}_2\}}} x^*_e + x^*_{\mathring{e}_2} - y^* = \sum_{e \in \delta_G(\mathring{b}_2)} x^*_e - y^* \le 1.$$

The degree of z equals $x^*_{\mathring{e}_1} + x^*_{\mathring{e}_2} - y^*$ which is not greater than one by the standard linearization constraint (6.7). Due to this, we can state that the blossom inequality (6.20) is never violated for any odd subset $\bar{U} \notin \mathcal{U}$:

$$w(\bar{U}) = \sum_{\substack{i \in \bar{U} \cap V'_a \\ j \in \bar{U} \cap V_b}} w_{ij} + w_{z\mathring{b}_2} = \sum_{\substack{i \in \bar{U} \cap V'_a \\ j \in \bar{U} \cap V_b \setminus \{\mathring{b}_2\}}} w_{ij} + \sum_{i \in \bar{U} \setminus \{\mathring{b}_2\}} w_{i\mathring{b}_2} \leq \left(\left\lfloor \frac{|\bar{U}|}{2} \right\rfloor - 1 \right) + 1 = \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor$$

$$\text{if } \mathring{a}_1 \notin \bar{U}, \mathring{b}_2, z \in \bar{U} \text{ and } |\bar{U} \cap V'_a| = |\bar{U} \cap V_b|,$$

$$w(\bar{U}) = \sum_{\substack{i \in \bar{U} \cap V'_a \\ j \in \bar{U} \cap V_b}} w_{ij} + w_{\mathring{a}_1 z} = \sum_{\substack{i \in \bar{U} \cap V'_a \setminus \{\mathring{a}_1\} \\ j \in \bar{U} \cap V_b}} w_{ij} + \sum_{j \in \bar{U} \setminus \{\mathring{a}_1\}} w_{\mathring{a}_1 j} \leq \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor$$

$$\text{if } \mathring{b}_2 \notin \bar{U}, \mathring{a}_1, z \in \bar{U} \text{ and } |\bar{U} \cap V'_a| = |\bar{U} \cap V_b|,$$

$$w(\bar{U}) = \sum_{\substack{i \in \bar{U} \cap V'_a \\ j \in \bar{U} \cap V_b}} w_{ij} \leq \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor \qquad \text{if } \mathring{a}_1, \mathring{b}_2 \notin \bar{U} \text{ or } z \notin \bar{U},$$

$$w(\bar{U}) = \sum_{\substack{i \in \bar{U} \cap V'_a \\ j \in \bar{U} \cap V_b}} w_{ij} + w_{\mathring{a}_1 z} + w_{z\mathring{b}_2} \leq \left(\left\lfloor \frac{|\bar{U}|}{2} \right\rfloor - 1 \right) + \left(x^*_{\mathring{e}_1} + x^*_{\mathring{e}_2} - y^* \right) \leq \left\lfloor \frac{|\bar{U}|}{2} \right\rfloor$$

$$\text{if } \mathring{a}_1, \mathring{b}_2, z \in \bar{U} \text{ and } |\bar{U} \cap V'_a| \neq |\bar{U} \cap V_b|.$$

In all cases where $\bar{U} \notin \mathcal{U}$ the blossom inequality is always satisfied such that any set U which violates (6.20) directly leads to the subsets T_1 and T_2 which violate one of the inequalities (6.18).

Thus, both classes of facet defining inequalities are separable in polynomial time by the blossom separation algorithm for odd sets U in the extended graphs G' and G'', respectively. Note that the separation is not needed for fractional solutions with $x^*_{\mathring{e}_1} = 0$ or $x^*_{\mathring{e}_2} = 0$ since in these cases (6.17) and (6.18) are always feasible due to $y^* = 0$ and the degree constraints.

6.4 Summary

In this chapter we investigated the assignment problem with one quadratic term. Other than in the studies of the previous optimization problems, a distinction of the connectedness of the monomial edges is not necessary since connected edges never appear in a feasible assignment solution such that the y-variable would always obtain a value of zero.

For the resulting linearized assignment polytope we could identify two new exponential sized classes of facet defining inequalities, the $\wedge$-clique and the $\vee$-clique constraints, which are both based on cliques in the bipartite graph that contain exactly two of the four monomial vertices. In fact, we conjecture that these two facet classes suffice to obtain a complete description of the polytope corresponding to the assignment problem with one quadratic term. According to this and the fact that a separation is possible in polynomial time, we could develop two polynomial time separation routines rendering an optimization possible also in practice.

One of the most surprising results we found during our investigations is the strongly increasing number of facets. Starting from a polynomial number of nonnegativity and degree constraints, which suffice to describe the assignment polytope in the linear case, one additional quadratic term causes an exponential number of facet defining inequalities and thus changes the shape of the polyhedron considerably.

Chapter 7

Quadratic Matchings

Finally, we consider the **quadratic matching problem** (QMP), which searches for a matching of maximum weight with respect to an objective function containing linear and quadratic weights c_e and q_{ef} on the (pairs of) edges. During this chapter we assume the underlying graph to be complete. Applications for the QMP come from image recognition problems, where two objects of nearly similar shape have to be recognized automatically [47] and other computer vision and neural modeling problems [168]. Considering the image recognition problem, it happens frequently that small parts or objects exist in one of the images which do not appear in the other or vice versa, for instance hidden by an object which slightly moves by comparing both images. Therefore, it is not reasonable to enforce a maximal or even perfect matching, such that this application should not be formulated as a quadratic assignment problem.

7.1 Properties and algorithms

As all optimization problems we considered in the previous chapters, the linear matching problem is easy to solve but becomes NP-hard when equipped with a quadratic objective function. This is due to its strong relation to the quadratic assignment problem.

Lemma 7.1.1.
QMP is NP-hard.

Proof. We show the statement by polynomially reducing the NP-hard assignment problem to QMP. The proof runs similarly to the proof of Lemma 4.1.1 where QMST is reduced to QMSF.

Consider a QAP instance on a bipartite graph $G = (V_a \dot{\cup} V_b, E)$ with $|V_a| = |V_b| =: n$ and with cost function $z(x) = c^\top x + x^\top Qx$. Extend G to a complete graph $\tilde{G} = (V_a \cup V_b, \tilde{E})$ and define $M := \max\{c_{\max}, q_{\max}, 0\} + 1$ with the maximal costs $c_{\max} := \max\{c_e \mid e \in E\}$ and $q_{\max} := \max\{q_{ef} \mid e, f \in E\}$. With these definitions modify the costs to $\tilde{c}_e := -c_e + M$ for all $e \in E$ and $\tilde{q}_{ef} := -q_{ef} + M$ for all non-adjacent edges $e, f \in E$, such that all new costs related to costs given by the original graph are strictly positive. Furthermore set $\tilde{c}_e := 0$ for all edges $e \in \tilde{E} \backslash E$ and $\tilde{q}_{ef} = 0$ for all pairs of edges with at least one edge in $\tilde{E}$.

By this construction, any maximal matching in $\tilde{G}$ is perfect and solely contains edges of the original graph, directly yielding an assignment in the original graph. Furthermore, the dependency of the objective values $z(x)$ and $\tilde{z}(x) := \tilde{c}^\top x + x^\top \tilde{Q}x$ of any optimal matching is given by $z(x) = -\tilde{z}(x) + nM + \frac{n(n-1)}{2}M$, such that any maximum matching in $\tilde{G}$ directly yields a minimum assignment in G. □

The "unknown brother" of the quadratic assignment problem, the QMP, has received much less research attention. Being NP-hard in general, the QMP commonly is solved by heuristical approaches. In particular, the main effort is put into application-tailored fast heuristics such as a dual decomposition approach for the image recognition problem [166]. For exact solutions, the universal branch-and-bound approach is used, potentially combined with cutting planes. Convenient cutting planes for the QMP are, for example, **target cuts** [28, 29], relatives of the **local cuts** introduced by Applegate et al. [7]. In the case of QMP target cuts are facets of the polytope corresponding to the same problem on a considerably smaller, edge-induced subgraph. As a matter of fact, the facet defining property disappears when considering the original graph again, but nevertheless the target cuts in general yield high dimensional faces and thus may speed up the B&B algorithm.

7.1.1 Formulation

Let again $\mathcal{Q}$ be the set of edge pairs with $q_{ef} \neq 0$. Since a quadratic term can only appear in a feasible solution if the corresponding edges are not adjacent, we restrict without loss of generality $\mathcal{Q}$ to consist of non-adjacent pairs only, as we already did for the QAP in Section 6.2.

A straightforward quadratic integer programming formulation of the quadratic matching problem is given by the ILP formulation of the corresponding linear problem, extended by the quadratic term $\sum_{\{e,f\}\in\mathcal{Q}} q_{ef} y_{ef}$ in the objective.

We linearize the quadratic formulation by the standard linearization approach such that the corresponding ILP formulation reads

$$
\begin{aligned}
(\mathrm{LQP_{QMP}}) \qquad \max\ & \sum_{e\in E} c_e x_e + \sum_{\{e,f\}\in\mathcal{Q}} q_{ef} y_{ef} \\
\text{s.t.}\ & \sum_{e\in\delta(v)} x_e \leq 1 && \forall\, v \in V_a \cup V_b && (7.1)\\
& y_{ef} \leq x_e, x_f && \forall\, \{e,f\} \in \mathcal{Q} && (7.2)\\
& y_{ef} \geq x_e + x_f - 1 && \forall\, \{e,f\} \in \mathcal{Q} && (7.3)\\
& x \in \{0,1\}^{|E|} \\
& y \in \{0,1\}^{|\mathcal{Q}|}.
\end{aligned}
$$

We define the **quadratic matching polytope**, or briefly **QMP polytope** as the convex hull of all feasible vectors of $(\mathrm{LQP_{QMP}})$, i.e.

$$
P_M^{ql} := \operatorname{conv}\left\{ (x,y) \in \{0,1\}^{|E|+|\mathcal{Q}|} \;\middle|\; x \text{ satisfies (7.1) and } y_{ef} = x_e x_f \ \ \forall\, e,f \in E \right\}.
$$

As a matter of fact, the blossom inequalities (2.12) remain valid for the quadratic matching polytope. They are not needed in the ILP formulation but, as in the linear case, they strengthen the description when integrality is relaxed. However their addition does not suffice to obtain a complete polyhedral description of the quadratic matching polytope, which actually can be seen in the case of only one quadratic term in Section 7.2.

7.1.2 The QMP polytope

In contrast to the linear assignment polytope, whose dimension is reduced by the degree equalities, the linear matching polytope is fulldimensional. In the quadratic case the affine hull of the QAP polytope is extended by additional equations, see Section 6.1.6. However, under the (reasonable) restriction that only quadratic terms of non-adjacent edge pairs are considered, there are no non-trivial affine equations which are satisfied by all feasible solutions, i.e. P_M^{ql} is fulldimensional.

Theorem 7.1.1.

$$\dim(P^{ql}_M) = |E| + |\mathcal{Q}|.$$

Proof. The incidence vectors of the following $1+|E|+|\mathcal{Q}|$ matchings are all affinely independent.

1. $M = \emptyset$
2. $M = \{e\}$ for all $e \in E$
3. $M = \{e, f\}$ for all $\{e, f\} \in \mathcal{Q}$ □

It was shown that the QMP polytope is a face of the boolean quadric polytope $P^{ql}_{\{0,1\}}$ [163].

Theorem 7.1.2.
P^{ql}_M is a face of $P^{ql}_{\{0,1\}}$.

Proof. Obviously, $P^{ql}_M \subseteq P^{ql}_{\{0,1\}}$ since each vector in P^{ql}_M is contained in $P^{ql}_{\{0,1\}}$. For all edges $e \in E$ the degree constraint (7.1) enforces $y_{ef} = 0$ for all edges f incident to e, thus P^{ql}_M is contained in a face of $P^{ql}_{\{0,1\}}$. Vice versa, for each vertex $i \in V$ and another vertex $j \neq i$, let $y_{ijik} = 0$ for all $k \in V\backslash\{i, j\}$. Then,

$$0 \geq \sum_{k\in V\backslash\{i,j\}} y_{ijik} = \sum_{k\in V\backslash\{i,j\}} x_{ij}x_{ik} = x_{ij} \sum_{k\in V\backslash\{i,j\}} x_{ik} = x_{ij} \sum_{k\in V\backslash\{i\}} x_{ik} - x_{ij}^2 = x_{ij}(\sum_{k\in V\backslash\{i\}} x_{ik} - 1).$$

The last step is due to $x_{ij}^2 = x_{ij}$ such that x_{ij} can be factored out. Therefore either $x_{ij} = 0$ or $\sum_{k\in V} x_{ik} - 1 \leq 0$, the degree constraint. □

In his diploma thesis, Stöcker derived several facet classes for the QMP polytope [163], which we summarize in the following theorem.

Theorem 7.1.3 (Stöcker)**.**

a) Let $G = (V, E)$ be a complete graph with $|V| \geq 6$. Let $\{f_1, f_2, f_3\}$ form a triangle in G, i. e. $f_1, f_2, f_3 \in E$ with $f_1 = \{a, b\}, f_2 = \{a, c\}$ and $f_1 = \{b, c\}$ for vertices $a, b, c \in V$. Furthermore, let $g_1, g_2, g_3 \in E$ with $g_1 = \{c, d\}, g_2 = \{b, d\}$ and $g_3 = \{a, d\}$ for another vertex $d \in V$. Finally, let $e \in E$ be an edge which is not incident to any of these edges. Then,

$$\begin{aligned}
&-x_e + \sum_{i=1}^{3} y_{ef_i} && \leq 0 && \\
&-x_e + \sum_{i=1}^{3} y_{ef_i} + y_{eg_j} - y_{g_jf_j} && \leq 0 && \text{for all } j \in \{1, 2, 3\} \\
&-x_e + \sum_{i=1}^{3} y_{ef_i} + y_{eg_j} + y_{eg_k} - y_{g_jf_j} - y_{g_kf_k} && \leq 0 && \text{for all } j \neq k \in \{1, 2, 3\} \\
&-x_e + \sum_{i=1}^{3} y_{ef_i} + y_{eg_1} + y_{eg_2} + y_{eg_3} - y_{g_1f_1} - y_{g_2f_2} - y_{g_3f_3} && \leq 0 &&
\end{aligned}$$

are facet defining for P^{ql}_M.

b) Let $G = (V, E)$ be an arbitrary graph with $e = \{a, b\} \in E$ for vertices $a, b \in V$ and let $c \in V$ be another vertex which has at least three adjacent vertices different from a and b. Then,

$$-x_e + \sum_{\substack{f \in \delta(c) \\ f \neq \{a,c\},\{b,c\}}} y_{ef} \leq 0$$

is facet defining for P_M^{ql}.

c) Let $G = (V, E)$ be an arbitrary graph. Let $F \subseteq E$ such that on the one hand for all non-incident pairs of edges $e_1, e_2 \in E \backslash F$ there exists another edge $f \in E \backslash F$ which is not incident to e_1 and e_2, and such that on the other hand for all edges $e \in E \backslash F$ there exist two edges $f_1, f_2 \in F$ such that all the three e, f_1, f_2 are not incident to each other. Then,

$$\sum_{f \in F} x_f - \sum_{e \in F} \sum_{\substack{f \in F \\ f \cap e = \emptyset}} y_{ef} \leq 1$$

is facet defining for P_M^{ql}.

d) Let $G = (V, E)$ be a complete graph with $|V| \geq 8$. Then, there exist facet defining inequalities of the form

$$\sum_{e \in E} a_e x_e + \sum_{e \in E} \sum_{\substack{f \in E \\ f \cap e = \emptyset}} b_{ef} y_{ef}$$

with $a_e, b_{ef} \in \{-1, 0, 1\}$ for all $e, f \in E$ and with $b_{ef} = 1$ for at least one non-incident pair of edges $e, f \in E$. The precise conditions for the facet inducing property can be found in [163].

In [163] it is stated that the inequalities presented in part *a*) also induce facets if the graph G is not complete but contains all edges which contribute to the respective inequality. Furthermore, ILP based exponential time separation algorithms and polynomial time separation heuristics are proposed for the inequality classes given in part *c*) and *d*) since their size is exponential in the number of vertices of G.

7.2 Matchings with one quadratic term

Although there exist some classifications of facets of the QMP polytope, the description of P_M^{ql} is far from being complete. Furthermore, including the exponentially many constraints in a branch-and-bound scheme leads to high running times since up to now there is no polynomial time separation algorithm. In the remainder of this chapter we again apply our approach and consider the matching problem with one quadratic term to find further valid inequalities and to possibly strengthen the polyhedral description of P_M^{ql}.

Without loss of generality we define the quadratic term to be the product of the edges $\mathring{e}_1 := \{\mathring{u}, \mathring{v}\}$ and $\mathring{e}_2 := \{\mathring{w}, \mathring{z}\}$. Thus, in the integral case, the product variable models $y := y_{\mathring{e}_1 \mathring{e}_2} = x_{\mathring{e}_1} x_{\mathring{e}_2}$ and we investigate the matching polytope with respect to the (disconnected) monomial $x_{\mathring{e}_1} x_{\mathring{e}_2}$, i. e.

$$P_M^d := \text{conv} \left\{ (x, y) \in \{0,1\}^{|E|+1} \;\middle|\; x \text{ satisfies (7.1) and } y = x_{mone_1} x_{mone_2} \right\}.$$

With the result of Theorem 7.1.1 it directly follows that the dimension of P_M^d equals $|E| + 1$.

Clearly, all inequalities that are valid for the linear matching polytope remain valid for the quadratic matching polytope. Moreover almost all of them remain facet inducing for P_M^d. In the following we always consider complete graphs $G = (V, E)$ and assume $|V| \geq 6$.

Lemma 7.2.1.

a) The degree inequalities $\sum_{e\in\delta(v)} x_e \le 1$ *for all* $v \in V$,

b) the nonnegativity constraints $x_e \ge 0$ *for all* $e \in E\backslash\{\mathring{e}_1, \mathring{e}_2\}$,

c) and the linearization constraints of the form $y \le x_{\mathring{e}_1}$, $y \le x_{\mathring{e}_2}$ *and* $y \ge 0$

are facet inducing for P_M^d.

Proof. To prove the facet inducing property, we list $\dim(P_M^d) = |E|+1$ many affinely independent vectors (x, y) that satisfy the corresponding inequality with equality.

a) Let $v \in V$.

1. $M = \{e\}$ for all $e \in \delta(v)$
2. $M = \{e, f\}$ for all $e \notin \delta(v)$, $f \in \delta(v)\backslash\{\mathring{e}_1, \mathring{e}_2\}$, f not adjacent to e
3. $M = \{e, \mathring{e}_1, \mathring{e}_2\}$ for e not adjacent to $\mathring{e}_1, \mathring{e}_2$, and $e \in \delta(v)$ if $v \notin \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$

b) Let $e \in E\backslash\{\mathring{e}_1, \mathring{e}_2\}$.

1. $M = \emptyset$
2. $M = \{f\}$ for all $f \in E\backslash\{e\}$
3. $M = \{\mathring{e}_1, \mathring{e}_2\}$

c) The proof is similar to *a)* and *b)* . □

The lemma shows that all inequalities that are facet inducing for the linear matching problem also induce a facet in P_M^d except for the nonnegativity constraints for the product edges $\mathring{e}_1$ and $\mathring{e}_2$. In fact these inequalities are dominated by the standard linearization constraints (7.2). Note that the linearization constraint (7.3) is not facet inducing. It can easily be shown that there do not exist enough affinely independent vectors that are tight for this inequality. Moreover it is shown in the remainder of this chapter that they are dominated by another class of inequalities.

For the description of the linear matching polytope the blossom inequalities (2.12) are facet inducing. In the case of one quadratic term this is not true for all blossom inequalities. However, most of the remaining constraints are dominated by very related facet classes.

Theorem 7.2.2.

Let $S \subseteq V$ *be a subset of nodes of odd cardinality.*

a) If both $\mathring{e}_1, \mathring{e}_2 \in \delta(S)$, *then the* $\wedge$***-blossom inequality***

$$\sum_{e\in E(G[S])} x_e + y \le \frac{|S|-1}{2} \tag{7.4}$$

induces a facet of P_M^d.

b) If $S = S_1 \in \{\{\mathring{u}, \mathring{v}, \mathring{w}\}, \{\mathring{u}, \mathring{v}, \mathring{z}\}\}$ *or if* $S = S_2 \in \{\{\mathring{u}, \mathring{w}, \mathring{z}\}, \{\mathring{v}, \mathring{w}, \mathring{z}\}\}$, *then the* $\dot{\vee}$***-blossom inequalities***

$$\sum_{e\in E(G[S_1])} x_e + (x_{\mathring{e}_2} - y) \le \frac{|S_1|-1}{2} \tag{7.5}$$

$$\sum_{e\in E(G[S_2])} x_e + (x_{\mathring{e}_1} - y) \le \frac{|S_2|-1}{2} \tag{7.6}$$

induce facets of P_M^d.

c) *In all other cases the linear blossom inequality*

$$\sum_{e\in E(G[S])} x_e \leq \frac{|S|-1}{2} \tag{7.7}$$

induces a facet of P_M^d.

In the following we denote the incidence vector of a matching M with x_M and call x_M **matching vector**. The corresponding product variable is denoted with y_M.

Proof.

a) Let $S \subseteq V$ be a subset of odd cardinality satisfying the conditions of 7.2.2 *a*). Without loss of generality let $\mathring{u}, \mathring{w} \in S$, $\mathring{v}, \mathring{z} \notin S$. If $y = 0$, the linear blossom inequality (7.7) is obtained. Its validity follows directly from the linear matching problem. If $y = 1$, the vertices $\mathring{u}$ and $\mathring{w}$ are matched by the edges $\mathring{e}_1$ and $\mathring{e}_2$ with the vertices $\mathring{v}, \mathring{z} \notin S$. As a result, only the remaining $|S| - 2$ vertices of $S \backslash \{\mathring{u}, \mathring{w}\}$ are matchable within S, which is restricted by

$$\sum_{e\in E(G[S\backslash\{\mathring{u},\mathring{w}\}])} x_e \leq \frac{|S|-3}{2}$$

due to the linear blossom inequality (7.7), see Figure 7.1. Adding $y = 1$ and increasing the right-hand side by one, we obtain inequality (7.4).

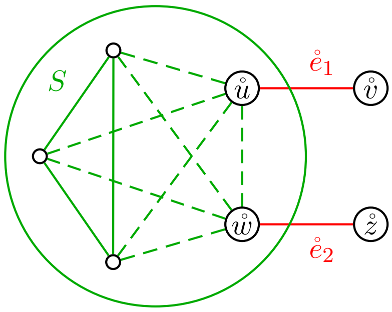


Figure 7.1: If both product edges are in the matching, the two vertices $\mathring{u}$ and $\mathring{w}$ cannot be matched with other vertices in the set S.

To prove the facet inducing property of (7.4), we show that the face induced by the inequality corresponding to S is not contained in any larger proper face. The main argumentation runs analogously to the proof in [48] verifying that blossom inequalities define facets in the linear case. Note that the here considered graph is complete and therefore two-connected and hypomatchable for each subset S, which is mandatory for the argumentation in [48].

Let $\mathcal{F}$ be the set of matching vectors that satisfy the $\wedge$-blossom inequality (7.4) with equality. Suppose that the valid inequality

$$\sum_{e\in E} c_e x_e + c_y y \leq d \tag{7.8}$$

is also satisfied with equality by every matching vector in $\mathcal{F}$. As P_M^d is a full dimensional polytope, it suffices to show that the two inequalities (7.4) and (7.8) only differ by a factor c, yielding the fact that (7.4) is not contained in any larger proper face of P_M^d.

In the first step we show $c_e = 0$ for all edges $e \in E \backslash E(G[S])$. For this, let $\bar{e}$ be such an edge and let x_M be a matching vector which satisfies $x_M, x_{M \cup \{\bar{e}\}} \in \mathcal{F}$. By this construction, $y_M, y_{M \cup \{\bar{e}\}} = 0$, and M and $M \cup \{\bar{e}\}$ both satisfy (7.8) with equality. A comparison of the coefficients yields

$$\sum_{e \in M} c_e = \sum_{e \in M} c_e + c_{\bar{e}},$$

and thus $c_{\bar{e}} = 0$.

In a second step, we show that $c_e = c_f =: c$ for all edges $e, f \in E(G[S])$ with $e \neq f$, which is done by contradiction. Assume that there exist two such edges with different coefficients. Then, there exists a vertex $v \in V$ which is adjacent to two edges f_1 and f_2 with $c_{f_1} \neq c_{f_2}$. Construct a graph G' by splitting v into two vertices v_1 and v_2, where all edges $e \in \delta(v) \cap E(G[S])$ with $c_e = c_{f_1}$ are incident to v_1 and incident to v_2 else. By this construction a matching M' exists which is perfect in $G'[S]$. Since $\mathring{e}_1, \mathring{e}_2 \in \delta(S)$, they are not matched by M such that $y_{M'} = 0$. Let $g_1 := M' \cap \delta(v_1)$ and $g_2 := M' \cap \delta(v_2)$ be the matching edges incident to v_1 and v_2 respectively. Define M_1 to be the matching on the original graph G that corresponds to $M' \backslash \{g_1\}$ and define M_2 on G corresponding to $M' \backslash \{g_2\}$. The construction is visualized in Figure 7.2. Then, the matching vectors $x_{M_1}, x_{M_2} \in \mathcal{F}$, i.e. x_{M_1}, x_{M_2} satisfy inequality (7.4) with equality. On the other hand $c_{g_1} < c_{g_2}$ by construction, such that not both x_{M_1} and x_{M_2} can satisfy (7.8) with equality since $y_{M_1}, y_{M_2} = 0$. This is a contradiction such that we obtain $c_e = c_f$ for all $e, f \in E(G[S])$.

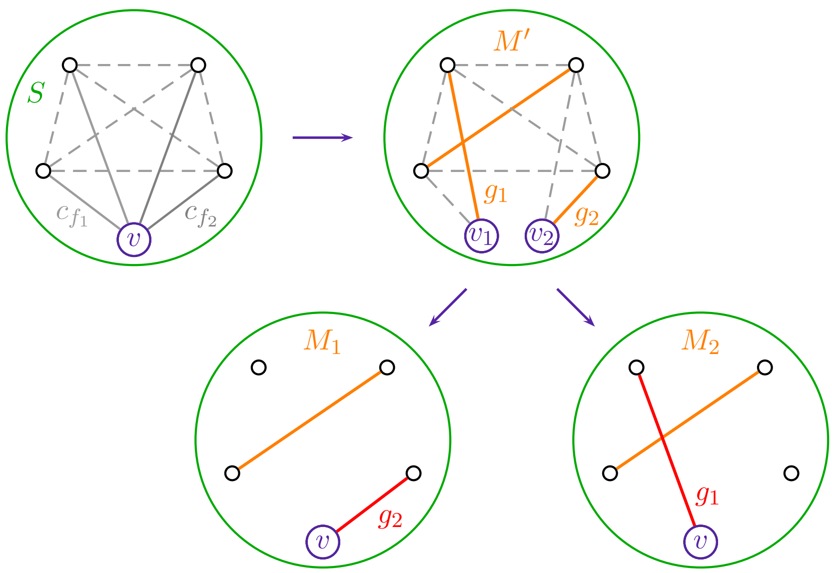


Figure 7.2: The vertex v is splitted into v_1 and v_2, and all edges with c_{f_1} are set adjacent to v_1, the others to v_2. The matchings M_1 and M_2 are derived from the perfect matching M' when shrinking v_1 and v_2 by omitting g_1 and g_2 respectively.

It remains to show that $c_y = 0$. Without loss of generality let $\mathring{u}, \mathring{w} \in S$ and $\mathring{v}, \mathring{z} \notin S$ such that $\mathring{e}_1, \mathring{e}_2 \in \delta(S)$. Let M be a matching which is maximal in $E(G[S \backslash \{\mathring{u}, \mathring{w}\}])$ and define the two matchings $M_1 := M \cup \{\{\mathring{u}, \mathring{w}\}\}$ and $M_2 := M \cup \{\{\mathring{u}, \mathring{v}\}, \{\mathring{w}, \mathring{z}\}\}$. By construction, both $x_{M_1}, x_{M_2} \in \mathcal{F}$ with $y_{M_1} = 0$ and $y_{M_2} = 1$. Thus, x_{M_1}, x_{M_2} both satisfy constraint (7.8) with equality, and since $c_e = 0$ for all $e \in E \backslash E(G[S])$ are zero, we obtain

$$\sum_{e \in M} c_e + c_{\{\mathring{u}, \mathring{w}\}} = \sum_{e \in M_1} c_e = \sum_{e \in M_2} c_e + c_y = \sum_{e \in M} c_e + c_y,$$

yielding $c_y = c_{\mathring{u}\mathring{w}} = c$, which completes the proof.

b) Let S satisfy the conditions of Theorem 7.2.2, without loss of generality let $S = \{\mathring{u}, \mathring{v}, \mathring{w}\}$. To show validity of the $\dot{\vee}$-blossom inequality (7.5) distinguish two cases. If $x_{\mathring{e}_2} = 0$ or $y = 1$, the term $x_{\mathring{e}_2} - y$ equals zero such that 7.2.2 equals a linear blossom inequality. If otherwise $x_{\mathring{e}_1} = 0$ and $x_{\mathring{e}_2} = 1$, there are no edges in $E(G[S])$ which are matchable since S consists of only the three monomial vertices, see Figure 7.3. Thus, $\sum_{e \in E(G[S])} x_e = 0$, yielding validity of (7.5).

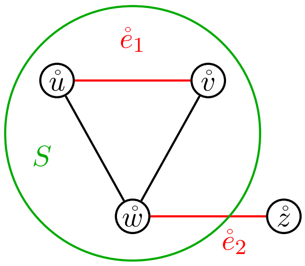


Figure 7.3: If $\mathring{e}_2$ is matched but not $\mathring{e}_1$, no edge in $E(G[S])$ can be in the matching since otherwise the degree constraints of vertex $\mathring{w}$ is violated.

For the facet inducing property, denote with $\mathcal{F}$ the set of matching vectors which satisfy the linear blossom inequality (7.5) with equality and again suppose that the valid inequality

$$\sum_{e \in E} c_e x_e + c_y y \leq d \tag{7.9}$$

is also satisfied with equality by every matching vector in $\mathcal{F}$. We can show $c_e = 0$ for all edges $e \in E \backslash (E(G[S]) \cup \mathring{e}_2)$ on the one hand and $c_{\mathring{e}_1} = c_{\{\mathring{u}, \mathring{w}\}} = c_{\{\mathring{v}, \mathring{w}\}} =: c$ on the other hand completely analogous to the two cases in a).

It remains to show that $c_{\mathring{e}_2} = c$ and that $c_y = -c$. For this, consider the three matching vectors $x_{M_1}, x_{M_2}, x_{M_3} \in \mathcal{F}$ with $M_1 := \{\mathring{e}_1\}$, $M_2 := \{\mathring{e}_2\}$ and $M_3 := \{\mathring{e}_1, \mathring{e}_2\}$. Then, the monomial variables $y_{M_1} = y_{M_2} = 0$ and $y_{M_3} = 1$ such that a comparison of the coefficients of (7.9) leads to $c = c_{\mathring{e}_1} = c_{\mathring{e}_2}$ on the one one hand and to $c = c_{\mathring{e}_2} = -c_y$ on the other hand

c) Let $S \subseteq V$ such that it does not satisfy the conditions of Theorem 7.2.2 a) and b). Validity of the linear blossom inequalities (7.7) follows from the linear case. The facet inducing property follows analogously to the other two parts. Define $\mathcal{F}$ as the set of matching vectors which satisfy the linear blossom inequality (7.7) with equality and suppose that the valid inequality

$$\sum_{e \in E} c_e x_e + c_y y \leq d \tag{7.10}$$

is also satisfied with equality by every matching vector in $\mathcal{F}$. Analogously to part a), we show $c_e = 0$ for all edges $e \in E \backslash E(G[S])$ and $c_e = c_f =: c$ for all edges $e, f \in E(G[S])$. Note that it is always possible to find appropriate matchings M and M', independent of the constellations of the monomial edges $\mathring{e}_1, \mathring{e}_2$ with respect to S as long as S satisfies the conditions in 7.2.2 c), even if $e = \mathring{e}_1$ or $e = \mathring{e}_2$.

It remains to show that $c_y = 0$. For this, we choose two matching vectors $x_{M_1}, x_{M_2} \in \mathcal{F}$ with $y_{M_1} = 0$ and $y_{M_2} = 1$. Since by construction $|M_1 \cap E(G[S])| = |M_2 \cap E(G[S])|$, a comparison of the coefficients of (7.9), exploiting the equality of the coefficients $c_e = c_f$ for all $e, f \in E(G[S])$, leads to $c_y = 0$. □

Note that there are only four inequalities satisfying the conditions in Theorem 7.2.2 *b*). This suggests that the special structure of the $\dot{\vee}$-blossom inequalities is generalizable. Indeed, when considering the subset $S = \{\mathring{u}, \mathring{v}, \mathring{w}, a, b\}$ with two additional vertices $a, b \in V$, it can be easily seen that the inequality

$$x_{\mathring{u}\mathring{v}} + x_{\mathring{u}\mathring{w}} + x_{\mathring{u}a} + x_{\mathring{u}b} + x_{\mathring{v}\mathring{w}} + x_{\mathring{v}a} + x_{\mathring{v}b} + 2x_{\mathring{w}a} + 2x_{\mathring{w}b} + 2x_{ab} + x_{\mathring{w}\mathring{z}} - y \leq 3 \tag{7.11}$$

is valid for P_M^d. For this, consider Figure 7.4. Here the edges which are counted twice in (7.11), i. e. with $c_e = 2$, are colored in blue, the others with $c_e = 1$ in green and red. By the degree constraints (7.1) at most two edges $e \in E(G[S])$ can be included in a matching among which at most one is blue, i. e. with a coefficient of 2, such that their contribution to (7.11) is not greater than three. If additionally $x_{\mathring{e}_2} = 1$, either two green edges, say $\{\mathring{u}, a\}$ and $\{\mathring{v}, b\}$ contributing $x_{\mathring{u}a} + x_{\mathring{v}b} = 2$, or $\{a, b\}$ and $\mathring{e}_1$ contributing $2x_{ab} + x_{\mathring{e}_1} = 3$, are in the matching and their value is added to $x_{\mathring{e}_2} = 1$, but in the latter case we have $y = 1$ which is subtracted again such that in both cases the sum cannot be greater than 3.

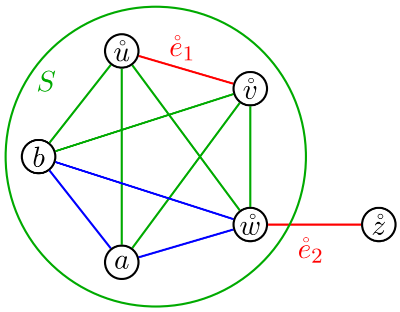


Figure 7.4: The green and the red edges are counted with a factor of one, the blue edges with a factor of two. If both red monomial edges are in the matching, a value of one has to be subtracted since $y = 1$.

At first sight, inequality (7.11) seems very different from the $\dot{\vee}$-blossom inequalities since some variables are counted with a coefficient of 2. However, a closer look at Figure 7.4 shows that inequality (7.11) can be seen as the sum of two nested blossom inequalities, strengthened by the nonnegative term $x_{\mathring{e}_2} - y$. For this, define $T := \{\mathring{w}, a, b\} = S \backslash \{\mathring{u}, \mathring{v}\}$, i. e. the set of vertices connected by the blue edges. Then, we can rewrite inequality (7.11) as

$$\sum_{e \in E(G[S])} x_e + \sum_{e \in E(G[T])} x_e + (x_{\mathring{e}_2} - y) \leq \frac{|S| - 1}{2} + \frac{|T| - 1}{2}.$$

The sum on the right-hand side in turn can be rewritten as $\frac{1}{2}((|S|-1) + ((|S|-2)-1)) = |S|-2$, and the construction indeed can be extended to odd cardinality subsets S of greater size, introducing a new facet class for P_M^d.

Theorem 7.2.3.

Let $S \subseteq V$ be a subset of nodes with odd cardinality and $\mathring{e}_1 \in E(G[S])$, $\mathring{e}_2 \in \delta(S)$ or conversely. Without loss of generality assume $\mathring{u}, \mathring{v}, \mathring{w} \in S$ and $\mathring{z} \in V \backslash S$. Define $T := S \backslash \{\mathring{u}, \mathring{v}\}$. Then, the ***nested blossom inequality***

$$\sum_{e \in E(G[S])} x_e + \sum_{e \in E(G[T])} x_e + x_{\mathring{e}_2} - y \leq |S| - 2 \tag{7.12}$$

induces a facet of P_M^d.

Proof. If $x_{\mathring{e}_2} = 0$ or if $y = 1$ we have $x_{\mathring{e}_2} - y = 0$ such that validity of (7.12) follows directly from the sum of the linear blossom inequalities for the two subsets S and T. Otherwise, if $x_{\mathring{e}_2} = 1$ and $x_{\mathring{e}_1} = 0$, each of the vertices $\mathring{u}$ and $\mathring{v}$ can either be matched with a vertex in $T\backslash\{\mathring{w}\}$ or not, leading to three cases which we distinguish in the following. If both $\mathring{u}, \mathring{v}$ are matched with vertices $t_1, t_2 \in T$ we obtain a left-hand side of (7.12) which is not greater than

$$\frac{|S\backslash\{\mathring{w}\}|}{2} + \frac{|T\backslash\{\mathring{w}, t_1, t_2\}|}{2} + 1 = |S| - 2,$$

since $\mathring{w}$ is matched with $\mathring{z} \notin T$. If exactly one of the vertices in $S\backslash T$, say $\mathring{u}$, is matched with a vertex $t_1 \in T$, the left-hand side of (7.12) is bounded by

$$\frac{|S\backslash\{\mathring{v}, \mathring{w}\}| - 1}{2} + \frac{|T\backslash\{\mathring{w}, t_1\}| - 1}{2} + 1 = |S| - 2$$

since $\mathring{v}$ is not matched with any vertex in S and T. If neither $\mathring{u}$ nor $\mathring{v}$ is matched with a vertex in T, the bound turns out to be

$$\frac{|S\backslash\{\mathring{u}, \mathring{v}, \mathring{w}\}|}{2} + \frac{|T\backslash\{\mathring{w}\}|}{2} + 1 = |S| - 2.$$

Therefore, in all cases the left-hand side of (7.12) is bounded by $|S| - 2$ and thus the inequality (7.12) is feasible for all vectors in P_M^d.

The facet inducing property is shown as in the case of the blossom inequalities, i. e., by proving that the face induced by inequality (7.12) is not contained in any larger proper face and hence is a facet of P_M^d. Let $\mathcal{F}$ be the set of matching vectors that satisfy (7.12) with equality, and suppose that the valid inequality

$$\sum_{e\in E} c_e x_e + c_y y \leq d \tag{7.13}$$

is also satisfied with equality by every matching vector in $\mathcal{F}$. Denote $E_S := E(G[S]) \cup \{\mathring{e}_2\}$.

In the first step we show $c_e = 0$ for all $e \in E\backslash E_S$. For such an edge $e \in E\backslash E_S$ let $x_M \in \mathcal{F}$ be a matching vector such that M does not cover the end nodes of e. Then, also $x_{M\cup\{e\}} \in \mathcal{F}$ since $e \notin E_S$. Thus, both, x_M and $x_{M\cup\{e\}}$ satisfy (7.13) with equality, and a comparison of coefficients leads to $c_e = 0$ for all edges $e = E\backslash E_S$.

Secondly, let $e, f \in E[G(S)] \cap \delta(\{\mathring{u}, \mathring{v}\})$. We show that $c_e = c_f =: c_1$. For this, let t be a vertex in T and let M be a perfect matching in $T\backslash\{t\}$. Then, the three matching vectors $x_{M\cup\{\{\mathring{u},\mathring{v}\}\}}$, $x_{M\cup\{\{\mathring{u},t\}\}}$ and $x_{M\cup\{\{\mathring{v},t\}\}}$ are in $\mathcal{F}$ and satisfy (7.13) with equality. Comparing the coefficients yields $c_{\mathring{u}\mathring{v}} = c_{\mathring{u}t} = c_{\mathring{v}t} := c_1$. Analogously we prove $c_{\mathring{e}_2} = c_1$ by considering a perfect matching M in $T\backslash\{\mathring{w}\}$. Then, both matching vectors $x_{M\cup\{\{\mathring{u},\mathring{w}\}\}}, x_{M\cup\{\mathring{e}_2\}} \in \mathcal{F}$ such that $c_{\mathring{e}_2} = c_{\mathring{u}\mathring{w}} = c_1$.

In a next step we show $c_y = -c_1$. Let M be a maximal matching in $T\backslash\{\mathring{w}\}$. Then, the two matching vectors $x_{M\cup\{\{\mathring{u},\mathring{v}\}\}}, x_{M\cup\{\{\mathring{u},\mathring{v}\},\{\mathring{w},\mathring{z}\}\}} \in \mathcal{F}$ since $y = x_{\mathring{e}_1}x_{\mathring{e}_2} = 1$ holds. As both matchings satisfy (7.13) with equality, we obtain $c_{\mathring{e}_2} + c_y = 0$, i. e. $c_y = -c_{\mathring{e}_2} = -c_1$.

Furthermore, we show that $c_e = c_f =: c_2$ for all $e, f \in E(G[T])$, which is proven by contradiction. For this, suppose that there exist edges $e, f \in E(G[T])$ with $c_e \neq c_f$. Then, there exists a vertex $v \in T$ which is adjacent to two edges f_1, f_2 with different coefficients $c_{f_1} \neq c_{f_2}$. We consider the same graph G' constructed in the proof of Theorem 7.2.2, and a matching M' which is perfect in $G'[T]$ and empty otherwise. Let $g_1 := M' \cap \delta(v_1)$ and $g_2 := M' \cap \delta(v_2)$ and define M_1 and M_2 to be the matchings on G that correspond to $M'\backslash\{g_1\}$ and $M'\backslash\{g_2\}$, respectively. Then, $x_{M_1\cup\{\mathring{e}_1\}}, x_{M_2\cup\{\mathring{e}_1\}} \in \mathcal{F}$ and satisfy (7.13) with equality. A comparison of the coefficients yields $c_{f_1} = c_{f_2}$, a contradiction.

It remains to show that $c_2 = 2c_1$. For two vertices $t_1, t_2 \in T \backslash \{\mathring{w}\}$ we choose a perfect matching M in $T \backslash \{t_1, t_2, \mathring{w}\}$ and define $M_1 := M \cup \{\{\mathring{u}, t_1\}, \{\mathring{v}, t_2\}, \mathring{e}_2\}$ and $M_2 := M \cup \{\{t_1, t_2\}, \mathring{e}_2\}$. Then, both $x_{M_1}, x_{M_2} \in \mathcal{F}$ such that $c_{\mathring{u}t_1} + c_{\mathring{v}t_2} + c_{\mathring{e}_2} = c_{t_1t_2} + c_{\mathring{e}_2}$, leading to $2c_1 = c_2$.

Summarizing, we showed that the inequality (7.13) is a positive scalar multiple of (7.12) and thus (7.12) induces a facet of P_M^d. □

Note that the $\dot{\vee}$-blossom inequalities are contained in the set of the nested blossom inequalities. Then, the set T only includes the one of the monomial vertices whose corresponding monomial edge is in $\delta(S)$.

In addition to the blossom constraints, we introduce two more facet defining inequalities. The first one is a facet class which looks like an hourglass when considering the smallest of the subsets satisfying the specified conditions. The second is an inequality which is based on even cliques.

Consider the four monomial vertices $\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}$ and two other vertices a and b. Then, the **hourglass inequality**

$$x_{\mathring{u}\mathring{v}} + x_{\mathring{u}a} + x_{\mathring{v}a} + x_{ab} + x_{\mathring{w}\mathring{z}} + x_{\mathring{w}b} + x_{\mathring{z}b} - y \leq 2 \tag{7.14}$$

is valid for all matchings in P_M^d, which can be seen in Figure 7.5(a). Obviously, the subgraph contains only one matching with three edges, the matching $M := \{\{\mathring{u}, \mathring{v}\}, \{a, b\}, \{\mathring{w}, \mathring{z}\}\}$. In all other cases the degree constrains would be violated. Since both monomial edges $\mathring{e}_1, \mathring{e}_2 \in M$, we obtain $y = 1$ which is subtracted in inequality (7.14) such that the left-hand side of (7.14) cannot be greater than 2.

The structure of the hourglass inequality can be generalized. Define $S := \{a, b\}$ and extend S by an even number of vertices which are all connected among themselves and with a and b. The construction is visualized in Figure 7.5(b).

(a) The subgraph corresponding to (7.14) contains the four monomial vertices and two vertices a and b as connectors.

(b) The subgraph corresponding to the extended hourglass inequalities is extended by an even number of vertices.

Figure 7.5: The only perfect matchings in the subgraphs are perfect matchings in the green subsets S combined with the two red monomial edges $\mathring{e}_1$ and $\mathring{e}_2$.

Theorem 7.2.4. *Let $S \subseteq V \backslash \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$ be a nonempty subset of even cardinality and let $a, b \in S$. Then, the* ***(extended) hourglass inequality***

$$x_{\mathring{u}\mathring{v}} + x_{\mathring{u}a} + x_{\mathring{v}a} + \sum_{e \in E(G[S])} x_e + x_{\mathring{w}\mathring{z}} + x_{\mathring{w}b} + x_{\mathring{z}b} - y \leq \frac{|S|}{2} + 1 \tag{7.15}$$

is facet defining for P_M^d.

Proof. Validity follows by the same arguments as for the hourglass inequalities (7.14). The only matchings with more edges in E' than $\frac{|S|}{2}+1$ are matchings which are perfect in S and contain both monomial edges. In these cases we have $y=1$ and this value is subtracted from the left-hand side of (7.15). Thus we obtain a value of $(\frac{|S|}{2}+2)-1$. In all other cases the inequality follows by the degree constraints.

To show the facet defining property we again define $\mathcal{F}$ as the set of matching vectors that satisfy (7.15) with equality and suppose that the valid inequality

$$\sum_{e\in E} c_e x_e + c_y y \le d \tag{7.16}$$

is also satisfied with equality by every matching vector in $\mathcal{F}$. Define $V' := S \cup \{\mathring{u},\mathring{v},\mathring{w},\mathring{z}\}$ and $E' := \{\{\mathring{u},\mathring{v}\},\{\mathring{u},a\},\{\mathring{v},a\},\{\mathring{w},\mathring{z}\},\{\mathring{w},b\},\{\mathring{z},b\}\} \cup E(S)$, the set of vertices and edges which contribute a value to (7.15).

Initially, let $e \in E(G[V\backslash V'])$ and let M be a matching that consists of only $\frac{|S|}{2}$ edges in S. The two matching vectors $x_{M\cup\{\mathring{e}_1\}}, x_{M\cup\{\mathring{e}_1,e\}} \in \mathcal{F}$ satisfy (7.18) with equality. A comparison of the coefficients yields $c_e = 0$ for all $e \in E(G[V\backslash V'])$.

Secondly, let $e \in \delta(V')$ with $e=\{i,j\}$, such that $i \in V'$ and $j \in V\backslash V'$. We again consider incidence vectors in $\mathcal{F}$ which satisfy (7.18) with equality and compare the corresponding coefficients:

- $i \in S\backslash\{a\}$: Let M be a perfect matching on $S\backslash\{a,i\}$. We consider the two matching vectors $x_{M\cup\{\{\mathring{u},a\},\mathring{e}_2\}}$ and $x_{M\cup\{\{\mathring{u},a\},\mathring{e}_2,e\}}$ and obtain $c_e=0$.
- $i=a$: Let M be a perfect matching on $S\backslash\{a,b\}$. Consider $x_{M\cup\{\{b,\mathring{w}\},\mathring{e}_1\}}$ and $x_{M\cup\{\{b,\mathring{w}\},\mathring{e}_1,e\}}$ to obtain $c_e=0$.
- $i \in \{\mathring{u},\mathring{v}\}$: Let M be a perfect matching on S. Comparing $x_{M\cup\{\mathring{e}_2\}}$ and $x_{M\cup\{\mathring{e}_2,e\}}$ yields $c_e=0$.
- $i \in \{\mathring{w},\mathring{z}\}$: Analogous.

All in all we obtain $c_e=0$ for all $e \in \delta(S')$.

Analogously we show that $c_e = c_f =: c_1$ for all $e \in E'$. Let M be a perfect matching on $S\backslash\{a,b\}$. If $|S| \ge 4$, let M_{ij} be a perfect matching on $S\backslash\{a,b,i,j\}$ for arbitrary $i,j \in S\backslash\{a,b\}$ with $i \ne j$.

- Comparing $x_{M\cup\{\{a,b\},\mathring{e}_2\}}$, $x_{M\cup\{\{\mathring{u},a\},\mathring{e}_2\}}$, $x_{M\cup\{\{\mathring{v},a\},\mathring{e}_2\}}$ yields $c_{ab} = c_{\mathring{u}a} = c_{\mathring{v}a} =: c_1$.
- Comparing $x_{M\cup\{\{a,b\},\mathring{e}_1\}}$, $x_{M\cup\{\{\mathring{w},b\},\mathring{e}_1\}}$, $x_{M\cup\{\{\mathring{z},b\},\mathring{e}_1\}}$ yields $c_1 = c_{ab} = c_{\mathring{w}b} = c_{\mathring{z}b}$.
- Comparing $x_{M\cup\{\{\mathring{u},a\},\mathring{e}_2\}}$, $x_{M\cup\{\{\mathring{u},a\},\{\mathring{w},b\}\}}$ yields $c_1 = c_{\mathring{w}b} = c_{\mathring{e}_2}$.
- Comparing $x_{M\cup\{\{a,b\},\mathring{e}_1\}}$, $x_{M\cup\{\{a,b\},\mathring{e}_2\}}$ yields $c_1 = c_{\mathring{e}_2} = c_{\mathring{e}_1}$.
- Comparing $x_{M_{ij}\cup\{\{i,j\},\{\mathring{u},a\},\mathring{e}_2\}}$, $x_{M_{ij}\cup\{\{i,b\},\{\mathring{u},a\},\mathring{e}_2\}}$ yields $c_{ij} = c_{ib} =: c_2$.
- Comparing $x_{M_{ij}\cup\{\{i,j\},\{\mathring{w},b\},\mathring{e}_1\}}$, $x_{M_{ij}\cup\{\{i,a\},\{\mathring{w},b\},\mathring{e}_1\}}$ yields $c_2 = c_{ij} = c_{ia}$.
- Comparing $x_{M_{ij}\cup\{\{i,j\},\{a,b\},\mathring{e}_1\}}$, $x_{M_{ij}\cup\{\{i,a\},\{j,b\},\mathring{e}_1\}}$ yields $c_1 = c_{ab} = c_{ia} = c_2$.

Finally we compare $x_{M\cup\{\{a,b\},\mathring{e}_1\}}$ and $x_{M\cup\{\{a,b\},\mathring{e}_1,\mathring{e}_2\}}$ and obtain $c_{\mathring{e}_2} + c_y = 0$, i.e. $c_y = -c_1$, which completes the proof. □

The facet class based on even cliques is composed of two constellations of the four monomial vertices $\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}$ and another vertex a with respect to a subset $S \subseteq V$ of even cardinality. In both cases, one of the vertices of $\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}$ is separated from the other three and combined with a. In the following we consider the case where $\mathring{u}$ is the separated monomial vertex, but as a matter of fact the following theorem can be formulated analogously for the three other constellations.

Theorem 7.2.5. *Let $S \subset V$ be a subset of nodes with even cardinality and either*

a) $\mathring{v}, \mathring{w}, \mathring{z} \in S$, $a, \mathring{u} \notin S$ *or*

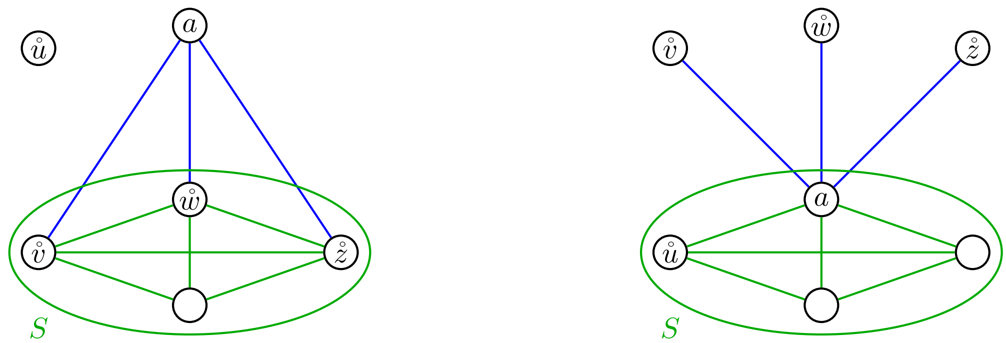
b) $\mathring{v}, \mathring{w}, \mathring{z} \notin S$, $a, \mathring{u} \in S$.

Then, the ***clique-a inequality***

$$\sum_{e \in E(G[S])} x_e + x_{\mathring{v}a} + x_{\mathring{w}a} + x_{\mathring{z}a} + y \leq \frac{|S|}{2} \tag{7.17}$$

is facet defining for P_M^d.

A visualization of the clique-a inequalities with respect to the two cases a) and b) is presented in Figure 7.6.



(a) S contains the vertices $\mathring{v}, \mathring{w}$ and $\mathring{z}$ but not a and $\mathring{u}$.

(b) S does not contain $\mathring{v}, \mathring{w}$ and $\mathring{z}$ but a and $\mathring{u}$.

Figure 7.6: The subgraphs corresponding to the subsets S specified in Theorem 7.2.5 a) and b).

Proof. We prove validity for sets S corresponding to the conditions in 7.2.5 a) and add the little differences with respect to b) in brackets. If $x_{\mathring{v}a} = x_{\mathring{w}a} = x_{\mathring{z}a} = y = 0$, validity is obvious for arbitrary $S \subseteq V$ of even cardinality. If vertex a is matched with one of the vertices $\mathring{v}, \mathring{w}, \mathring{z}$, say $\mathring{v}$, it follows from the degree inequalities that $x_{\mathring{w}a} = x_{\mathring{z}a} = y = 0$. The set of unmatched vertices in $S \backslash \{\mathring{v}\}$ (or in $S \backslash \{a\}$) can, by blossom inequality (7.7), contain at most $\frac{|S|-2}{2}$ matching edges and, summed up, the left-hand side does not exceed $\frac{|S|}{2}$. Finally, if $y = 1$ and therefore $x_{\mathring{u}\mathring{v}} = x_{\mathring{w}\mathring{z}} = 1$, the degree inequality (7.1) leads to $x_{ka} = 0$ for $k \in \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$. The set of matchable vertices in S reduces by $\mathring{v}$ (or $\mathring{u}$) since $x_{\mathring{u}\mathring{v}} = 1$, This compensates the value of the additional term $y = 1$, leading to validity of constraint (7.17).

Next, we prove the facet inducing property. Define $\mathcal{F}$ as before, with respect to (7.17), and suppose that the valid inequality

$$\sum_{e \in E} c_e x_e + c_y y \leq d \tag{7.18}$$

is satisfied with equality by every matching vector in $\mathcal{F}$. Define E' as the set of edges which contribute a value to (7.17), i. e. $E' := E(G[S]) \cup \{\{a, \mathring{v}\}, \{a, \mathring{w}\}, \{a, \mathring{z}\}\}$.

For the first part of the proof let S satisfy the conditions of 7.2.5 a), i. e., let $\mathring{v}, \mathring{w}, \mathring{z} \in S$ and $a, \mathring{u} \notin S$. First we show that $c_e = 0$ for all edges which do not contribute to inequality (7.17), i. e. for all $e = \{i, j\} \in E \backslash E'$. Let $j \in V \backslash S$.

- $e \in E(G[V \backslash S])$: Let M be a perfect matching in S. The matching vectors x_M and $x_{M \cup \{e\}}$ both are in $\mathcal{F}$ and thus $c_e = 0$.
- $e \in \delta(S),\ i \neq \mathring{v},\ j \neq a$: Let M be a perfect matching in $S \backslash \{\mathring{v}, i\}$. Consider the matching vectors $x_{M \cup \{\{\mathring{v},a\}\}}$ and $x_{M \cup \{\{\mathring{v},a\},e\}}$ in $\mathcal{F}$ to obtain $c_e = 0$.
- $e \in \delta(S),\ i = \mathring{v},\ j \neq a$: Let M be a perfect matching in $S \backslash \{\mathring{w}, i\}$. Then, $x_{M \cup \{\{\mathring{w},a\}\}}$ and $x_{M \cup \{\{\mathring{w},a\},e\}}$ in $\mathcal{F}$ yield $c_e = 0$.
- $e \in \delta(S),\ j = a,\ i \neq \mathring{v}, \mathring{w}, \mathring{z}$: Let M be a perfect matching in $S \backslash \{\mathring{v}, \mathring{w}, \mathring{z}, i\}$. With the matching vectors $x_{M \cup \{\mathring{e}_1, \mathring{e}_2\}}, x_{M \cup \{\mathring{e}_1, \mathring{e}_2, e\}} \in \mathcal{F}$ we obtain $c_e = 0$.

In the following we prove that $c_e = c_f =: c$ holds for all remaining edges e and f, i. e. for all edges $e, f \in E(G[S]) \cup \{\{a, \mathring{v}\}, \{a, \mathring{w}\}, \{a, \mathring{z}\}\}$.

- Let M be a perfect matching in $S \backslash \{\mathring{v}, \mathring{w}\}$. Then, $x_{M \cup \{\{\mathring{v},\mathring{w}\}\}}$, $x_{M \cup \{\{\mathring{v},a\}\}}$ and $x_{M \cup \{\{\mathring{w},a\}\}}$ in $\mathcal{F}$ yield $c_{\mathring{v}\mathring{w}} = c_{\mathring{v}a} = c_{\mathring{w}a} =: c$.
- Analogous for $c_{\mathring{v}\mathring{z}} = c_{\mathring{w}\mathring{z}} = c_{\mathring{z}a} = c$.
- Let $i \in S \backslash \{\mathring{v}\}$ and M a perfect matching in $S \backslash \{\mathring{v}, i\}$. Comparison of the matching vectors $x_{M \cup \{\{\mathring{v},a\}\}}$, $x_{M \cup \{\{\mathring{v},i\}\}} \in \mathcal{F}$ yields $c_{\mathring{v}i} = c$.
- Analogous for $c_{\mathring{w}i} = c$ for all $i \in S \backslash \{\mathring{w}\}$ and $c_{\mathring{z}i} = c$ for all $i \in S \backslash \{\mathring{z}\}$.

Finally, for an arbitrary $i \in S \backslash \{\mathring{v}, \mathring{w}, \mathring{z}\}$ let M be a perfect matching in $S \backslash \{\mathring{v}, \mathring{w}, \mathring{z}, i\}$. We compare $x_{M \cup \{\{\mathring{v},\mathring{w}\},\{\mathring{z},i\}\}}$ and $x_{M \cup \{\mathring{e}_1, \mathring{e}_2\}}$ to obtain the equation $c_{\mathring{v}\mathring{w}} + c_{\mathring{z}i} = c_{\mathring{e}_2} + c_y$. This results in $c_y = c$ proving that (7.18) is a positive multiple of (7.17) and completing the proof for subsets S that satisfy the conditions of a).

For the second part of the proof let S be a subset with $\mathring{v}, \mathring{w}, \mathring{z} \notin S$ and $a, \mathring{u} \in S$. Similar to the first part of the proof we compare the coefficients of different matching vectors. In the first step we show that $c_e = 0$ for all $e = \{i, j\} \in E \backslash E'$. Let $j \in V \backslash S$.

- $e \in E(G[V \backslash S])$: Let M be a perfect matching in S. The matching vectors x_M and $x_{M \cup \{e\}}$ both are in $\mathcal{F}$ and thus $c_e = 0$.
- $e \in \delta(S),\ i \neq a,\ j \neq \mathring{v}$: Let M be a perfect matching in $S \backslash \{a, i\}$. Consider the matching vectors $x_{M \cup \{\{\mathring{v},a\}\}}$ and $x_{M \cup \{\{\mathring{v},a\},e\}}$ in $\mathcal{F}$ to obtain $c_e = 0$.
- $e \in \delta(S),\ i \neq a,\ j = \mathring{v}$: Let M be a perfect matching in $S \backslash \{a, i\}$. Then, $x_{M \cup \{\{\mathring{w},a\}\}}$ and $x_{M \cup \{\{\mathring{w},a\},e\}}$ in $\mathcal{F}$ yield $c_e = 0$.
- $e \in \delta(S),\ i = a,\ j \neq \mathring{v}, \mathring{w}, \mathring{z}$: Let M be a perfect matching in $S \backslash \{\mathring{u}, i\}$. With the matching vectors $x_{M \cup \{\mathring{e}_1, \mathring{e}_2\}}, x_{M \cup \{\mathring{e}_1, \mathring{e}_2, e\}} \in \mathcal{F}$ we obtain $c_e = 0$.

For the remaining edges $e, f \in E(G[S]) \cup \{\{a, \mathring{v}\}, \{a, \mathring{w}\}, \{a, \mathring{z}\}\}$ we again show $c_e = c_f$.

- Let M be a perfect matching in $S \backslash \{\mathring{u}, a\}$. Then, $x_{M\cup\{\{\mathring{u},a\}\}}$, $x_{M\cup\{\{\mathring{v},a\}\}}$, $x_{M\cup\{\{\mathring{w},a\}\}}$ and $x_{M\cup\{\{\mathring{z},a\}\}}$ in $\mathcal{F}$ yield $c_{\mathring{u}a} = c_{\mathring{v}a} = c_{\mathring{w}a} = c_{\mathring{z}a} =: c$.
- Let $i \in S\backslash\{a\}$ and M a perfect matching in $S\backslash\{a, i\}$. Comparison of the matching vectors $x_{M\cup\{\{a,i\}\}}$, $x_{M\cup\{\{\mathring{v},a\}\}} \in \mathcal{F}$ yields $c_{ai} = c$.
- Analogous for $c_{\mathring{u}i} = c$ for all $i \in S\backslash\{a\}$.

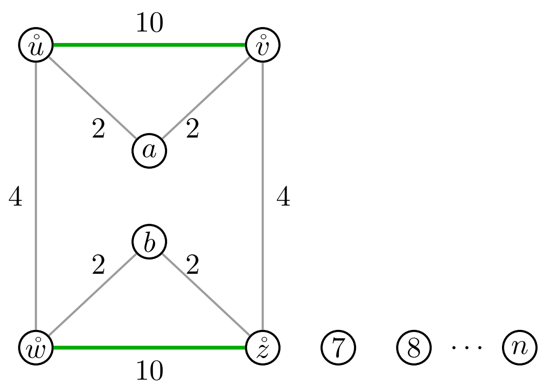
Finally, let M be a perfect matching in $S\backslash\{\mathring{u}, a\}$. Comparing $x_{M\cup\{\mathring{e}_1,\{\mathring{w},a\}\}}$ and $x_{M\cup\{\mathring{e}_1,\mathring{e}_2\}}$ yields $c_y = c_{\mathring{w}a} = c$. This completes the proof for subsets S satisfying the conditions of b). □

When considering facet defining inequalities for P_M^d we always assume to have complete graphs. However, considering the proofs of Theorems 7.2.4 and 7.2.5 one can see that inequalities of the corresponding forms remain valid and even facet inducing in a non-complete graph G as long as all edges which contribute a value to the respective inequality exist in G.

Considering the different facet classes we have to assert that the matching problem becomes more complicated when adding a single quadratic term. In fact, there exist even more classes of facets since the previous constraints do not suffice for an integral description of the polytope. The following example shows that there exist fractional solutions with better objective values than the integral optimum, which are not cut off by the previous constraints.

Example 7.2.6.

Consider the graph $K_n = (V, E)$. The costs of single edges are indicated in the illustration on the right; the omitted edges have negative cost such that they never appear in any optimal solution. The quadratic costs are $q_{\mathring{e}_1\mathring{e}_2} = -10$ for the edges $\mathring{e}_1 = \{\mathring{u}, \mathring{v}\}$ and $\mathring{e}_2 = \{\mathring{w}, \mathring{z}\}$.
The optimal integral solution of the matching problem with one quadratic term has an objective value of 10 and is given by the highlighted edges $\{\mathring{u}, \mathring{v}\}$ and $\{\mathring{w}, \mathring{z}\}$. However, there exists a better fractional solution with a value of 11 given as follows.



- $x_{\mathring{u}\mathring{v}} = x_{\mathring{w}\mathring{z}} = 0.5$, $y = 0.3$
- $x_{\mathring{u}\mathring{w}} = x_{\mathring{v}\mathring{z}} = 0.3$,
- $x_{\mathring{u}a} = x_{\mathring{v}a} = x_{\mathring{w}b} = x_{\mathring{z}b} = 0.2$,
- $x_e = 0$ *otherwise.*

Note that this fractional solution satisfies all of the previously formulated matching constraints, i. e. the degree, the nonnegativity and the linearization constraints, all blossom inequalities (7.4)–(7.7) *and* (7.12)*, the extended hourglass inequalities* (7.15) *and the clique-a inequalities* (7.17).

The example shows that the previously discussed constraints do not suffice for an integral description of P_M^d. Nevertheless the derived constraints containing the quadratic variable yield a tighter description of P_M^d, and also of P_M^{ql}. As they all depend on subsets S of V, there clearly exist exponentially many inequalities of each class making an enumeration in a B&B scheme inefficient. To nevertheless make use of such inequalities, approaches for polynomial time separation algorithms are required. In the following section we present two detailed algorithms for (7.4) and (7.17) to explain the idea for a polynomial time separation of classes depending on either even or odd subsets. For the remaining of the derived facet classes we shortly present some ideas how to adapt the previous approaches.

7.3 Separation routines

The similarity of the $\wedge$-blossom inequalities (7.4) and the linear ones is obvious as they only differ by the y-value on the left-hand side. Thus, a straightforward idea for a separation approach for the $\wedge$-blossom inequalities is to slightly modify the linear blossom separation of Padberg an Rao (c. f. Section 2.4.3) to reuse it for the quadratic case. Having a closer look at the clique-a facets, the main difference lies in the cardinality of S since both new quadratic facet classes depend on the choice of an even subset $S \subseteq V$, instead of an odd one as in the case of the blossom inequalities. The blossom separation is based on the calculation of a minimum T-odd cut, which suggests to modify the separation routine such that the calculation of minimum T-even cuts provides the desired result.

Recall that, for a set T of even cardinality, a T-odd cut is a cut $\delta(S)$ with $|T \cap S|$ odd. Analogously, a ***T*-even cut** is a cut $\delta(S)$ with $|T \cap S|$ even, and an ***s*-*t* *T*-even (odd) cut** is a cut $\delta(S)$ with $|T \cap S|$ even (odd) and with $s \in S,\ t \notin S$ or $s \notin S,\ t \in S$. The latter two cuts are needed for the following separation strategies. Goemans and Ramakrishnan stated in [85] that these problems are solvable in polynomial time with an algorithm of Grötschel et al. [91, 92]. This leads to polynomial time separation strategies for the considered facet classes.

The $\wedge$-blossom inequalities

First, we consider the facets induced by the inequalities of (7.4),

$$\sum_{e \in E(G[S])} x_e + y \leq \frac{|S| - 1}{2}.$$

Recall that the inequalities are facet defining for odd subsets S with $\mathring{e}_1, \mathring{e}_2 \in \delta(S)$. For the resulting four cases, depending on how $\mathring{u}, \mathring{v}, \mathring{w}$ and $\mathring{z}$ are related to S, two at a time are combinable. The construction presented in the following yields odd subsets S where $\mathring{u}, \mathring{w} \in S,\ \mathring{v}, \mathring{z} \notin S$ and conversely. The other two cases can be calculated analogously.

We introduce, as in Section 2.4.3, the term $s_i := 1 - \sum_{e \in \delta(i)} x_e$ for each vertex $i \in V$, which represents the slack of the corresponding degree inequality (7.1). Re-writing the $\wedge$-blossom inequality (7.4) then leads to

$$\sum_{i \in S} s_i + \sum_{e \in \delta(S)} x_e \geq 1 + 2y \tag{7.19}$$

for $S \subset V$ with $|S|$ odd and the required relations of $\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}$ to S.

For a given vector $(x^*, y^*) \in [0,1]^{|E|+1}$ satisfying the degree and the linearization inequalities, we create an extended graph $G_d = (V_d, E_d)$ similarly to the linear case by adding a new dummy vertex d and new edges $\{d,i\}$ for every vertex $i \in V$. Furthermore, we assign the weight x_e^* to each edge $e \in E$ and the weight $s_i^* = 1 - \sum_{e\in\delta(i)} x_e^*$ to each edge $\{d,i\}$ and call this weight function w.

Inequality (7.4) is violated if and only if there exists a cut $\delta_{G_d}(S)$ in the extended graph with respect to an odd set S, with a cut value less than $1 + 2y^*$ and $\mathring{u}, \mathring{w} \in S$, $\mathring{v}, \mathring{z} \notin S$ (or conversely). This holds since, with respect to the extended graph and the new edge weights w_e, inequality (7.19) can be re-written as

$$\sum_{e\in\delta_{G_d}(S)} w_e \geq 1 + 2y^*, \tag{7.20}$$

with $d \notin S$. To consider the additional restriction for S to (not) contain particular vertices, we construct another graph G_d^- from G_d by shrinking the vertices $\mathring{u}, \mathring{w}$ and $\mathring{v}, \mathring{z}$ to supernodes s and t, respectively. The construction of graph G_d^- is visualized in Figure 7.7.

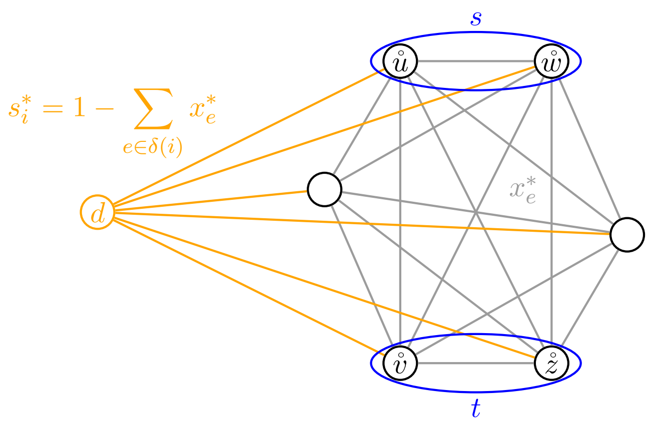


Figure 7.7: The graph G_d^- results from the extended graph G_d by shrinking the vertices $\mathring{u}, \mathring{w}$ to a supernode s and the vertices $\mathring{v}, \mathring{z}$ to a supernode t.

By this construction a violation of the $\wedge$-blossom inequality (7.4) is given if an even cut in G_d^- with s on the one side, t on the other and a value less than $1 + 2y^*$ exists. To test violation, either define the set $T := (V \setminus \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}) \cup \{s,t\}$ if $|V|$ is even, otherwise, if $|V|$ is odd, define the set $T := (V_d \setminus \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}) \cup \{s,t\}$, such that in both cases $|T|$ is even. Then, inequality (7.20) is violated if there exists an s-t T-even cut in G_d^- with a weight less than $1+2y^*$. The s-t T-even cut partitions the vertices of G_d^- into two subsets of even cardinality out of which the one is chosen which does not contain d. Then, after expansion of s and t, the resulting subset S has odd cardinality and satisfies either $\mathring{u}, \mathring{w} \in S$ and $\mathring{v}, \mathring{z} \notin S$ or $\mathring{v}, \mathring{z} \in S$ and $\mathring{u}, \mathring{w} \notin S$. Furthermore, it violates (7.20) and thus, a set S is found which violates a $\wedge$-blossom inequality (7.4).

To separate all possible constellations of the monomial vertices with $\mathring{e}_1, \mathring{e}_2 \in S$, this routine has to be carried out for two different fixings. Thus, the running time amounts to two times the running time needed to calculate an s-t T-even cut.

The clique-a inequalities

For a separation algorithm for the clique-a inequalities (7.17), the previous algorithm can be modified again. As in the formulation and the context of Theorem 7.2.5, we consider without loss of generality $\mathring{u}$ to be the vertex which is separated from $\mathring{v}, \mathring{w}$ and $\mathring{z}$. The other cases can be separated analogously. Remind that the clique-a inequalities in the considered case hold for subsets S of even cardinality with either a) $a, \mathring{u} \in S$ and $\mathring{v}, \mathring{w}, \mathring{z} \notin S$ or b) vice versa, and read

$$\sum_{e \in E(G[S])} x_e + x_{\mathring{v}a} + x_{\mathring{w}a} + x_{\mathring{z}a} + y \leq \frac{|S|}{2}.$$

The two cases a) and b) are combinable, i. e., if the inequality is violated in one of the cases, the separation algorithm returns a corresponding even subset S. Note that the clique-a inequality (7.17) depends on the choice of a, such that the following separation strategy has to be applied for all $a \in V \backslash \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$.

First, by the same arguments as in the derivation of the reformulation (2.13) for the separation of the linear blossom inequalities, we reformulate the clique-a inequalities (7.17) as

$$\sum_{i \in S} s_i + \sum_{e \in \delta(S)} x_e \geq 2x_{\mathring{v}a} + 2x_{\mathring{w}a} + 2x_{\mathring{z}a} + 2y. \tag{7.21}$$

For a given fractional solution $(x^*, y^*) \in [0,1]^{|E|+1}$ that satisfies the degree and the linearization inequalities we define the slack variables s_i^* and the extended graph G_d as in the previous subsection such that inequality (7.21) can be re-written as

$$\sum_{e \in \delta_{G_d}(S)} x_e^* \geq 2x^*_{\mathring{v}a} + 2x^*_{\mathring{w}a} + 2x^*_{\mathring{z}a} + 2y^*, \tag{7.22}$$

and a violation of the clique-a inequalities is given if and only if there exists a cut $\delta_{G_d}(S)$ for an even subset S not containing d, with $a, \mathring{u} \in S$ and $\mathring{v}, \mathring{w}, \mathring{z} \notin S$ or vice versa, and with a cut value less than $2x^*_{\mathring{v}a} + 2x^*_{\mathring{w}a} + 2x^*_{\mathring{z}a} + 2y^*$.

To guarantee the desired partition of the monomial vertices and a in $\delta_{G_d}(S)$, perform the following steps for each $b \in V \backslash \{a, \mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$. Shrink the vertices $a, \mathring{u}$ and the vertices $b, \mathring{v}, \mathring{w}, \mathring{z}$ to supernodes s and t, respectively. Denote the resulting shrunk graph with G_d^-. Furthermore, define the set $T := (V \backslash \{a, b, \mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}) \cup \{s, t\}$ if $|V|$ is even and define the set $T := (V_d \backslash \{a, b, \mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}) \cup \{s, t\}$ if $|V|$ is odd, such that $|T|$ again is even in both cases. Then, each s-t T-odd cut on the shrunk graph G_d^- partitions G_d^- into two subsets out of which the one which does not contain d is odd. After expanding the vertices s and t, this subset S becomes even with either $a, \mathring{u} \in S$ and $\mathring{v}, \mathring{w}, \mathring{z} \notin S$ or conversely, as desired. Thus, if for each fixed vertex b the value of the minimum s-t T-odd cut is not less than $2x^*_{\mathring{v}a} + 2x^*_{\mathring{w}a} + 2x^*_{\mathring{z}a} + 2y^*$, all clique-$a$ inequalities are satisfied by (x^*, y^*), otherwise one or more violating subsets S are found. The running time for this separation algorithm is $n - 5$ times the running time for the calculation of an s-t T-odd cut, since this has to be done for each $b \in V \backslash \{a, \mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$.

The nested blossom and the hourglass inequalities

For the remaining two classes of facet defining inequalities the proposed algorithms can be transferred analogously. By reconsidering the slack variables s_i, the nested blossom inequalities (7.12) can be rewritten as

$$\sum_{i\in T} s_i + \sum_{e\in\delta(T)} x_e - \underbrace{\sum_{i\in T}(x_{\mathring{u}i} + x_{\mathring{v}i})}_{(*)} \geq x_{\mathring{e}_2} - y.$$

For a given fractional solution $(x^*, y^*) \in [0,1]^{|E|+1}$ that satisfies the degree and the linearization inequalities, the extended graph G_d can be constructed similarly. To take account of the respective position of the monomial vertices with respect to the subset T, reasonable shrinking steps have to be added. Furthermore, the additional sum $(*)$ can be handled by slight changes in the construction of the weight function of G_d.

The hourglass inequalities (7.15) in turn can be reformulated as

$$\sum_{i\in S} s_i + \sum_{e\in\delta(S)} x_e \geq x_{\mathring{u}\mathring{v}} + x_{\mathring{u}a} + x_{\mathring{v}a} + x_{\mathring{w}\mathring{z}} + x_{\mathring{w}b} + x_{\mathring{z}b} - y - 2,$$

where the right hand side is a constant for a given solution $(x^*, y^*) \in [0,1]^{|E|+1}$ if the vertices a and b are fixed. Thus, the construction of the extended graph G_d has to be carried out for each pair of vertices $a, b \in V \backslash \{\mathring{u}, \mathring{v}, \mathring{w}, \mathring{z}\}$. It can be done similar to the construction for the other classes of inequalities.

7.4 Summary

In this chapter we investigated the matching problem with one quadratic term in the objective function. Although the matching problem is related to the assignment problem, the classification of facets of the corresponding polytope turned out to be much more complicated in the matching case, assuming that Conjecture 6.2.4 holds. Nonetheless we could classify several facets. The linear blossom inequalities remain facet defining in only some constellations but can be strengthened in two ways otherwise. On the one hand, if both monomial edges are in the blossom cut, an additional y-term yields the $\wedge$-blossom inequalities. On the other hand, if the blossom set S consists of exactly three of the four monomial vertices, the $\dot{\vee}$-blossom inequalities are obtained. The latter in turn are included in the nested blossom inequalities, which are a strengthened combination of two nested blossoms. Furthermore we could classify two classes which are based on cliques of even cardinality, the hourglass and the clique-a inequalities. For all of these new classes of facet defining inequalities we either presented detailed constructions for polynomial time separation routines or sketched out ideas for analogous constructions.

However we could show that all these constraints still do not yield an integral description of the polytope. In fact, further studies showed that there are several facet defining inequalities which remain unclassified so far. It seems that very different combinations of blossoms and even cliques, strengthened by product terms with large integral coefficients, can lead to facet defining inequalities. Thus, there is wide space for further research on this topic of matching problems with one quadratic term.

Chapter 8

Practical Results

In the previous sections, we could derive several facet defining inequalities with corresponding efficient separation algorithms for the polytopes obtained from adding and linearizing a single quadratic term to different optimization problems. Our ultimate motivation, however, is to solve the problems in the case where more or all quadratic terms are present in the objective function. Since all inequalities obtained in the case of a single quadratic term remain valid in this setting, we can apply our results to each quadratic term individually, one after another. By this we obtain separation algorithms for the general optimization problems.

Our aim in the following is to determine the impact of such a separation algorithm in terms of the bound improvement. For the minimum spanning forest and the minimum spanning tree problem with one quadratic term we succeeded in deriving a complete polyhedral description, which motivates to investigate at the example of these two problems. We implemented the devised separation algorithms for the quadratic subtour elimination constraints and embedded them into the branch-and-cut software SCIL [159]. We considered the basic spanning forest problem formulation using the constraints (4.2)–(4.4) where the subtour elimination constraints were separated dynamically and no further reformulation was applied (called *stdlin* in the following). For comparison, we then separated the quadratic subtour elimination constraints (4.9) and (4.10) for each of the appearing products (*qsec*). As it turns out that the constraints (4.10) often do not lead to a significant improvement, and since in many application we only have connected quadratic terms in the objective function, we also consider the separation approach only using the constraints (4.9), denoted by $qsec^c$.

We tested random graphs generated as in [49]. For a given number n and a given density d, we produce a random graph with n vertices and $\lfloor \binom{n}{2} d \rfloor$ edges. All edges obtain random integer coefficients in the range $\{1, \ldots, 10\}$. We consider instances where either all possible products of variables have non-zero coefficients or where only connected products are present. All non-zero quadratic coefficients are chosen either from $\{-100, \ldots, -1\}$ or $\{1, \ldots, 100\}$.

All experiments were carried out on Intel Xeon E5-2670 processors, running at 2.60 GHz with 64 GB of RAM. All computing times are stated in cpu seconds. We are mostly interested in the root gaps obtained (*rootgap*), computed as

$$\frac{OPT - rootDB}{|OPT|},$$

i. e. the relative difference between the optimal solution (OPT) and the dual bound (*rootDB*) in the root node of the branch-and-bound tree, and in the number of subproblems that have to be enumerated to solve the instance to optimality (*# subs*). These two values indicate the strength of the additional cutting planes. Moreover, we report the time needed for separation (*septime*), the total time needed to solve the instance to optimality (*cputime*), and the total number of LPs to be solved (*# LPs*). All lines in the following tables report average results over 10 random instances.

We start by considering the spanning forest problem. As the case of positive coefficients of the quadratic terms is trivial then, we consider only instances with quadratic coefficients in $\{-100, \ldots, -1\}$. When only connected product terms are present in the original instance, as is the case for typical applications involving reload or changeover costs, we obtain the results summarized in Table 8.1. The results show that the new inequalities can improve the root gap significantly with respect to the standard linearization for instances on sparse graphs. For denser graphs, the improvement in the root gap is much smaller, but the number of subproblems to be enumerated is still decreased significantly, showing that the new inequalities are effective in deeper levels of the enumeration tree. Nevertheless, the separation time remains small compared to the total time. In summary, this results in a decrease of computational times for all instances considered.

When considering instances with all quadratic terms having non-zero coefficients, our results are weaker in general, see Table 8.2. While the root gaps are only slightly improved, the number of subproblems can still be decreased by adding both inequalities for the connected and the disconnected quadratic terms. However, while the former also lead to a slight improvement in terms of computational times, the latter lead to longer times due to the higher computational effort of separation. Also the gap improvement obtained by adding the latter inequalities is very small even for sparse instances, which suggests that the constraints of type (4.9) are much more effective in practice than those of type (4.10).

We next investigate quadratic spanning trees. Then also the case of positive quadratic coefficients is non-trivial. However, by Proposition 4.3.4, we cannot expect to obtain any improvement in this case by adding constraints of type (4.9) or (4.10). For this reason, we reformulate the cardinality constraint (4.5) in a quadratic fashion: we add the constraint

$$\sum_{e,f \in E, e \neq f} y_{ef} = \binom{|V|-1}{2} \tag{8.1}$$

to our linear problem formulation. This constraint fixes the sum of all product variables, so that the signs of the corresponding coefficients become irrelevant. Note that this additional constraint has a positive impact on bounds even if added to the standard linearization. Whenever adding (8.1) to our model, we denote this by *qref* in our tables.

In Tables 8.3 and 8.4, we state the results for the cases of negative and positive quadratic coefficients, respectively. The results in the first case turn out to be much better than those obtained for QMSF. However, this improvement is apparent in all methods and partly due to the reformulation qref. Indeed, when comparing different methods, the relative behaviour is very similar to the QMSF case. Comparing positive and negative coefficients, it turns out that the latter case is slightly easier to solve than the former, but the difference is comparably small.

To conclude, we also tested our approach on the original instances of Cordone and Passeri [49]. For given $n = 10, 15, 20$ and given density $d = 33, 67, 100$, we have coefficient ranges $\{1, \ldots, 10\}$ or $\{1, \ldots, 100\}$ for linear and quadratic variables in each combination, leading to four different instances per row. Results are given in Table 8.5. Of course our method cannot achieve the same computational times as the approach presented in [49]. However, just by separating our constraints (4.9) and the quadratic reformulation (8.1), we can solve 18 of these instances within the time limit of 5 hours.

Summarizing we can state that our approach yields significant improvements considering the root gaps and thus an improvement of the polyhedral description. Of course this approach in itself is not able to – and not meant to – compete with tailored, fully-fletched approaches to the quadratic spanning tree problem presented recently in the literature. However, it can be combined with any other linearization-based approach, leading to improved bounds and thus to faster computational times if applied carefully.

vertices	density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin	1.00	2.00	0.00	0.00	0.00 %
		+qsec^c	1.00	2.00	0.00	0.00	0.00 %
	30%	stdlin	20.40	23.10	0.01	0.00	31.01 %
		+qsec^c	8.20	12.70	0.01	0.00	17.30 %
	40%	stdlin	62.60	63.90	0.05	0.00	47.73 %
		+qsec^c	26.20	34.00	0.05	0.01	41.06 %
	50%	stdlin	308.20	284.50	0.35	0.01	69.61 %
		+qsec^c	128.20	149.70	0.41	0.07	63.25 %
12	20%	stdlin	7.20	8.30	0.00	0.00	12.65 %
		+qsec^c	3.20	5.30	0.00	0.00	4.75 %
	30%	stdlin	64.20	62.70	0.04	0.00	38.71 %
		+qsec^c	27.40	33.80	0.04	0.01	31.52 %
	40%	stdlin	358.20	317.20	0.45	0.04	57.46 %
		+qsec^c	112.80	141.60	0.38	0.08	52.26 %
	50%	stdlin	1473.80	1396.90	3.90	0.16	72.68 %
		+qsec^c	606.40	683.00	3.64	0.68	68.58 %
14	20%	stdlin	22.40	26.30	0.01	0.00	19.53 %
		+qsec^c	8.00	12.50	0.01	0.00	11.74 %
	30%	stdlin	328.40	327.40	0.47	0.04	47.30 %
		+qsec^c	124.00	155.70	0.41	0.10	40.87 %
	40%	stdlin	3138.20	3126.90	8.81	0.52	71.56 %
		+qsec^c	1102.20	1331.10	7.42	1.42	68.66 %
	50%	stdlin	9921.80	9340.20	59.57	2.09	72.08 %
		+qsec^c	3864.00	4022.80	59.43	8.63	70.13 %
16	20%	stdlin	90.80	90.20	0.08	0.01	24.95 %
		+qsec^c	27.00	38.20	0.05	0.01	15.92 %
	30%	stdlin	3472.80	3348.40	8.51	0.65	64.03 %
		+qsec^c	977.60	1333.90	5.93	1.25	59.05 %
	40%	stdlin	20305.20	20690.90	139.12	5.06	72.46 %
		+qsec^c	7327.00	8708.60	124.09	17.76	69.64 %
	50%	stdlin	94662.60	92729.60	1673.11	25.54	81.54 %
		+qsec^c	31323.40	34508.20	1402.86	125.14	79.53 %
18	20%	stdlin	289.40	277.40	0.46	0.05	31.92 %
		+qsec^c	82.00	109.20	0.28	0.07	26.02 %
	30%	stdlin	5760.00	6283.50	30.13	1.64	48.52 %
		+qsec^c	2132.00	2685.50	22.34	5.12	44.89 %
20	20%	stdlin	1056.40	1072.80	2.58	0.26	38.32 %
		+qsec^c	318.40	431.80	1.62	0.53	33.12 %
	30%	stdlin	130753.40	138239.90	2582.81	50.28	67.01 %
		+qsec^c	38619.40	47254.30	935.33	151.21	63.67 %

Table 8.1: Results for spanning forests with negative coefficients on connected terms; each line reports averages over ten random instances

vertices	density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin	1.00	2.00	0.00	0.00	0.00 %
		+qsec^c	1.00	2.00	0.00	0.00	0.00 %
		+qsec	1.00	2.00	0.00	0.00	0.00 %
	30%	stdlin	65.40	56.90	0.07	0.01	31.49 %
		+qsec^c	42.00	40.90	0.07	0.01	23.70 %
		+qsec	33.40	37.80	0.10	0.02	23.33 %
	40%	stdlin	767.60	683.50	1.67	0.05	72.10 %
		+qsec^c	494.00	482.60	1.59	0.09	68.85 %
		+qsec	465.60	481.20	2.69	0.43	68.85 %
	50%	stdlin	6690.80	6569.40	37.33	0.48	123.55 %
		+qsec^c	4153.00	4410.30	32.03	1.28	118.88 %
		+qsec	3780.20	4204.50	53.00	6.12	118.88 %
12	20%	stdlin	8.80	11.00	0.01	0.00	4.55 %
		+qsec^c	4.60	6.40	0.01	0.00	1.72 %
		+qsec	2.60	4.50	0.01	0.00	1.34 %
	30%	stdlin	941.20	865.80	3.11	0.06	55.32 %
		+qsec^c	635.80	634.50	2.84	0.14	51.32 %
		+qsec	570.00	615.40	4.59	0.87	51.29 %
	40%	stdlin	20128.00	19650.60	179.53	1.97	101.70 %
		+qsec^c	12729.00	13399.10	155.41	5.21	98.44 %
		+qsec	11191.40	12627.90	244.01	29.83	98.44 %
14	20%	stdlin	126.20	121.20	0.30	0.01	19.99 %
		+qsec^c	90.20	77.60	0.27	0.01	15.84 %
		+qsec	66.40	71.30	0.42	0.12	15.12 %
	30%	stdlin	23322.20	22434.80	241.62	2.73	77.96 %
		+qsec^c	15781.00	15969.10	212.94	6.77	74.17 %
		+qsec	13288.80	15035.90	336.70	45.75	74.15 %
16	20%	stdlin	1858.40	1691.80	10.98	0.23	36.53 %
		+qsec^c	1194.60	1116.70	8.77	0.39	32.23 %
		+qsec	1026.80	1102.60	14.69	3.73	31.92 %
18	20%	stdlin	64032.60	61917.50	1126.54	10.80	57.08 %
		+qsec^c	43881.40	45018.20	1069.21	23.64	54.72 %
		+qsec	40006.40	43786.40	1763.52	233.87	54.64 %

Table 8.2: Results for spanning forests with negative coefficients on all terms; each line reports averages over ten random instances

vertices	density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin +qref	1.00	2.00	0.00	0.00	0.00 %
		+qsec^c+qref	1.00	2.00	0.00	0.00	0.00 %
		+qsec +qref	1.00	2.00	0.00	0.00	0.00 %
	30%	stdlin +qref	7.20	9.10	0.01	0.00	2.81 %
		+qsec^c+qref	5.40	8.40	0.03	0.00	1.79 %
		+qsec +qref	5.00	8.10	0.01	0.00	1.62 %
	40%	stdlin +qref	93.20	93.90	0.28	0.01	18.99 %
		+qsec^c+qref	75.00	85.10	0.31	0.01	18.39 %
		+qsec +qref	74.20	85.60	0.30	0.04	18.39 %
	50%	stdlin +qref	320.00	309.00	2.01	0.03	25.48 %
		+qsec^c+qref	264.60	300.80	1.78	0.08	24.57 %
		+qsec +qref	253.60	296.60	1.97	0.30	24.57 %
12	20%	stdlin +qref	1.40	3.90	0.00	0.00	0.06 %
		+qsec^c+qref	1.00	3.20	0.00	0.00	0.00 %
		+qsec +qref	1.00	3.10	0.01	0.00	0.00 %
	30%	stdlin +qref	103.20	100.60	0.41	0.01	14.64 %
		+qsec^c+qref	80.20	81.90	0.42	0.02	13.93 %
		+qsec +qref	75.80	80.20	0.45	0.09	13.86 %
	40%	stdlin +qref	1041.00	934.70	9.24	0.08	25.34 %
		+qsec^c+qref	852.60	909.20	8.27	0.28	24.81 %
		+qsec +qref	825.60	919.70	9.64	1.73	24.81 %
	50%	stdlin +qref	3186.00	3088.60	68.95	0.47	27.55 %
		+qsec^c+qref	2636.00	3101.20	61.10	1.35	27.30 %
		+qsec +qref	2707.00	3191.70	68.15	8.56	27.30 %
14	20%	stdlin +qref	10.40	13.00	0.04	0.00	1.81 %
		+qsec^c+qref	7.60	10.10	0.04	0.00	1.38 %
		+qsec +qref	7.20	10.10	0.05	0.02	1.32 %
	30%	stdlin +qref	1619.20	1570.30	18.38	0.19	24.47 %
		+qsec^c+qref	1245.40	1344.50	15.24	0.39	23.71 %
		+qsec +qref	1215.40	1353.10	17.77	3.14	23.69 %
	40%	stdlin +qref	11139.60	10738.60	329.38	2.04	29.81 %
		+qsec^c+qref	9074.00	10699.70	291.47	6.47	29.60 %
		+qsec +qref	8775.20	10628.00	328.23	44.66	29.60 %
	50%	stdlin +qref	47158.00	46778.60	3566.61	11.04	31.87 %
		+qsec^c+qref	38313.00	46052.40	2948.17	40.41	31.77 %
		+qsec +qref	37098.40	45462.00	3141.08	281.16	31.77 %
16	20%	stdlin +qref	110.00	102.30	0.77	0.01	6.99 %
		+qsec^c+qref	94.60	91.30	0.75	0.03	6.41 %
		+qsec +qref	81.40	87.40	0.95	0.28	6.36 %
	30%	stdlin +qref	17712.20	16830.00	547.16	3.35	29.66 %
		+qsec^c+qref	14413.40	16305.90	474.70	9.52	29.21 %
		+qsec +qref	14446.40	16675.70	542.13	85.00	29.21 %
18	20%	stdlin +qref	3913.60	3763.10	72.69	0.66	18.61 %
		+qsec^c+qref	3286.00	3241.00	65.59	1.53	18.18 %
		+qsec +qref	3187.20	3275.30	76.48	14.33	18.17 %
20	20%	stdlin +qref	29314.00	26738.60	1083.51	6.87	22.90 %
		+qsec^c+qref	24940.60	24314.30	950.09	17.09	22.52 %
		+qsec +qref	23675.20	24371.10	1095.19	184.61	22.52 %

Table 8.3: Results for spanning trees with negative coefficients on all terms; each line reports averages over ten random instances

vertices	density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin +qref	1.00	2.00	0.00	0.00	0.00 %
		+qsec^c+qref	1.00	2.00	0.00	0.00	0.00 %
		+qsec +qref	1.00	2.00	0.00	0.00	0.00 %
	30%	stdlin +qref	12.00	12.90	0.02	0.00	3.09 %
		+qsec^c+qref	9.60	11.10	0.02	0.00	2.68 %
		+qsec +qref	8.40	11.60	0.04	0.01	2.64 %
	40%	stdlin +qref	53.80	49.90	0.14	0.00	18.56 %
		+qsec^c+qref	45.40	49.90	0.17	0.01	17.87 %
		+qsec +qref	49.00	53.10	0.22	0.04	17.87 %
	50%	stdlin +qref	249.00	211.20	1.30	0.02	31.07 %
		+qsec^c+qref	209.00	218.40	1.23	0.04	30.64 %
		+qsec +qref	199.40	223.80	1.43	0.22	30.64 %
12	20%	stdlin +qref	1.20	3.10	0.00	0.00	0.03 %
		+qsec^c+qref	1.20	3.10	0.00	0.00	0.03 %
		+qsec +qref	1.00	2.70	0.01	0.00	0.00 %
	30%	stdlin +qref	83.60	73.70	0.35	0.00	14.68 %
		+qsec^c+qref	58.60	61.80	0.28	0.02	13.19 %
		+qsec +qref	59.00	62.70	0.38	0.11	13.15 %
	40%	stdlin +qref	507.20	429.00	4.11	0.06	29.55 %
		+qsec^c+qref	381.60	403.90	3.66	0.12	28.79 %
		+qsec +qref	385.40	418.60	4.18	0.68	28.79 %
	50%	stdlin +qref	2220.40	1973.30	42.57	0.24	38.30 %
		+qsec^c+qref	1728.40	2023.70	37.99	0.76	37.79 %
		+qsec +qref	1709.80	2039.60	40.95	4.32	37.79 %
14	20%	stdlin +qref	5.60	8.70	0.03	0.00	1.07 %
		+qsec^c+qref	5.40	7.70	0.03	0.00	0.70 %
		+qsec +qref	4.80	7.90	0.05	0.01	0.64 %
	30%	stdlin +qref	867.80	801.50	9.11	0.10	29.04 %
		+qsec^c+qref	750.40	756.10	8.30	0.24	28.37 %
		+qsec +qref	713.60	774.10	9.78	1.80	28.37 %
	40%	stdlin +qref	9603.60	8968.90	279.73	1.55	39.89 %
		+qsec^c+qref	8116.60	8924.50	246.27	4.46	39.50 %
		+qsec +qref	7797.00	9071.10	265.74	27.56	39.50 %
	50%	stdlin +qref	35372.40	33993.00	2705.89	7.08	46.05 %
		+qsec^c+qref	29163.40	35036.70	2160.54	24.29	45.82 %
		+qsec +qref	28799.60	35463.50	2269.69	171.40	45.82 %
16	20%	stdlin +qref	83.40	82.30	0.67	0.02	7.03 %
		+qsec^c+qref	59.80	66.60	0.55	0.02	6.32 %
		+qsec +qref	56.00	65.30	0.75	0.19	6.28 %
	30%	stdlin +qref	12745.00	11304.90	356.06	2.29	37.61 %
		+qsec^c+qref	10495.20	11130.20	318.35	5.62	36.98 %
		+qsec +qref	10602.80	11499.10	361.48	51.18	36.98 %
18	20%	stdlin +qref	1444.60	1258.70	22.37	0.27	19.43 %
		+qsec^c+qref	1089.00	1067.30	19.10	0.57	18.68 %
		+qsec +qref	1028.20	1095.30	24.85	5.90	18.67 %
20	20%	stdlin +qref	13318.40	11128.30	439.46	3.15	26.59 %
		+qsec^c+qref	10307.60	10218.80	366.25	7.21	25.97 %
		+qsec +qref	9590.20	10359.60	447.28	81.86	25.96 %

Table 8.4: Results for spanning trees with positive coefficients on all terms; each line reports averages over ten random instances

vertices	density	sep	solved	# subs	# LPs	cputime	septime	rootgap
10	33%	+qsec^c+qref	4	4.00	5.25	0.02	0.00	1.31 %
	67%	+qsec^c+qref	4	867.50	922.75	12.63	0.26	34.74 %
	100%	+qsec^c+qref	4	2803.50	3503.75	197.79	2.06	43.96%
15	33%	+qsec^c+qref	4	5432.50	6226.25	146.38	2.46	33.57 %
	67%	+qsec^c+qref	1	*3781.00*	*4231.00*	*1075.26*	*7.96*	*21.33 %*
	100%	+qsec^c+qref	0	-	-	-	-	-
20	33%	+qsec^c+qref	1	*80969.00*	*99098.00*	*16014.59*	*203.46*	*24.14 %*
	67%	+qsec^c+qref	0	-	-	-	-	-
	100%	+qsec^c+qref	0	-	-	-	-	-

Table 8.5: Results for instances of Cordone and Passeri [49]

Conclusions

The aim of this thesis is to establish a new polyhedral approach for quadratic combinatorial optimization problems. It is based on the idea of not considering all product terms simultaneously but only a single product term at a time; assuming that the underlying linear problem is tractable, the same is true for optimizing the problem with one quadratic term, given by case distinction on the four possible fixings of the two product variables. Furthermore, from a theoretical point of view, the corresponding separation problem is tractable, too, since separation and optimization are equivalent in terms of complexity. To make such a theoretical approach practical and abandon the dependency on an abstract optimization oracle, one needs to consider specific underlying optimization problems. Thus, the idea of this thesis is to investigate the facetial structures of concrete problems, finding good polyhedral descriptions and to develop concrete separation algorithms.

The first of the here considered optimization problems are the minimimum spanning forest and the minimum spanning tree problem. Depending on the connectedness of the edges which correspond to the quadratic term, two different cases, the connected and the disconnected case, needed to be considered. For both cases we present a new class of facet defining inequalities, the quadratic subtour elimination constraints, which are highly related to the linear ones. If the monomial edges are connected, the quadratic subtour elimination constraints strengthen a subclass of the linear ones by an additional y-term. Otherwise, if the monomial edges are disconnected, the quadratic subtour elimination constraints can be seen as the sum of two linear ones, also strengthened by the additional y-term. The main result in this chapter is the complete polyhedral description of the polytopes corresponding to the minimum spanning forest and the minimum spanning tree problem with one quadratic term. We showed that, in addition to the standard linearization and the constraints which are needed for the description of the two linear polytopes, the quadratic subtour elimination constraints indeed suffice to obtain a complete description of the polytopes corresponding to the problems with one quadratic term. To make these results applicable in practice we devised two efficient separation algorithms, one for the connected and one for the disconnected case.

In connection with this we afterwards showed that a transfer of our positive results from the spanning forest and the spanning tree problem to the corresponding directed versions, the branching and the arborescence problem, is only partially possible. One the one hand we showed that the quadratic subtour elimination constraints and the corresponding separation algorithms are one-to-one transferrable. However, we also introduced another new facet class, the tail-in constraints, and created an example which showed that there still exist fractional solutions which are not in the integral hull but which are not cut off by all considered constraints. Thus, we had to assert that the classified constraints do not suffice to obtain an integral description of the polytopes corresponding to the branching and the arborescence problem with one quadratic term and that the results from the undirected cases are not completely transferrable to the directed cases.

Further positive results have been obtained when investigating the minimum assignment problem with one quadratic term. We classified exponentially many facet defining constraints, the $\wedge$-clique and the $\vee$-clique inequalities. In particular we discovered the surprising fact that, although the problem complexity remains polynomial, the addition of one product term can increase the number of facets of the polyhedron from polynomial to exponential. However, we derived two efficient separation algorithms and establish the significant conjecture that these two inequality classes indeed yield a complete description of the polytope corresponding to the assignment problem with one quadratic term.

Last but not least we analyzed the maximum matching problem with one quadratic term, which seems to be the hardest one in terms of a polyhedral description. We classified several new facet defining constraints, i. e. the $\wedge$-blossom, the $\dot{\vee}$-blossom and the nested blossom inequalities, the hourglass and the clique-a inequalities but, however, we also created an example where we showed that this variety of constraints does not suffice to yield a complete description of the corresponding polytope. Nonetheless we presented polynomial time separation routines for a practical application.

To verify that the idea of individually considering single quadratic terms also has a practical impact, we computationally tested the influence of the new constraints containing one product term in the cases of quadratic spanning forests and spanning trees. For this, we embedded the quadratic subtour elimination constraints into a branch-and-cut scheme. Indeed we obtained significant improvements of the root gaps and the LP-bounds, particularly in the connected case and when the underlying graph structure is sparse.

Summarizing, we can state that the approach of considering only one quadratic term at a time yielded a deeper insight into the polyhedral structure and the dependency of monomials and subgraphs. We could not only derive interesting theoretical results concerning structures and numbers of facets and information about complete descriptions, but also verify the practical impact of the new inequalities on the example of the quadratic minimum spanning forest and the quadratic minimum spanning tree problem. However, there remain some open questions. The most interesting questions are obviously the missing complete polyhedral descriptions, in the cases of quadratic branchings, arborescences and matchings, but of course especially in the assignment case, where we conjecture that we already classified all facets. To determine the impact of the new constraint classes, further experimental studies are necessary.

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