HIGHER-ORDER CONTINUOUS FORMULATIONS FOR DISCRETE OPTIMIZATION PROBLEMS

A Dissertation

by

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ABSTRACT

This dissertation is focused on the developing a set of novel mathematical programming formulations for a class of problems related to community detection in networks. The proposed approach is based on the extension of quadratic formulations that were proposed by Motzkin and Strauss in 1967. These formulations are related to the Maximum Clique problem, which asks to find the largest complete subgraph. The main result is the establishing of a family of higher-order polynomial optimization problems which exhibits a hierarchical structure of local and global optima, different from previously known hierarchies in the field of optimization. Additional results obtained include a tighter description for the set of local and global maxima of the proposed formulations, improving the previously obtained results for the original Motzkin-Strauss problem as a side-result. The second part of the thesis is dedicated to a discussion on the regularized version of the proposed formulations, analogous to what was established by Bomze in 1997 for the original Motzkin-Strauss formulation. We discuss the required properties of the regularization and analyze the different options regarding the selection of the regularization term. A set of conditions is established for the regularization term, so that the required properties are satisfied. Finally, a set of computational experiments is presented to evaluate the performance of the proposed formulations over the set of standard benchmarks.

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NOMENCLATURE

LP	Linear Program
IP	Integer Program
QP	Quadratic Program
M-S	Motzkin-Strauss Formulation
MSQP	Motzkin-Strauss Quadratic Program
BR	Bomze's Quadratically Regularized Motzkin-Strauss Polynomial Program
GR	Hungerford and Rinaldi Φ-Regularized Motzkin-Strauss Polynomial Program
MSPP	Motzkin-Strauss Polynomial Program
QR	Quadratically Regularized Motzkin-Strauss Polynomial Program
PR	Polynomially Regularized Motzkin-Strauss Polynomial Program
$\mathbf{P}^k$	An instance of MSPP of order k
$\mathbf{P}^{k,\Phi}$	An instance of General Regularized Motzkin-Strauss Polynomial Program of order k given regularization function Φ
$\mathbb{R}^n$	Euclidean space of n dimensions
$\mathbb{R}^n_{\geq 0}$	Positive orthant of $\mathbb{R}^n$
2^S	Power set of S, set of all subsets of S
$\binom{S}{k}$	A set of subsets of a set S of size $k \in \mathbb{Z}_+$
$\|S\|$	cardinality of the set S
Δ^n	A standard simplex of dimension n
$S(x)$	The support of x
$[n]$	Range, a set of integers from 1 to n
0_n	An all-zero vector of size n

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1. INTRODUCTION

It is widely known that some problems, whose structure appears to be fairly simple, can be extremely hard to solve under the modern computational framework. The most widely commonly known examples of such problems are the ones from complexity class NP and its subclass NP-complete (or NPC) [1]. Informally, NP is a class of problems for which a solution is easy to verify but hard to obtain. Moreover, being able to solve a specific NP-complete problem fast-enough would guarantee that any other problem from NP class can also be solved fast. The classical examples of such problems are Knapsack problem, Vertex Cover problem, and Clique problem.

Last two examples represent problems from Graph Theory, a fruitful field of Discrete Mathematics, which was first introduced by Leonard Euler back in 1735 with a famous Köningsberg bridges problem [2]. He used the idea of analyzing a structure consisting of nodes connected with edges to answer if it is possible to visit every island and bridge in Köningsberg, while only crossing each bridge once. The answer to this question turned out to be negative, and since then this nodes-and-edges framework has been extensively applied to real-life problems. Most commonly, applications of Graph Theory arise when describing transportation networks [3], where nodes represent transportation terminals, warehouses, depots and other locations of interest, such as power plants [4], while edges model connections between them, such as roads, airline routes [5], or power-lines. Another example are social networks [6], where nodes represent social entities, such as people or communities, while arcs represent the relationships between them. Some other examples are neural networks of living beings [7], financial networks [8], graph-theoretic models in linguistics [9] and so on [10].

One of the directions of Graph Theory is community detection problems [11]. In these problems, researches are interested in inferring some communal relationship from the network provided. For example, the Six degree of separation problem [12], perhaps more widely known as Six handshakes rule, suggests that and two people are at most six social connections away from each other. Technically, this problem asks to verify if the social network of all humanity is a 6-

club. Community detection problems (also known as clustering problems) are quite commonly constructed based on the concept of a clique, which represents the most tightly-knit group possible: each node is connected to every other node. Of course, such conditions are often too extreme [11], so it makes sense to employ less restrictive structures, which are, nevertheless, originate from cliques. Such structures are called clique relaxations and, as it was shown, the problem of finding such structures can often be reformulated in terms of finding cliques in some transformed graph. This motivates us to study cliques in depth and detail.

The maximum clique problem is a classical optimization problem [13] which asks to find the largest clique in a given graph. Some of the most theoretically interesting and computationally successful approaches to this problem are based on the Motzkin-Straus formulation, expressing the clique number in terms of the maximal value of a standard quadratic program [14]. This quadratic program is known as Motzkin-Strauss Quadratic Program, or MSQP, and it was proposed in 1967 as a mean to provide an alternative proof for Turán's graph theorem, which establishes an upper bound on the clique number of a graph (i.e., the size of the maximum clique of a graph) as a function of the number of edges and vertices of the graph. In 1990's, MSQP gained attention from the global optimization community [15], [16], [17], which lead to a series of results characterizing the combinatorial structure of local and global optima of MSQP. Additionally significant developments in quadratic optimization, copositive programming [18], and complexity in nonlinear optimization were motivated by the study of this problem.

1.1 Preliminaries

In section 1.2 we present the summary of contributions of this thesis. To ensure that the reader is familiar with the basic concepts, terminology and notation used in the discussion that follows, in this section we introduce the necessary concepts and results regarding the Graph Theory and Mathematical Optimization.

Set notation

Throughout this proposal we will be working with finite sets only. Sets are denoted using capital latin letters, e.g: V, E, S. For a positive integer k, a range k is $[k] := \{1, 2, \ldots, k\}$. Given a set S, $|S|$ denotes the cardinality of the set S, i.e. the number of elements present in the set. We will assume the existence of a naive order (or enumeration) for any given set S, a bijective function o: $S \to [|S|]$. We will implicitly assume a one-to-one correspondence between set elements and positive integer number from here on, i.e., we will assume any set S consists of integers: $S := \{1, 2, \ldots, |S|\} = [|S|]$, unless specifically stated otherwise.

For a subset C of a set S, an indicator vector $x_C \in \mathbb{R}^{|S|}$ is defined as

$$x_i = \begin{cases} 1, & i \in C, \\ 0, & i \notin C, \end{cases} \qquad i \in S. \tag{1.1}$$

Note that x_C is a vertex of a standard hypercube of dimension $|S|$. Correspondingly, a characteristic vector x^C is defined as a normalized indicator vector, $x^C := \frac{1}{|C|} x_C$. Again, note that x^C is a vertex of a *standard simplex* $\Delta^{|S|}$ of dimension $|S|$, defined as:

$$\Delta^n := \left\{ x \in \mathbb{R}^n \mid \sum_{i=1}^{n} x_i = 1, x_i \geq 0, i \in [n] \right\}. \tag{1.2}$$

For a set S and a non-negative integer k, by $\binom{S}{k}$ we denote a set of all subsets of S of size k. Specifically,

$$\binom{S}{k} := \left\{ C \in 2^S \mid |C| = k \right\}, \tag{1.3}$$

where 2^S is the power set of S, i.e., a set of all subsets of S. Note that

$$\binom{S}{0} = \{\emptyset\}, \quad \binom{S}{|S|} = \{S\}, \quad \left| \binom{S}{k} \right| = \binom{|S|}{k}. \tag{1.4}$$

Given a set S and a vector $x \in \mathbb{R}^{|S|}$, *the support* $S(x) \subseteq S$ is defined as

$$S(x) \coloneqq \{i \in S \mid x_i \neq 0\}. \tag{1.5}$$

Given a vector x in $R^{|V|}$, a subset product $\pi_C(x)$, where $C \subseteq V$, is defined as

$$\pi_C(x) \coloneqq \prod_{i \in C} x_i. \tag{1.6}$$

1.1.1 Graph theory terminology

This thesis heavily relies on the concepts of from Graph Theory. The basic concepts are *vertices* and *edges*. Interchangeably, term *node* can be used to denote vertices and term *arc* to denote edges. We will use the former vocabulary, however, in literature, the reader might encounter the latter.

A *graph* is a pair of sets, vertex set and edges set, and is denoted as $G = (V, E)$, where V is the vertex set and E is the edge set. We will only consider finite simple undirected graphs, so $V = \{v_1, v_2, \dots, v_n\}$ is a set of n nodes, while $E \subset \binom{V}{2}$ is a set of edges (unordered pairs of vertices). The number of edges of a given graph G is usually denoted by $m(G) \coloneqq |E|$. We will refer to $m(G)$ as m when the graph is clear from the context.

Given an edge $e = \{u, v\} \in E$, we say that u and v are *adjacent* or *neighbor*, while the edge e is *incident* to u and v. The set of all vertices adjacent to a given vertex $v \in V$ is called the *neighborhood* of v and is denoted as $N_G(v) \coloneqq \{u \mid \{u, v\} \in E\}$. When it is convenient and the graph is clear from the context, G is dropped from the notation, shortening it to $N(v)$.

For a vertex v in graph G, a degree of v is defined as the size of the neighborhood of v in G: $d_G(v) \coloneqq |\mathrm{N}(N_G(v))|$. The minimum and maximum degree of a given graph are defined as $\delta(G) \coloneqq \min_{v \in V} d_G(v)$ and $\Delta(G) \coloneqq \max_{v \in V} d_G(v)$ respectively.

A graph $G' = (V', E')$ is called a *subgraph* of graph G if $V' \subseteq V$ and $E' \subseteq \binom{V'}{2} \cup E$. Given a subset of vertices $V' \subseteq V$, an *induced subgraph* $G[V'] = (V', E[V'])$ is the graph obtained from G by removing vertices that are not in V' and any edges incident to those vertices: $E[V'] \coloneqq \binom{V'}{2} \cup E$.

For a graph G, A_G denotes its *adjacency matrix* $(a_{i,j})_{i,j\in V}$ defined as

$$a_{i,j} \coloneqq \begin{cases} 1, & \{i,j\} \in E, \\ 0, & \{i,j\} \notin E, \end{cases} \quad i,j \in V. \tag{1.7}$$

For a subset U of V, the neighborhood of U in G is defined as

$$N_U \coloneqq \{v \in V \mid \{v, u_i\} \in E \; \forall u_i \in U\}, \tag{1.8}$$

i.e., it is the set of vertices in V that are adjacent to every vertex in U. Note that, by definition, $N_U \cap U = \emptyset$, as $\{u, u\} \notin E$ for any $u \in V$, as G is a simple graph.

Given a vector $x \in \mathbb{R}^n$, we will occasionally refer to the support $S(x)$ as the set of vertices corresponding to x.

1.1.2 Clique and related concepts

The following special cases of graphs (or subgraphs) are of a major interest in network analytics:

Definition 1 (Clique)**.** *Given a graph $G = (V, E)$, we say that G is a clique (a complete graph) if $E = \binom{V}{2}$.*

For a graph G, we will say that $\mathcal{C}_k(G)$ is a set of all cliques of cardinality k in graph G. We assume that the empty set is the only clique with zero vertices. Note that $\mathcal{C}_2(G) = E$. When G is clear from the context, we will use the shortened notation $\mathcal{C}_k \coloneqq \mathcal{C}_k(G)$. Additionally, given two sets $U = \{u_1, u_2, \ldots u_p\} \subseteq V$ and $W = \{w_1, w_2, \ldots, w_t\} \subseteq V$ we define a set of restricted cliques or cardinality k in G as

$$\mathcal{C}^U_{k;W} \coloneqq \mathcal{C}^{u_1,\ldots,u_p}_{k;w_1,\ldots,w_t} \coloneqq \mathcal{C}_k(N_U \setminus W).$$

That is, both $\mathcal{C}^U_{k;W}$ and $\mathcal{C}^{u_1,\ldots,u_p}_{k;w_1,\ldots,w_t}$ denote the set of all cliques consisting of k vertices that are adjacent to every vertex in $U = \{u_1, \dots, u_p\}$ and containing no vertex from $W = \{w_1, \dots, w_t\}$. If $U = \emptyset$ or $W = \emptyset$, we will use the notations

$$\mathcal{C}_{k;W} := \mathcal{C}_{k;w_1,\dots,w_t} := \mathcal{C}_k(V \setminus W) \quad \text{and} \quad \mathcal{C}_k^U := \mathcal{C}_k^{u_1,\dots,u_p} := \mathcal{C}_k(N_U), \tag{1.9}$$

respectively. The introduced notations allow us to invoke various alternative representations of $\sum\limits_{C \in \mathcal{C}_k} \pi_C(x)$ using a set of one or more vertices in our derivations. For example, by observing that for any vertex v the set $\mathcal{C}_k$ of k-vertex cliques is a disjoint union of $\{C \cup \{v\} \mid C \in \mathcal{C}_{k-1}^v\}$ and $\mathcal{C}_{k;v}$, we obtain the following representation:

$$\sum_{C \in \mathcal{C}_k} \pi_C(x) = x_v \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x) + \sum_{C \in \mathcal{C}_{k;v}} \pi_C(x). \tag{1.10}$$

Definition 2 (Multipartite graph)**.** *Given a graph $G = (V, E)$, we say that G is a multipartite graph with p parts if there exists a partition of V into p non-empty sets P_1, P_2, $\dots$, P_p, such that*

$$E \subseteq \binom{V}{2} \setminus \bigcup_{i=1}^{p} \binom{P_i}{2}.$$

A concept closely related to a clique is *complete multipartite graph*, also referred to as a *multi-clique*. Among all multipartite graphs on the same set of parts, the one with the most possible number of edges is called a multi-clique. For a multi-clique, any two vertices from two different parts are necessarily adjacent.

Definition 3 (Multi-clique)**.** *Given a graph $G = (V, E)$, we say that G is a multi-clique with p parts (a p-partite clique) if G is a multipartite graph with p parts $P_1, P_2, \dots, P_p \subset V$ and*

$$E = \binom{V}{2} \setminus \bigcup_{i=1}^{p} \binom{P_i}{2}.$$

Clearly, a clique is a special case of a multi-clique, when each part contains exactly one vertex. On multiple occasions, we will deal with x such that $S(x) = \bigsqcup_{s=1}^{p} P_s$ is a p-partite clique with the parts $P_s, s \in [p]$, where $p \geq k$. We can use the fact that no two vertices from the same part P_s can belong to the same clique to obtain the following alternative representation using P_s (assuming $k \leq p$):

$$\sum_{C \in \mathcal{C}_k} \pi_C(x) = \sum_{v \in P_s} x_v \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x) + \sum_{C \in \mathcal{C}_{k;P_s}} \pi_C(x). \tag{1.11}$$

In this case, each term $\pi_C(x^*)$ for $C \in \mathcal{C}_k$ is a product of k entries of x^*, each corresponding to a different part P_s of $S(x^*)$. Hence, the sum can be rewritten as follows:

$$\sum_{C \in \mathcal{C}_k} \pi_C(x^*) = \sum_{D \in \binom{[p]}{k}} \prod_{s \in D} \sum_{v \in P_s} x_v^*. \tag{1.12}$$

(This can be easily shown by induction on $p - k$ using (1.11).)

The following definition is proposed in [19]:

Definition 4 (Regular Multi-clique)**.** *Given a graph $G = (V, E)$, we say that G is a regular multi-clique with p parts if G is a complete multipartite graph and*

$$|P_i| = |P_j| \;\; \forall i, j \in [p].$$

Clearly, a regular multi-clique is a *Turàn's graph* [20], which is a family of complete multipartite graphs $T(n, \omega)$ on n vertices with w parts of equal or nearly equal (up to one vertex difference) size.

There are other generalizations of a clique concept [11]. While not the main topic of this thesis, we will use some of them in the discussion. Some common relaxations are:

Definition 5 (s-plex, [21])**.** *Given a graph $G = (V, E)$, we say that G is an s-plex if $\delta(G) \geq |V| - k$.*

Definition 6 (s-defective clique, [22])**.** *Given a graph $G = (V, E)$, we say that G is an s-defective clique if $|E| \geq \binom{|V|}{2} - s$.*

Given a combinatorial structure property (clique, multiclique, etc.), we will say that a $S \subseteq V$ of vertices is *maximal* structure if it is not a proper subset of any $S' \subseteq V$ such that S' also has the same property. Correspondingly, $S \subseteq V$ is *maximum* if there is no $S' \subseteq V$ such that S' has the property and $|S'| > |S|$.

1.1.3 Optimization and Mathematical Programming

The area of Mathematical Programming, or Optimization, deals, in a nutshell, with a process of selection of the best element among the set of possible alternatives. Optimization problems arise in almost every modern science field, while being a cornerstone part of Economics, Computer Science, Operations Research and Engineering [23]. Nowadays, with advances in computational and experimental capabilities, Mathematical Programming finds extensive applications in Medicine (e.g.: automatic MRI scans recognition and diagnosis), Physics (calibrating the parameters of theoretical models based on the large datasets) or Sociology (studying the implied communities).

In this thesis, we will mostly concentrate on *combinatorial optimization* problems. Being quite an umbrella term without a rigorous definition, it generally describes a problem of considering a finite set of discrete objects while trying to find the "optimal" one. The goal is to find a "smart" or "quick" way to find such an optimal object without considering every possible element. In this specific case, the set is a set of subsets of vertices which satisfy some property, while the "optimal" object is the largest one of those subsets.

Definition 7 (MAXIMUM CLIQUE)**.** *Given a graph $G = (V, E)$,* MAXIMUM CLIQUE *problem asks to find a subset $S \subseteq V$ such that S is a clique and $|S|$ is maximized.*

Given a graph, the size of its maximal clique is denoted by $\omega(G)$, which is called the *clique number* of graph G.

Clearly, not every clique in a given graph is a maximal clique. Among all cliques in a given graph, we can, given some definition of a neighborhood, define a set of local maxima. Specifically:

Definition 8 (Maximal Clique)**.** *Given a graph $G = (V, E)$, set $S \subseteq V$ is called maximal clique if S is not a proper subset of any other clique.*

A concept similar to strict local maximum was introduced for maximal cliques in [16] as following:

Definition 9 (Strictly Maximal Clique)**.** *A maximal clique S is called strictly maximal if it is not a proper subset of an 1-defective clique of size $|S| + 1$.*

This definition, in a nutshell, requires that any vertex in S can not be exchanged with a vertex from $V \setminus S$ such that the resulting set is a clique. Analogous definition can then be established for strictly maximum clique:

Definition 10 (Maximal Clique)**.** *Given a graph $G = (V, E)$, set $S \subseteq V$ is called strictly maximum clique if S is a maximum clique and a strictly maximal clique.*

Is is clear that any maximum clique is necessarily a maximal clique.

Similarly to clique, we define local maxima for multi-clique as:

Definition 11 (Part-maximal Multi-clique)**.** *We will call a multipartite clique $C = \bigsqcup_{s=1}^{p} P_s$ in G* part-maximal *if it is not a subset of a $(p + 1)$-partite clique in G.*

Definition 12 (Strongly Part-maximal Multi-clique)**.** *We will call a multipartite clique $C = \bigsqcup_{s=1}^{p} P_s$ in G* strongly part-maximal *if there does not exist $s \in [p]$ and $D \subseteq P_s$ such that $C \setminus D$ is a subset of a $(p + 1)$-partite clique in G.*

1.1.4 Mathematical Programming Formulations

Mathematical Programming is usually applied in situations when decisions and their impacts can be quantified. The usual setup is as follows: Each decision is represented with a value associated with one or more *decision variables* $x = \{x_i\}_{i=1}^{n} \in X$. With each decision, an *objective*, $f : X \to \mathbb{R}$, is associated, a numeric value to measure the quality or the desirability of the option. Additionally, there are constraints $f_i : X \to \mathbb{R}$, $i \in I$, that define a *feasible region* $\mathcal{F} \coloneqq \{x \in X \mid \forall i \in I : f_i(x) = 0\}$.

The most general form of a Mathematical Programming formulation, then, is

$$\begin{aligned} \text{maximize} \quad & f(x), \\ \text{subject to} \quad & x \in \mathcal{F}. \end{aligned} \tag{Generic program}$$

It is said that the formulation is *feasible* if $\mathcal{F} \neq \emptyset$. It is usually assumed that the feasible region $\mathcal{F}$ defines a compact (closed and bounded) set over X, which allows to guarantee the existence of a set of optimal solutions [24].

A formulation in its most generic form is often impossible to solve, as it provides almost no guarantees regarding the structure of the feasible set and the behavior of the objective function over $\mathcal{F}$. To overcome this, restrictions are often imposed on f, f_i and X that allow us to resolve the complexity of finding the global optimal solution. If both f and f_i are required to be linear functions, while set X is $\mathbb{R}^n$, then such formulation is called a *linear programming* or LP formulation. Linear programs can then be represented as

$$\begin{aligned} \text{maximize} \quad & c^T x, \\ \text{subject to} \quad & Ax \geq 0_m, \\ & x \in \mathbb{R}^n, \end{aligned} \tag{Linear program}$$

where $c \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$. It is known that linear programs can be efficiently (in polynomial time) solved to their global optima by employing the ellipsoid method [25]. In practice, simplex method is usually preferred, as it, while not guaranteeing polynomial execution time, usually performs much faster compared to the ellipsoid method [26].

Unfortunately, not every process behavior can be captured in sufficient detail while relying only on linear constraints and decision variables in $\mathbb{R}^n$. To overcome this issue, multiple approaches were developed. The first one lies in imposing the integrality constraints on some of the decision vector components. Such formulations are known as *integer linear* (or IP), *mixed integer* linear (MIP) and *binary* programs, depending on the specifics of the integrality constraints:

$$\begin{aligned} \text{maximize} \quad & c^T x, \\ \text{subject to} \quad & Ax \geq 0, \\ & x \in \mathbb{Z}^n. \end{aligned} \tag{Integer linear program}$$

$$
\begin{aligned}
\text{maximize} \quad & c_l^T x + c_i^T y, \\
\text{subject to} \quad & Ax + By \geq 0, \\
& x \in \mathbb{R}^{n_l},\ y \in \mathbb{Z}^{n_i}.
\end{aligned}
\tag{Mixed integer linear program}
$$

$$
\begin{aligned}
\text{maximize} \quad & c^T x, \\
\text{subject to} \quad & Ax \geq 0, \\
& x \in \mathbb{B}^n.
\end{aligned}
\tag{Binary linear program}
$$

Unfortunately, being able to efficiently solve any of this class of problems would mean that $P = NP$, as, for example, Maximum Clique problem can be modeled as a binary linear program for graph $G = (V, E)$ as:

$$
\begin{aligned}
\text{maximize} \quad & 1_n^T x, \\
\text{subject to} \quad & -x_i - x_j + 1 \geq 0, \quad \forall \{i, j\} \in \binom{V}{2} \setminus E \\
& x \in \mathbb{B}^n.
\end{aligned}
\tag{Binary Max. Clique}
$$

Another approach can be pursued by allowing the objective function or the constraints to be non-linear. One of such relaxations is known as *quadratic programming*, which allows for the objective function to be a polynomial of order 2. Specifically

$$
\begin{aligned}
\text{maximize} \quad & x^T Q x + c^T x, \\
\text{subject to} \quad & Ax \geq 0.
\end{aligned}
\tag{Quadratic program}
$$

Depending on the properties of matrix $Q \in \mathbb{R}^{n \times n}$, a quadratic program can be either easy or hard to solve. When Q is a positive semi-definite matrix, the ellipsoid method can be employed to find the optimal solution in (weak) polynomial time [27]. On the other hand, if no guarantees are made regarding the structure of Q, quadratic program can be NP-hard. An example of such case is the Motzkin-Strauss quadratic program for Maximal Clique for a graph $G = (V, E)$ with an adjacency matrix A_G:

$$\begin{aligned} \text{maximize} \quad & x^T A_G x, \\ \text{subject to} \quad & 1_n^T x - 1 = 0, \\ & x \in \mathbb{R}^n_{\geq 0}. \end{aligned} \tag{Motzkin-Strauss QP}$$

Finally, a generalization of quadratic programming known as *polynomial programming* allows for the objective function and constraints to be polynomials. Specifically, we will be interested in polynomial programs of form

$$\begin{aligned} \text{maximize} \quad & P(x), \\ \text{subject to} \quad & Ax \geq 0, \end{aligned} \tag{Polynomial program}$$

or, in other words, a problem of optimizing a polynomial function over a set defined by linear constraints. Polynomial optimization problems have found various and extensive applications in operations research, production planning, engineering design, physics, signal processing, VLSI, financial engineering, etc [28]. The idea of applying convex optimization techniques to multivariate polynomials was proposed by Shor [29]. Further advances were made by, among others, Nesterov [30] and Lasserre [31]. Lasserre offered to construct a sequence of semi-definite programming relaxations whose optima eventually converge to the optimum of the original polynomial optimization problem. Unfortunately, the approach comes with a trade-off, as the dimensionality of the sequence of the SDP relaxations grows exponentially.

1.1.5 Motzkin-Strauss formulation in Mathematical Optimization

The maximum clique problem is one of the first problems shown to be NP-hard [32] and is known to be hard to approximate [33, 34]. It is among the most popular problems in operations research and mathematical optimization [35, 17, 36], and the Motzkin-Straus formulation is the cornerstone of research bridging continuous and discrete optimization. The first algorithm for the maximum clique problem based on the Motzkin-Straus formulation was published in [37]. Since then, the formulation has been used to develop new optimality conditions and several successful heuristics for the maximum clique problem based on continuous optimization [38, 39, 16, 40, 41]. This non-traditional approach also inspired some interesting developments in quadratic programming [42, 43, 44, 45], copositive programming [46, 47, 48], and complexity analysis in nonlinear optimization [49, 50, 51]. In addition, generalizations to uniform hypergraphs [52] and hypergraphs with $\{1, 2\}$-edges [53] have been formulated.

More recently, the Motzkin-Straus formulation has been extended to two clique relaxation models, s-defective clique and s-plex [54]. Furthermore, a regularization of the cubic formulation for the maximum s-defective clique proposed in [54] was studied in [55].

Optimality conditions for the Motzkin-Straus quadratic program (QP) have been studied in several works [16, 40, 41, 15]. In particular, the correspondence of its (strict) local maxima to (strictly) maximal cliques and multipartite cliques in the considered graph has been investigated, and several related concepts concerning cliques and multipartite cliques have been defined in connection with optimality conditions for the Motzkin-Straus QP.

1.2 Summary of Contributions

Inspired by the developments described above, in Chapter 2 we propose a hierarchy of polynomial programming formulations, which we call MSPP (or specifically ($\mathbf{P}^k$), $k \in \{2, \dots, \omega\}$, when k is needed to specify the order explicitly) for the maximum clique problem, relating the clique number ω of a given graph $G = (V, E)$ to the global maximal value of a multilinear polynomial function $f_k(x)$ of degree k over the standard simplex in $\mathbb{R}^{|V|}$. Based on the proposed formulations, we establish a series of results regarding the combinatorial structure of local/global optima. The case of $k = 2$ corresponds to the Motzkin-Straus formulation. To the best of our knowledge, the results established for MSPP, when applied for MSQP, give the most complete characterization of local/global optima, as, previously, only feasible points that are characteristic vectors were considered.

In Chapter 3, we study the hierarchical structure of the proposed formulations, which lies in the fact that the set of local maxima of ($\mathbf{P}^{k+1}$) is a subset of the set of local maxima of ($\mathbf{P}^k$),

$k \in \{2, \ldots, \omega - 1\}$. In particular, every local maximum of ($\mathbf{P}^{\omega}$) is global. We show that given a local maximum of MSPP, a corresponding clique can be easily computed by utilizing the multilinear structure of the objective function. From the combinatorial structure point of view, this result arises from the fact that the support of any local maximum of MSPP can be represented as a union of cliques of the same size.

In Chapter 4, we study the regularization approaches for MSPP. Specifically, Bomze [38] has shown that adding a diagonal terms to the Hessian matrix of the objective function guarantees a strict correspondence between local maxima of MSQP and maximal cliques in the graph. Recently, the result was generalized by Hungerford and Rinaldi [41], who have shown that there exists a set of generalized conditions for a regularization term added to the objective function of MSQP such that, again, a strict correspondence is guaranteed. Based on these developments, we investigate the possibility of implementing a regularization approach for higher order formulations. To achieve that goal, we firstly identify the requirements that the regularized formulation must satisfy (one of them being strict correspondence of local maxima to cliques).

The performance of a local solver on the original and regularized formulations of degrees 2 and 3 and 4 (when computationally feasible) is compared through extensive numerical experiments.

Finally, we provide conclusions and discuss possible future directions of research in Chapter 5.

2. STANDARD POLYNOMIAL FORMULATIONS FOR MAXCLIQUE PROBLEM*

2.1 Background and research questions

2.1.1 Motzkin-Strauss Formulation

Given a graph $G = (V, E)$, the maximum clique problem asks for a clique of the largest cardinality in G. This cardinality is referred to as the clique number, denoted by $\omega(G)$, which is simplified to ω throughout this proposal when the graph G is apparent from the context.

The classical Turán's graph theorem [20] provides the following relation between the number of edges m, the number of vertices n, and the clique number ω:

$$m \leq \left(1 - \frac{1}{\omega}\right)\frac{n^2}{2}, \tag{2.1}$$

which holds at equality for the Turán graph $T(n, \omega)$.

Over the years, multiple different proofs were developed for Turán's theorem [56], based on combinatorial analysis, probabilistic methods, or global optimization approaches. The former one is of the interest for us. This proof was proposed by Motzkin and Straus [14] and it relies on the study of a quadratic optimization problem with an objective function given as $f\colon \Delta^n \to \mathbb{R}$:

$$f(x) = \sum_{\{i,j\}\in E} x_i x_j = \sum_{C\in\mathcal{C}_2}\prod_{v\in C} x_v = \sum_{C\in\mathcal{C}_2}\pi_C(x) = \frac{1}{2}x' A_G x. \tag{2.2}$$

They prove that the global maximum of $f(x)$ over $\Delta^{|V|}$ is

$$\max_{x\in\Delta^n} f(x) = \max_{x\in\Delta^n}\sum_{\{i,j\}\in E} x_i x_j = \frac{1}{2}\left(1 - \frac{1}{\omega}\right), \tag{2.3}$$

*Parts of the content in this chapter were first published in "A Hierarchy of Standard Polynomial Programming Formulations for the Maximum Clique Problem" by Sergiy Butenko, Mykyta Makovenko, Miltiades Pardalos in SIAM Journal on Optimization, Vol. 32, 2022, pp. 2102-2128, published by the Society for Industrial and Applied Mathematics (SIAM), Copyright 2022 by Society for Industrial and Applied Mathematics while the result of the Turán's theorem is obtained by setting $x = x^V$ in (2.3)

The cornerstone of all of the mentioned approaches is the Motzkin-Strauss Quadratic Program. As we are introducing multiple optimization problems in this thesis, we will use a standard notation for optimization problems, given as:

$$\begin{aligned} \text{maximize} \quad & f(x) := \sum_{\{i,j\}\in E} x_i x_j, \\ \text{subject to} \quad & x \in \Delta^{|V|}. \end{aligned} \tag{MSQP}$$

Optimality conditions for the Motzkin-Straus Quadratic Program have been studied in several works [16, 40, 41, 15]. In particular, the correspondence of its (strict) local maxima to (strictly) maximal cliques and multipartite cliques in the considered graph has been investigated, and several related concepts concerning cliques and multipartite cliques have been defined in connection with optimality conditions for the Motzkin-Straus QP. A (multipartite) clique is *maximal* if it is not a subset of a larger (multipartite) clique in the graph. In [15], Pellilo and Jagota claim that the following proposition holds:

Proposition 1. *A subset C of vertices in G is a maximum clique if and only if its characteristic vector x^C is a global maximum of Equation 2.3.*

Unfortunately, this claim is not entirely correct. Hungerford and Rinaldi [41] and Tang et. al. [19] have both recently reported the existence of counterexamples for this proposition. Specifically, while a characteristic vector of a maximum clique is a global maximum for MSQP, there can exist alternative global optima not corresponding to any maximum clique. Consider Figure 2.1. Clearly, $C = \{1, 2\}$ is a maximum clique in the given graph and $x^C = \left(\frac{1}{2}, \frac{1}{2}, 0, 0\right)$ is the global maximum with the objective value of $\frac{1}{4}$. But $C' = \{1, 2, 3, 4\}$, which is not a clique, also results in the same objective value for $x^{C'} = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$. Note that the counterexample is a $T(4, 2)$ Turán graph.

To resolve this issue, the correspondence of its (strict) local maxima to (strictly) maximal cliques and multipartite cliques in the considered graph has been reinvestigated, and several related concepts concerning cliques and multipartite cliques have been defined in connection with

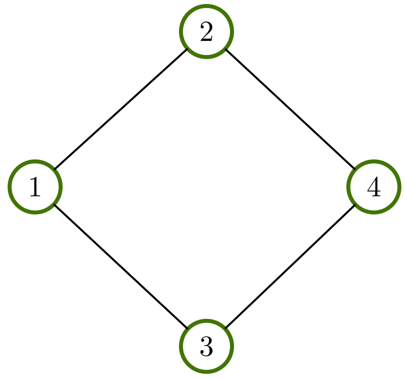

Figure 2.1: A counterexample to Proposition 1

optimality conditions for the Motzkin-Straus QP. Specifically, the following set of theorems is proven in [19]. The first one characterizes a subset of global maxima of MSQP that corresponds to characteristic vectors:

Theorem 1. *C is a maximum regular multipartite clique of G if and only if x^C is a global maximizer of MSQP.*

The second one characterizes the subset of local maxima of MSQP, again, in therms of characteristic vectors:

Theorem 2. *If C is a regular multipartite clique in G, then x^C is a local maximizer of* (MSQP)*, if and only if C satisfies the following requirements:*

1. *Each vertex in $V \setminus C$ is adjacent to at most $\frac{p-1}{p}|C|$ vertices in C;*

2. *Each vertex in $V \setminus C$ is not adjacent to $\frac{p-1}{p}|M|$ vertices from p different parts of C;*

3. *And pair of adjacent vertices in $V \setminus C$, are not adjacent to $\frac{p-1}{p}|C|$ in the same different $p-1$ parts of C.*

To the best of out knowledge, these results were the state of the art for characterizations of global/local maxima of MSQP. Note that both of them do not offer complete characterizations, as only characteristic vectors are considered.

2.1.2 Higher Order Formulations

As we have mentioned before, in the recent years multiple new formulations were proposed, based on generalizations of MSQP, to tackle optimization problems related to clique relaxations. For example, a set of formulations were presented in [54] for an s-defective clique and an s-plex. The core of the proposed approach was to introduce a trilinear function

$$f(x,Y) := \sum_{\{i,j\}\in E} x_i x_j + \sum_{\{i,j\}\in\binom{V}{2}\setminus E} x_i y_{i,j} x_j = \frac{1}{2} x' \left(A_G + Y\right) x. \tag{2.4}$$

Depending on the type of a clique relaxation, additional constraints are introduced for matrix Y. Either

$$\sum_{\{i,j\}\in\binom{V}{2}\setminus E} y_{i,j} \leq s$$

for an s-defective clique, or

$$\sum_{j\in V} y_{i,j} \leq s-1, \quad \forall i \in V$$

for an s-plex. The authors show that the results analogous to Equation 2.3 hold, which allows them to extend Turán's theorem and related bounds to clique relaxations. Inspired, in part, by this approach, and, in part, by the relaxation techniques proposed by Lasserre, we propose to explore the possibility of formulating a family of Motzkin-Strauss Polynomial Programs. Note that, in the original MSQP, the objective function is written to account for every edge. On the other hand, an edge is a clique of size 2. A natural question arises what will happen if cliques of size 2 are replaced with cliques of higher cardinality? More specifically, our goal would be to study the following optimization problem, parametrized by the degree k:

$$\begin{aligned} \text{maximize} \quad & f_k(x) := \sum_{C\in\mathcal{C}_k} \prod_{i\in C} x_i, \\ \text{subject to} \quad & x \in \Delta^{|V|}. \end{aligned} \tag{MSPP}$$

Note that the objective function $f_k(x)$ in this case is a multi-linear (k-linear, to be precise), polynomial, and, for $k = 2$, MSPP coincides with MSQP. This leads to a question if results analogous to Equation 2.3, Theorem 1, Theorem 2 hold for MSPP.

If that is true, then the hierarchical aspect of the proposed formulations lies in the fact that, by increasing the value of k, the set of local maxima that are not global is narrowed down, to eventually yield a formulation with each local maximum being global for $k = \omega$. Indeed, assuming that there is a local optimum of size $k \leq \omega$, which corresponds to a multiclique, a formulation of order $k + 1$ would not have those subcliques present, which suggests that the set of local optima is shrinking.

To the best of our knowledge, this type of hierarchy is new in mathematical optimization and is fundamentally different from existing hierarchies focusing on convex relaxations, such as Sherali-Adams [57], Lovász-Schrijver [58] and Lasserre [31]. More specifically, the existing methods rely on hierarchies of convex relaxations and proceed by introducing additional variables and constraints in order to improve the quality of the relaxation at each next level of the hierarchy. The convex relaxation obtained at the final level is tight and yields a global optimal solution to the original problem. In contrast to the existing hierarchies, our approach works with the original feasible region; instead, it alters the objective function at each level of the hierarchy.

This approach would also allow us to establish a set of benchmark instances for modern state-of-the-art solvers for convex and non-convex problems, as, for a lot of standard benchmark graph instances, the size of maximal clique is known.

Since MSQP is a special case of MSPP, developing a series of results characterizing optimal points and corresponding combinatorial structures would allow us to simultaneously resolve the open questions for order $k = 2$ formulation.

2.2 Optimality structure of MSPP

Now we are ready to establish our main results regarding the structure of the global and local optima of the Motzkin-Strauss Polynomial Program. First, we will establish some basic observations and results.

2.2.1 Basic Observations

2.2.1.1 Structure of global maxima

Firstly, we directly derive a theorem analogous to Motzkin-Strauss theorem, which links some of the global optima of MSPP to the maximum cliques in G and guarantees the objective value at global optima.

Theorem 3. *Consider the following problem of maximizing a multilinear polynomial of degree $k \in \{2, \ldots, \omega\}$ over the standard simplex:*

$$f_k(G) := \max_{x \in \Delta^n} \sum_{C \in \mathcal{C}_k} \prod_{i \in C} x_i = \max_{x \in \Delta^n} \sum_{C \in \mathcal{C}_k} \pi_C(x). \tag{$\mathbf{P}^k$}$$

Then for any maximum clique C of G, x^C is a global maximum of ($\mathbf{P}^k$) *and*

$$f_k(G) = \binom{\omega}{k} \left(\frac{1}{\omega}\right)^k. \tag{2.5}$$

Proof. Let $x' \in \Delta^n$ be an optimal solution of ($\mathbf{P}^k$) with the minimum number of missing edges in the subgraph $G[S(x')]$ induced by its corresponding set of vertices. First, we will show that $S(x')$ is a clique in G. Assume there is a pair of vertices $i, j \in S(x')$ such that $\{i, j\} \notin E$. Then, since no clique can include both i and j,

$$f_k(x') = x'_i \sum_{C \in \mathcal{C}^i_{k-1}} \pi_C(x') + x'_j \sum_{C \in \mathcal{C}^j_{k-1}} \pi_C(x') + \sum_{C \in \mathcal{C}_{k;i,j}} \pi_C(x').$$

Without loss of generality, assume that $\sum\limits_{C \in \mathcal{C}^i_{k-1}} \pi_C(x') \geq \sum\limits_{C \in \mathcal{C}^j_{k-1}} \pi_C(x')$. For $v \in V$, set

$$x''_v := \begin{cases} x'_i + x'_j, & v = i, \\ 0, & v = j, \\ x'_v, & v \in V \setminus \{i, j\}. \end{cases}$$

Then $\sum\limits_{C\in\mathcal{C}^i_{k-1}} \pi_C(x') = \sum\limits_{C\in\mathcal{C}^i_{k-1}} \pi_C(x'')$, $\sum\limits_{C\in\mathcal{C}^j_{k-1}} \pi_C(x') = \sum\limits_{C\in\mathcal{C}^j_{k-1}} \pi_C(x'')$, $x'' \in \Delta^n$, and

$$f(x'') - f(x') = \Big(\sum_{C\in\mathcal{C}^i_{k-1}} \pi_C(x') - \sum_{C\in\mathcal{C}^j_{k-1}} \pi_C(x') \Big) x'_j \geq 0.$$

Hence, x'' is an alternative optimal solution, such that $G[S(x'')]$ has at least one less missing edge than $G[S(x')]$, which contradicts the definition of x'. Thus, $S(x')$ is a clique in G. This clique must contain at least k vertices, otherwise $f_k(x') = 0 < f_k(x^V)$. Next, we show that $x'_i = x'_j$ for any $i, j \in S(x')$. Assume the opposite, then there exists ε such that $x'_i - x'_j > \varepsilon > 0$. For $v \in V$, set

$$x''_v := \begin{cases} x'_i - \varepsilon, & v = i, \\ x'_j + \varepsilon, & v = j, \\ x'_v, & v \in V \setminus \{i, j\}. \end{cases}$$

Since $S(x')$ is a clique, $\sum\limits_{C\in\mathcal{C}^i_{k-1;j}} \pi_C(x') = \sum\limits_{C\in\mathcal{C}^j_{k-1;i}} \pi_C(x')$; hence, we have:

$$\begin{aligned} f(x'') - f(x') &= (x'_i - \varepsilon)(x'_j + \varepsilon) \sum_{C\in\mathcal{C}^{i,j}_{k-2}} \pi_C(x') - x'_i x'_j \sum_{C\in\mathcal{C}^{i,j}_{k-2}} \pi_C(x') \\ &= \varepsilon(x'_i - x'_j - \varepsilon) \sum_{C\in\mathcal{C}^{i,j}_{k-2}} \pi_C(x') > 0. \end{aligned}$$

This contradicts the optimality of x'. Thus, $x'_i = x'_j$ for any $i, j \in S(x')$, implying that $x' = x^{S(x')}$ and

$$f_k(x') = \binom{|S(x')|}{k} \left(\frac{1}{|S(x')|} \right)^k.$$

Finally, observe that $f_k(x')$ increases with the increase in $|S(x')|$, hence it achieves its maximum at x' if $S(x')$ is a maximum clique of G. $\square$

Observe that the Motzkin-Straus formulation is obtained by setting $k = 2$ in Theorem 3. In this case, the corresponding quadratic optimization problem is referred to as the Motzkin-Straus QP. While the focus of this paper is on studying the properties of formulations presented in Theorem 3, in the reminder of this section we state several relevant results that follow directly from this theorem. First, note that formulation ($\mathbf{P}^k$) can be used to obtain a generalization of Turán's graph theorem as follows.

Corollary 1. *The number c_k of cliques with k vertices in $G = (V, E)$ satisfies the following inequality:*

$$c_k \leq \binom{\omega}{k} \left(\frac{n}{\omega}\right)^k, \tag{2.6}$$

where $n = |V|$.

Proof. Set $x_i = \frac{1}{n},\ i \in V$ in ($\mathbf{P}^k$), then by Theorem 3,

$$\binom{\omega}{k} \left(\frac{1}{\omega}\right)^k \geq c_k \left(\frac{1}{n}\right)^k,$$

which is equivalent to (2.6). □

It should be pointed out that (2.6) is also implied by the following inequality established by Fisher and Ryan [59]:

$$\left(\frac{c_1}{\binom{\omega}{1}}\right)^{1/1} \geq \left(\frac{c_2}{\binom{\omega}{2}}\right)^{1/2} \geq \left(\frac{c_3}{\binom{\omega}{3}}\right)^{1/3} \geq \cdots \geq \left(\frac{c_\omega}{\binom{\omega}{\omega}}\right)^{1/\omega}. \tag{2.7}$$

Note that for $k = 2$, we have $c_2 = m$ and (2.6) coincides with the Turán's bound (2.1). In addition, (2.6) is sharp for Moon-Moser graphs [60], which are known to contain the largest possible number of maximal cliques among all n-vertex graphs. Specifically, the Moon-Moser graph on $n = 3p$ vertices is a complete balanced p-partite graph, in which each of the p parts consists of 3 vertices, and hence there are $3^p = 3^{n/3}$ distinct maximum cliques of cardinality p.

2.2.1.2 Structure of local maxima

In our analysis of local maxima structure, we will heavily rely on KKT first order necessary optimality conditions. For MSPP of order k, let $\lambda^{(k)} \in \mathbb{R}$ and $\mu^{(k)} \in \mathbb{R}^{|V|}$ be the dual variables, where $\lambda^{(k)}$ corresponds to the single equality constraint and $\mu^{(k)}$ corresponds to the non-negativity constrains. As before, $n \coloneqq |V|$. Then the conditions can be formulated as

- Stationarity:

$$\sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) + \mu_v^{(k)} = \lambda^{(k)}, \quad \forall v \in V; \tag{2.8}$$

- Primal feasibility:

$$\sum_{v \in V} x_v^* = 1; \quad x_v^* \geq 0, \quad \forall v \in V; \tag{2.9}$$

- Dual feasibility and complementary slackness:

$$x_v^* \mu_v^{(k)} = 0, \quad \mu_v^{(k)} \geq 0, \quad \forall v \in V; \tag{2.10}$$

In particular, due to (2.10), $\mu_i^{(k)} = 0$ for any $i \in S\left(x^*\right)$. Hence, from (2.8) we have

$$\lambda^{(k)} = \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*), \quad \forall i \in S\left(x^*\right). \tag{2.11}$$

Also, since $\mathcal{C}_{k-1}^i$ is the disjoint union of $\mathcal{C}_{k-1;j}^i$ and $\left\{C \cup \{j\} \mid C \in \mathcal{C}_{k-2}^{i,j}\right\}$ for $j \in V \setminus \{i\}$, we have

$$\lambda^{(k)} = \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-1;j}^i} \pi_C(x^*) + x_j^* \sum_{C \in \mathcal{C}_{k-2}^{i,j}} \pi_C(x^*), \quad \forall i \in S\left(x^*\right), j \in V \setminus \{i\}. \tag{2.12}$$

In the following lemma, we show that every vertex from $S\left(x^*\right)$ belongs to some k-vertex clique contained in $S\left(x^*\right)$.

Lemma 1. *If x^* is a local maximum of* $(\mathbf{P}^k)$ *for a given $k \in \{2, \ldots, \omega\}$, then each $v \in S\left(x^*\right)$ belongs to some clique in $\mathcal{C}_k\left(G\left[S\left(x^*\right)\right]\right)$.*

Proof. Let $v \in S\left(x^*\right)$ and suppose there is no k-vertex clique in $S\left(x^*\right)$ containing v. Then $\sum\limits_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) = 0$ and using (1.10),

$$f_k(x^*) = \sum_{C \in \mathcal{C}_k} \pi_C(x^*) = x_v^* \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) + \sum_{C \in \mathcal{C}_{k;v}} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k;v}} \pi_C(x^*). \tag{2.13}$$

Since $2 \leq k \leq \omega, \mathcal{C}_k \neq \emptyset$. Consider an arbitrary clique $K \in \mathcal{C}_k$. Then it is evident from (2.13) that the direction d given by

$$d_i := \begin{cases} 1, & i \in K \setminus \{v\}, \\ -|K \setminus \{v\}|, & i = v, \\ 0, & \text{otherwise} \end{cases}$$

is a feasible direction of increase for $f_k(x)$ at x^*, a contradiction. $\square$

Next, we show that two adjacent vertices from $S(x^*)$ that have a common non-neighbor in $S(x^*)$ both belong to a k-vertex clique in $G[S(x^*)]$.

Lemma 2. *Suppose x^* is a local maximum of ($\mathbf{P}^k$) for a given $k \in \{2, \ldots, \omega\}$ and there exist $u, v, w \in S(x^*)$ such that $\{u, v\} \in E$ and $\{u, w\}, \{v, w\} \notin E$. Then $u, v \in K$ for some $K \in \mathcal{C}_k(G[S(x^*)])$.*

Proof. Clearly, the statement holds for $k = 2$. Hence, in the remainder of the proof we assume that $k \geq 3$. Suppose there does not exist a clique in $\mathcal{C}_k(G[S(x^*)])$ containing both u and v. By Lemma 1, $S(x^*)$ contains a clique $\tilde{C} \in \mathcal{C}_k$ such that $w \in \tilde{C}$. Let $w' \in \tilde{C} \setminus \{w\}$. Then

$$\sum_{C \in \mathcal{C}_{k-2}^{w,w'}} \pi_C(x^*) > 0. \tag{2.14}$$

Consider $d \in \mathbb{R}^n$ such that

$$\sum_{i \in V} d_i = 0, \quad d_i = 0 \; \forall i \in V \setminus \{u, v, w, w'\}. \tag{2.15}$$

Due to the local optimality of x^*, the KKT conditions (2.8)–(2.10) as well as (2.11)-(2.12) hold for some $\lambda^{(k)} \in \mathbb{R}$ and $\mu^{(k)} \in \mathbb{R}^n$. From (2.10), $\mu_{w'}^{(k)} = 0$. Using (2.8) with $v = w'$ and considering that $\mathcal{C}_{k-1}^{w'}$ is the disjoint union $\mathcal{C}_{k-1;u,v,w}^{w'} \cup \left\{C \cup \{u\} \mid C \in \mathcal{C}_{k-2}^{u,w'}\right\} \cup \left\{C \cup \{v\} \mid C \in \mathcal{C}_{k-2}^{v,w'}\right\} \cup$

$\left\{C \cup \{w\} \mid C \in \mathcal{C}_{k-2}^{w,w'}\right\}$, we have

$$\lambda^{(k)} = \sum_{C \in \mathcal{C}_{k-1;u,v,w}^{w'}} \pi_C(x^*) + x_u^* \sum_{C \in \mathcal{C}_{k-2}^{u,w'}} \pi_C(x^*) + x_v^* \sum_{C \in \mathcal{C}_{k-2}^{v,w'}} \pi_C(x^*) + x_w^* \sum_{C \in \mathcal{C}_{k-2}^{w,w'}} \pi_C(x^*). \tag{2.16}$$

Since no two of the vertices $\{u, v, w\}$ can belong to the same k-vertex clique in $G[S(x^*)]$, we have

$$\begin{aligned} f_k(x^* + \varepsilon d) = &\sum_{C \in \mathcal{C}_{k;u,v,w,w'}} \pi_C(x^*) + (x_u^* + \varepsilon d_u) \sum_{C \in \mathcal{C}_{k-1;w'}^{u}} \pi_C(x^*) + (x_v^* + \varepsilon d_v) \sum_{C \in \mathcal{C}_{k-1;w'}^{v}} \pi_C(x^*) \\ &+ (x_w^* + \varepsilon d_w) \sum_{C \in \mathcal{C}_{k-1;w'}^{w}} \pi_C(x^*) + (x_{w'}^* + \varepsilon d_{w'}) \Big(\sum_{C \in \mathcal{C}_{k-1;u,v,w}^{w'}} \pi_C(x^*) + (x_u^* + \varepsilon d_u) \sum_{C \in \mathcal{C}_{k-2}^{u,w'}} \pi_C(x^*) \\ &+ (x_v^* + \varepsilon d_v) \textstyle\sum_{C \in \mathcal{C}_{k-2}^{v,w'}} \pi_C(x^*) + (x_w^* + \varepsilon d_w) \displaystyle\sum_{C \in \mathcal{C}_{k-2}^{w,w'}} \pi_C(x^*) \Big). \end{aligned}$$

Therefore, using (2.16) and (2.12) for $(i, j) \in \{(u, w'), (v, w'), (w, w')\}$ we obtain:

$$\begin{aligned} f_k(x^* + \varepsilon d) - f_k(x^*) = &\, \varepsilon \lambda^{(k)} (d_u + d_v + d_w + d_{w'}) \\ &+ \varepsilon^2 d_{w'} \Big(d_u \sum_{C \in \mathcal{C}_{k-2}^{u,w'}} \pi_C(x^*) + d_v \sum_{C \in \mathcal{C}_{k-2}^{v,w'}} \pi_C(x^*) + d_w \sum_{C \in \mathcal{C}_{k-2}^{w,w'}} \pi_C(x^*) \Big). \end{aligned}$$

Since $d_u + d_v + d_w + d_{w'} = 0$ due to (2.15), for d to be a direction of improvement, it is sufficient for it to be a solution to the following system:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & \sum_{C \in \mathcal{C}_{k-2}^{u,w'}} \pi_C(x^*) & \sum_{C \in \mathcal{C}_{k-2}^{v,w'}} \pi_C(x^*) & \sum_{C \in \mathcal{C}_{k-2}^{w,w'}} \pi_C(x^*) \end{pmatrix} \begin{pmatrix} d_{w'} \\ d_u \\ d_v \\ d_w \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}. \tag{2.17}$$

If the matrix above has full row rank, the system has a solution d, which is a direction of improvement, contradicting the local maximality of x^*. Otherwise, the second row of the matrix must be proportional to the third row, and since (2.14) holds,

$$\sum_{C \in \mathcal{C}_{k-2}^{u,w'}} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-2}^{w,w'}} \pi_C(x^*) > 0,$$

which implies that $\exists \hat{C} \in \mathcal{C}_k\left(G\left[S\left(x^*\right)\right]\right)$ such that $u, w' \in \hat{C}$ as $k \geq 3$. Since u and v do not belong to the same k-vertex clique in $G[S\left(x^*\right)]$, there must exist $w'' \in \hat{C}$ such that $\{v, w''\} \notin E$. Now let

$$d'_i := \begin{cases} 1, & i \in \{u, w''\}, \\ -2, & i = v, \\ 0, & \text{otherwise,} \end{cases}$$

and observe that

$$\begin{aligned} f_k(x^* + \varepsilon d') &= \sum_{C \in \mathcal{C}_{k;u,v,w''}} \pi_C(x^*) + (x_u^* + \varepsilon) \sum_{C \in \mathcal{C}_{k-1;w''}^{u}} \pi_C(x^*) + (x_v^* - 2\varepsilon) \sum_{C \in \mathcal{C}_{k-1}^{v}} \pi_C(x^*) \\ &\quad + (x_{w''}^* + \varepsilon) \sum_{C \in \mathcal{C}_{k-1;u}^{w''}} \pi_C(x^*) + (x_u^* + \varepsilon)(x_{w''}^* + \varepsilon) \sum_{C \in \mathcal{C}_{k-2}^{u,w''}} \pi_C(x^*). \end{aligned}$$

Hence, using (2.11) for $i = v$ and (2.12) for $(i, j) = (u, w'')$ and (w'', u), we obtain:

$$f_k(x^* + \varepsilon d') - f_k(x^*) = \varepsilon^2 \sum_{C \in \mathcal{C}_{k-2}^{u,w''}} \pi_C(x^*) > 0.$$

Thus, d' is a feasible ascent direction at x^*, a contradiction with the local maximality of x^*. $\square$

Next we show that the support of a local maximum of (**P**^{k}) is a multipartite clique in G. In the proof, we use the fact that a complete multipartite graph is, equivalently, a $\bar{P}_3$-free graph, where $\bar{P}_3$ is the complement graph of the path on 3 vertices.

Theorem 4. *If x^* is a local maximum of* (**P**^{k}) *for a given $k \in \{2, \ldots, \omega\}$, then $S\left(x^*\right)$ is a multipartite clique with at least k parts.*

Proof. Suppose that x^* is a local maximum of ($\mathbf{P}^k$), but $S(x^*)$ is not a multipartite clique. Due to the local optimality of x^*, the KKT conditions (2.8)–(2.10) as well as (2.11)-(2.12) hold for some $\lambda^{(k)} \in \mathbb{R}$ and $\mu^{(k)} \in \mathbb{R}^n$.

Since $S(x^*)$ is not a multipartite clique, there exist $u, v, w \in S(x^*)$ such that $\{u, v\} \in E$ and $\{u, w\}, \{v, w\} \notin E$. By Lemma 2, there exists a k-vertex clique in $G[S(x^*)]$ containing both u and v. This implies that

$$\sum_{C \in \mathcal{C}_{k-2}^{u,v}} \pi_C(x^*) > 0. \tag{2.18}$$

Let $d \in \mathbb{R}^n$ be the direction defined as

$$d_i := \begin{cases} -1, & i \in \{u, v\}, \\ 2, & i = w, \\ 0, & \text{otherwise}. \end{cases} \tag{2.19}$$

Note that $\mathcal{C}_k$ can be represented as the disjoint union of the following five sets:

- the set $\mathcal{C}_{k;u,v,w}$ of cliques in $\mathcal{C}_k$ that contain none of the vertices u, v, w,
- the set $\left\{C \cup \{u\} \mid C \in \mathcal{C}_{k-1;v}^{u}\right\}$ of cliques in $\mathcal{C}_k$ that contain u but not v,
- the set $\left\{C \cup \{v\} \mid C \in \mathcal{C}_{k-1;u}^{v}\right\}$ of cliques in $\mathcal{C}_k$ that contain v but not u,
- the set $\left\{C \cup \{u, v\} \mid C \in \mathcal{C}_{k-2}^{u,v}\right\}$ of cliques in $\mathcal{C}_k$ that contain both u and v, and
- the set $\left\{C \cup \{w\} \mid C \in \mathcal{C}_{k-1}^{w}\right\}$ of cliques in $\mathcal{C}_k$ that contain w.

We have

$$\begin{aligned} f_k(x^* + \varepsilon d) &= \sum_{C \in \mathcal{C}_{k;u,v,w}} \pi_C(x^*) + (x_u^* - \varepsilon) \sum_{C \in \mathcal{C}_{k-1;v}^{u}} \pi_C(x^*) + (x_v^* - \varepsilon) \sum_{C \in \mathcal{C}_{k-1;u}^{v}} \pi_C(x^*) \\ &\quad + (x_u^* - \varepsilon)(x_v^* - \varepsilon) \sum_{C \in \mathcal{C}_{k-2}^{u,v}} \pi_C(x^*) + (x_w^* + 2\varepsilon) \sum_{C \in \mathcal{C}_{k-1}^{w}} \pi_C(x^*). \end{aligned}$$

Hence, using (2.11) for $i \in \{u, v, w\}$ and (2.12) for $(i, j) \in \{(u, v), (v, u)\}$ we obtain:

$$
\begin{aligned}
& f_k\left(x^* + \varepsilon d\right) - f_k\left(x^*\right) \\
&= -\varepsilon \sum_{C \in \mathcal{C}^u_{k-1;v}} \pi_C(x^*) - \varepsilon \sum_{C \in \mathcal{C}^v_{k-1;u}} \pi_C(x^*) + 2\varepsilon \sum_{C \in \mathcal{C}^w_{k-1}} \pi_C(x^*) \\
&\qquad\qquad + \left(\varepsilon^2 - \varepsilon x^*_u - \varepsilon x^*_v\right) \sum_{C \in \mathcal{C}^{u,v}_{k-2}} \pi_C(x^*) \\
&= -\varepsilon \sum_{C \in \mathcal{C}^u_{k-1}} \pi_C(x^*) - \varepsilon \sum_{C \in \mathcal{C}^v_{k-1}} \pi_C(x^*) + 2\varepsilon \sum_{C \in \mathcal{C}^w_{k-1}} \pi_C(x^*) + \varepsilon^2 \sum_{C \in \mathcal{C}^{u,v}_{k-2}} \pi_C(x^*) \\
&= -\varepsilon\lambda^{(k)} - \varepsilon\lambda^{(k)} + 2\varepsilon\lambda^{(k)} + \varepsilon^2 \sum_{C \in \mathcal{C}^{u,v}_{k-2}} \pi_C(x^*) = \varepsilon^2 \sum_{C \in \mathcal{C}^{u,v}_{k-2}} \pi_C(x^*) > 0,
\end{aligned}
$$

where the inequality follows from (2.18). Clearly, d is a feasible ascent direction for the objective function $f_k(x)$ of ($\mathbf{P}^k$) at x^*, a contradiction with the local maximality of x^*. This proves that $S\left(x^*\right)$ is a multipartite clique.

Finally, due to Lemma 1, every vertex from $S\left(x^*\right)$ belongs to a k-vertex clique in $G[S\left(x^*\right)]$. This implies that the complete multipartite graph $G[S\left(x^*\right)]$ has at least k parts. $\square$

The following theorem further refines the structure of a local maximum x^* of ($\mathbf{P}^k$).

Theorem 5. *Suppose that* $S\left(x^*\right) = \bigsqcup_{s=1}^{p} P_s$, *where* $P_s, s \in [p]$ *are the parts of the multipartite clique* $S\left(x^*\right)$ *defined by a local maximum* x^* *of* ($\mathbf{P}^k$). *Then*

$$\sum_{u \in P_s} x^*_u = \frac{1}{p}, \quad \forall s \in [p]. \tag{2.20}$$

Moreover,

$$f_k(x^*) = \binom{p}{k} \frac{1}{p^k}. \tag{2.21}$$

Proof. Let $u \in P_r$, $v \in P_s$ for some distinct $r, s \in [p]$. Consider (2.8) for u and v. Since x^* is a local maximum, the following must hold:

$$\lambda^{(k)} = \sum_{C \in \mathcal{C}^u_{k-1}} \pi_C(x^*) = \sum_{C \in \mathcal{C}^v_{k-1}} \pi_C(x^*) \Longrightarrow \sum_{C \in \mathcal{C}^u_{k-1}} \pi_C(x^*) - \sum_{C \in \mathcal{C}^v_{k-1}} \pi_C(x^*) = 0. \tag{2.22}$$

Using the alternative representation in the form (1.11), we can rewrite (2.22) as

$$\sum_{w\in P_s} x_w^* \sum_{C\in\mathcal{C}_{k-2}^{u,w}} \pi_C(x^*) + \sum_{C\in\mathcal{C}_{k-1;P_s}^{u}} \pi_C(x^*) - \sum_{w\in P_r} x_w^* \sum_{C\in\mathcal{C}_{k-2}^{v,w}} \pi_C(x^*) - \sum_{C\in\mathcal{C}_{k-1;P_r}^{v}} \pi_C(x^*) = 0. \tag{2.23}$$

Since $S(x^*)$ is a multipartite clique, $\forall w \in P_s, w' \in P_r$ we have

$$\sum_{C\in\mathcal{C}_{k-1;P_s}^{u}} \pi_C(x^*) = \sum_{C\in\mathcal{C}_{k-1;P_r}^{v}} \pi_C(x^*), \quad \sum_{C\in\mathcal{C}_{k-2}^{u,v}} \pi_C(x^*) = \sum_{C\in\mathcal{C}_{k-2}^{u,w}} \pi_C(x^*) = \sum_{C\in\mathcal{C}_{k-2}^{v,w'}} \pi_C(x^*) \neq 0.$$

Then (2.23) becomes

$$\sum_{w\in P_s} x_w^* \sum_{C\in\mathcal{C}_{k-2}^{u,w}} \pi_C(x^*) - \sum_{w\in P_r} x_w^* \sum_{C\in\mathcal{C}_{k-2}^{v,w}} \pi_C(x^*) = \sum_{C\in\mathcal{C}_{k-2}^{u,v}} \pi_C(x^*) \Big(\sum_{w\in P_s} x_w^* - \sum_{w\in P_r} x_w^* \Big) = 0,$$

and, therefore,

$$\sum_{w\in P_s} x_w^* = \sum_{w\in P_r} x_w^* = \frac{1}{p}, \quad \forall i, j \in [p].$$

Finally, the fact that $S(x^*)$ is a multipartite clique implies that (1.12) holds, hence

$$f_k(x^*) = \sum_{C\in\mathcal{C}_k} \pi_C(x^*) = \sum_{D\in\binom{[p]}{k}} \prod_{r\in D} \sum_{v\in P_r} x_v^* = \sum_{D\in\binom{[p]}{k}} \prod_{r\in D} \frac{1}{p} = \sum_{D\in\binom{[p]}{k}} \frac{1}{p^k} = \binom{p}{k} \frac{1}{p^k}, \tag{2.24}$$

which completes the proof. $\square$

Corollary 2. *Suppose x^* and $\bar{x}$ are two local maxima of $(\mathbf{P}^k)$ such that $S(x^*)$ is a p-partite clique and $S(\bar{x})$ is a $\bar{p}$-partite clique. If $p > \bar{p}$ then $f_k(x^*) > f_k(\bar{x})$.*

Proof. Note that by Theorem 5, $p > \bar{p} \geq k$. It is sufficient to show that the statement holds for $p = \bar{p} + 1$. From (2.24) we have

$$\begin{aligned} f_k(x^*) - f_k(\bar{x}) &= \binom{p}{k}\frac{1}{p^k} - \binom{p-1}{k}\frac{1}{(p-1)^k} \\ &= \frac{(p-1)!}{k!(p-k-1)!}\left[\frac{(p-1)^k - (p-k)p^{k-1}}{(p-k)p^{k-1}(p-1)^k}\right]. \end{aligned}$$

Since $(p-1)^k - (p-k)p^{k-1} = kp^{k-1} - \sum_{i=0}^{k-1}(p-1)^i p^{k-1-i} > kp^{k-1} - \sum_{i=0}^{k-1} p^{k-1} = 0$, the statement of the corollary holds. $\square$

Corollary 3. *If x^* is a local maximum of* ($\mathbf{P}^k$)*, then the KKT multiplier $\lambda^{(k)}$ in* (2.8) *is given by*

$$\lambda^{(k)} = \binom{p-1}{k-1}\frac{1}{p^{k-1}}. \tag{2.25}$$

Proof. As before, we assume that $P_1, \ldots, P_p$ are the parts of the complete multipartite clique $S(x^*)$. Let u be a vertex from P_1. From (2.8) and the result of Theorem 5:

$$\lambda^{(k)} = \sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) = \sum_{D \in \binom{\{2,\ldots,p\}}{k-1}} \prod_{s \in D} \sum_{v \in P_s} x_v^* = \binom{p-1}{k-1}\frac{1}{p^{k-1}}.$$

$\square$

The following corollary provides an alternative proof of Theorem 3.

Corollary 4. *If x^* is a global maximum of* ($\mathbf{P}^k$)*, then*

$$f_k(x^*) = \binom{\omega}{k}\frac{1}{\omega^k}.$$

Proof. There is no complete multipartite subgraph with $\omega + 1$ parts in G. Therefore, due to Theorem 5 and Corollary 2, the statement of the corollary holds. $\square$

Corollary 5. *For $k = \omega$, every local maximum of* ($\mathbf{P}^k$) *is global.*

Proof. Let x^* be a local maximum of ($\mathbf{P}^k$) with $k = \omega$. According to Theorem 4, $S(x^*)$ is a multipartite clique with at least ω parts. Since the graph cannot contain a multipartite clique with more than ω parts, $f_\omega(x^*) = \frac{1}{\omega^\omega}$ by Theorem 5. Hence, x^* is a global maximum by Corollary 4. $\square$

Corollary 6. *If x^* is a strict local maximum of* ($\mathbf{P}^k$) *then $S(x^*)$ is a clique in G and $x^* = x^{S(x^*)}$.*

Proof. Note that (2.24) implies that $f_k(x^*) = f(x')$ for any $x' \in \left\{x \in \mathbb{R}^n \mid \sum_{u \in P_s} x_u = \frac{1}{p}, s \in [p]\right\}$. Hence, x^* can be a strict local maximum only if $|P_s| = 1 \; \forall s \in [p]$, that is, if C is a clique. $\square$

Lemma 3. *If x^* is a local maximum of* ($\mathbf{P}^k$) *then $S(x^*)$ is a part-maximal multipartite clique in G.*

Proof. By Theorem 4, $S(x^*) = \bigsqcup_{s=1}^{p} P_s$ is a p-partite clique for some $p \geq k$. Assume it is not part-maximal. Then there exists $v \in V \setminus S(x^*)$ such that $S(x^*) \cup \{v\}$ is a $(p+1)$-partite clique in G. Consider the following direction $d \in \mathbb{R}^n$:

$$d_i \coloneqq \begin{cases} -1, & i \in P_1, \\ |P_1|, & i = v, \\ 0, & \text{otherwise.} \end{cases}$$

Then

$$f_k(x^* + \varepsilon d) - f_k(x^*) = \sum_{i \in P_1} (-\varepsilon) \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) + \varepsilon |P_1| \sum_{C \in \mathcal{C}_{k-1;P_1}^v} \pi_C(x^*) + \varepsilon |P_1| \sum_{i \in P_1} (x_i^* - \varepsilon) \sum_{C \in \mathcal{C}_{k-2}^i} \pi_C(x^*).$$

Note that due to the optimality conditions (2.8)-(2.10), since $S(x^*) \cup \{v\}$ is a multipartite clique and $x_v^* = 0$, for $i \in P_1$ we have

$$\lambda^{(k)} = \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-1;P_1}^v} \pi_C(x^*).$$

Hence, for $\varepsilon < \min\limits_{i \in P_1} \{x_i\}$, we obtain

$$f_k(x^* + \varepsilon d) - f_k(x^*) = -\varepsilon |P_1| \lambda^{(k)} + \varepsilon |P_1| \lambda^{(k)} + \varepsilon |P_1| \sum_{i \in P_1} (x_i^* - \varepsilon) \sum_{C \in \mathcal{C}_{k-2}^i} \pi_C(x^*) > 0.$$

Thus, d is a feasible direction of improvement for ($\mathbf{P}^k$) at x^*, a contradiction. $\square$

Theorem 6. *If x^* is a local maximum of* $(\mathbf{P}^k)$ *then $S(x^*)$ is a strongly part-maximal multipartite clique in G.*

Proof. By Lemma 3, $S(x^*) = \bigsqcup_{s=1}^{p} P_s$ is a part-maximal p-partite clique for some $p \geq k$. Assume it is not strongly part-maximal. Then, according to Definition 12, for some $r \in [p]$ there exists $D \subset P_r$ such that $S(x^*) \setminus D$ is a subset of a $(p+1)$-partite clique in G. Since $S(x^*)$ is part-maximal, D has to be non-empty. We will consider two possible cases, $D \neq P_r$ and $D = P_r$. We will provide a direction of improvement for each case to obtain a contradiction with the local maximality of x^*.

Case 1: $D \neq P_r$. Then there exists a vertex $u \in V \setminus S(x^*)$ such that u is adjacent to all vertices in $S(x^*) \setminus D$, while $D \cup \{u\}$ is an independent set. Consider $d \in \mathbb{R}^n$ defined as follows:

$$d_i := \begin{cases} -1, & i \in D, \\ |D| & i = u, \\ 0, & \text{otherwise}. \end{cases}$$

Then

$$f_k(x^* + \varepsilon d) = \sum_{i \in D} (x_i^* - \varepsilon) \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) + \varepsilon |D| \sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) + \sum_{i \in P_r \setminus D} x_i^* \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*).$$

Note that, according to (2.11), $\sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) = \lambda^{(k)}$ for all $i \in S(x^*)$, including all $i \in D$. Also, since $S(x^*)$ is a multipartite clique and $x_u^* = 0$, for any $v \in P_r$ we have $\sum_{C \in \mathcal{C}_{k-1;P_r}^u} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) = \lambda^{(k)}$. Hence,

$$\sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) = \sum_{i \in P_r \setminus D} x_i^* \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) + \sum_{C \in \mathcal{C}_{k-1;P_r}^u} \pi_C(x^*) = \lambda^{(k)} \sum_{i \in P_j \setminus D} x_i^* + \lambda^{(k)},$$

and

$$f_k(x^* + \varepsilon d) - f_k(x^*) = -\varepsilon|D|\lambda^{(k)} + \varepsilon|D|\Big(\lambda^{(k)} \sum_{i \in P_r \setminus D} x_i^* + \lambda^{(k)}\Big) = \varepsilon|D|\lambda^{(k)} \sum_{i \in P_r \setminus D} x_i^* > 0.$$

<u>Case 2:</u> $D = P_r$. Then there exist two vertices $u, v \in V \setminus S\,(x^*)$ such that $\{u, v\} \in E$ and both u and v are adjacent to all vertices in $S\,(x^*) \setminus P_r$. Consider $d \in \mathbb{R}^n$ defined as follows:

$$d_i := \begin{cases} -1, & i \in P_r, \\ |P_r|/2 & i \in \{u, v\} \\ 0, & \text{otherwise.} \end{cases}$$

Then

$$f_k(x^* + \varepsilon d) - f_k(x^*) = \sum_{i \in P_r} (-\varepsilon) \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) + \frac{1}{2}\varepsilon|P_r|\Big(\sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) + \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*)\Big) + \delta,$$

where

$$\delta := \frac{1}{4}\varepsilon^2 |P_r|^2 \sum_{C \in \mathcal{C}_{k-2}^{u,v}} \pi_C(x^*).$$

Noting that for $i \in P_r$

$$\sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) = \lambda^{(k)}, \quad \sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) \geq \lambda^{(k)}, \quad \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) \geq \lambda^{(k)},$$

and $\delta > 0$, we conclude that $f_k(x^* + \varepsilon d) - f_k(x^*) > 0$. □

It is interesting to observe that if a feasible point x' for ($\mathbf{P}^k$) corresponds to a strongly part-maximal multipartite clique in G and the KKT conditions are satisfied at some λ', μ', this does not imply local maximality of x' for ($\mathbf{P}^k$). Indeed, consider an example graph and a feasible x' shown in Figure 2.2 for $k = 3$. Note that x' satisfies the KKT conditions with $\lambda' = 1/9, \mu' = 0$, and

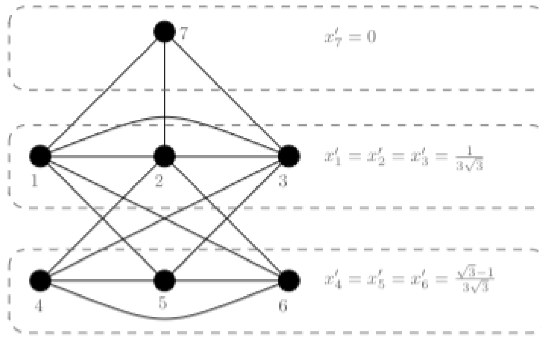

Figure 2.2: A graph in which $\{1, \ldots, 6\}$ is a strongly part-maximal 3-partite clique, x' satisfies the KKT conditions for ($\mathbf{P}^k$) with $k = 3$, but x' is not a local maximum of ($\mathbf{P}^k$). Reprinted with permission from "A Hierarchy of Standard Polynomial Programming Formulations for the Maximum Clique Problem" by Sergiy Butenko, Mykyta Makovenko, Miltiades Pardalos, 2022. SIAM Journal on Optimization, Vol. 32, pp. 2102-2128, Copyright 2022 by Society for Industrial and Applied Mathematics

$\{1, 2, 3, 4, 5, 6\}$ forms a 3-partite clique, but x' is not a local maximum, as the direction d given by

$$d_i = \begin{cases} 0, & i \in \{1, 2, 3\}, \\ -1, & i \in \{4, 5, 6\}, \\ 3, & i = 7 \end{cases}$$

is a direction of improvement.

2.2.2 Computational results

We evaluate the performance of both the original standard polynomial formulations MSPP using the CONOPT solver [61], which aims to compute a local optimum satisfying the KKT optimality conditions. We focus on the cases of $k = 2$ and $k = 3$, since the time required to formulate and solve the considered models is rather large for higher values of k, making the approach impractical at this point. For some smaller instances ($|V| \leq 100$) we also consider formulations of orders $k = 4$ and 5. The solutions obtained using CONOPT are then converted into cliques, yielding heuristic solutions to the maximum clique problem. The extracting of a maximal clique

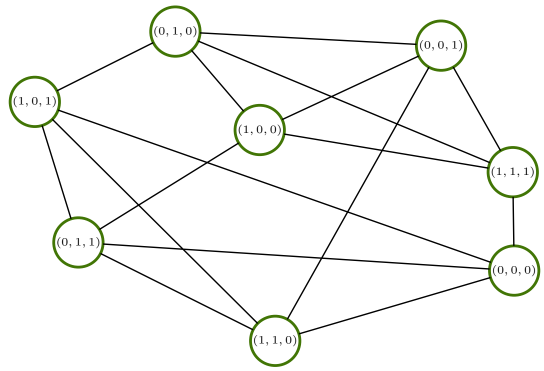

Figure 2.3: Hamming 3-2 graph. $x = x^V$ is a KKT point but not a local maximum.

corresponding to a local maximum found by CONOPT a trivial task: since any local optimum is a strongly part-maximal multipartite clique, it is sufficient to identify the parts and then pick an arbitrary vertex from each part. It is possible, however, for the solver to output a KKT point that does not correspond to a clique (see Figure 2.3). The instances where this case occurs are often highly symmetrical (e.g., "hammingX-Y" instances are representations of X-dimensional hypercubes with vertices adjacent if the diagonal between them is at least Y-dimensional). Since we are relying on the convex optimization problem solver, the obtained local maximum highly depends on the choice of the starting point, which we address by . We perform two sets of numerical experiments, based on the density of the considered graphs. The description of benchmark instances are available in Table 4.1 and Table 4.2. The computational experiments results are presented in Table 4.3 – Table 4.8. A more detailed description of the experiment setup is presented in section 4.4.

3. HIERARCHICAL STRUCTURE OF MSPP*

3.1 Background and research questions

As mentioned in the introduction, one possible approach to solving hard optimization problems lies in constructing a series of problems that approximate the original problem and are more tractable than the original. This is known as hierarchical approach. It provides a powerful framework for reasoning about the bounds on the objective value of the original problem, by providing a way to construct valid upper/lower bounds in an automated, controllable way, as the user is able to decide the trade off between the quality of the bound and the computational complexity of the relaxation by selecting the appropriate hierarchy level.

More specifically, the existing hierarchies rely on convex relaxations and proceed by introducing additional variables and constraints in order to improve the quality of the relaxation at each next level of the hierarchy. The convex relaxation obtained at the final level is tight and yields a global optimal solution to the original problem. In contrast to the existing methods, our approach works with the original feasible region; instead, it alters the objective function at each level of the hierarchy. Rather than building a tighter and tighter convex *outer* approximation for the original problem, we construct its equivalent non-convex reformulation aiming to reduce the set of local maxima that are not global. This process can be viewed as an *inner* transformation of the original problem, such that a global maximum of each reformulation is also a global maximum of the original problem, whereas a local maximum of a reformulation yields a heuristic solution to the original problem. The worst-case quality of a local maximum is expected to improve with each next reformulation in the hierarchy, and every local maximum is guaranteed to be global at the final level of the hierarchy. Hence, instead of taking advantage of convexity, as in the previous approaches, we shift the effort towards building an "equi-maximal" reformulation of the original

*Parts of the content in this chapter were first published in "A Hierarchy of Standard Polynomial Programming Formulations for the Maximum Clique Problem" by Sergiy Butenko, Mykyta Makovenko, Miltiades Pardalos in SIAM Journal on Optimization, Vol. 32, 2022, pp. 2102-2128, published by the Society for Industrial and Applied Mathematics (SIAM), Copyright 2022 by Society for Industrial and Applied Mathematics problem, in which every local maximum would be global. This property is eventually achieved at the final level of the hierarchy. In terms of computational complexity, the improved quality of local maxima in our approach comes with an increased cost of objective function evaluation, which is in contrast to the existing hierarchies, where the increase in computational expense is due to the increase in the number of variables and constraints.

3.2 Hierarchical Properties of MSPP

Now we are ready to discuss the hierarchical properties of the proposed formulations. Namely, in Theorem 7 we show that given $k \in \{2, \ldots, \omega - 1\}$, any local maximum of ($\mathbf{P}^{k+1}$) is also a local maximum of ($\mathbf{P}^{k}$). The proof of this result takes advantage of properties of local maxima established in several lemmata stated and proved before Theorem 7.

Before we can begin, we need to establish a set of helpful lemmata. They will be used to guarantee that a local optima of a higher-order problem corresponds can be used as a KKT point for a formulations of lower order.

Lemma 4. *Given three integers, $p \geq k \geq t \geq 0$, where $p \geq 1$, the following inequality holds:*

$$\frac{1}{p^{k-t}} \leq \binom{p-t}{k-t}\left(\frac{1}{p}\right)^{k-t} \leq \frac{1}{(k-t)!} \leq 1. \tag{3.1}$$

Proof. The statement clearly holds for $k = t$, which includes the case of $k = 0$. Now assume that $k > t$ (in particular, $k \geq 1$) and consider a straightforward expansion:

$$\begin{aligned} \frac{1}{p^{k-t}} &\leq \binom{p-t}{k-t}\left(\frac{1}{p}\right)^{k-t} = \frac{(p-t)!}{(p-k)!(k-t)!p^{k-t}} = \frac{(p-k+1)^{\overline{k-t}}}{(k-t)!p^{k-t}} \\ &\leq \frac{p^{k-t}}{(k-t)!p^{k-t}} = \frac{1}{(k-t)!} \leq 1. \end{aligned}$$

(Here $p^{\overline{n}} := p(p+1)\cdots(p+n-1)$ is the rising factorial.) $\square$

To establish the next result, some background on elementary symmetric polynomials is required. Given $x \in \mathbb{R}^p$, we denote by

$$e_{k,p}(x) \coloneqq \sum_{I \in \binom{[p]}{k}} \prod_{i \in I} x_i, \quad k \geq 1 \tag{3.2}$$

the k-th order elementary symmetric polynomial in p variables given by vector $x = (x_1, \ldots, x_p)$. In the following lemma, we will use Newton's inequality [62], which states that

$$\left(\frac{e_{k,p}(x)}{\binom{p}{k}} \right)^2 \geq \left(\frac{e_{k+1,p}(x)}{\binom{p}{k+1}} \right) \left(\frac{e_{k-1,p}(x)}{\binom{p}{k-1}} \right). \tag{3.3}$$

It is easy to check that (3.3) can be equivalently written as follows:

$$(e_{k,p}(x))^2 \geq e_{k-1,p}(x) e_{k+1,p}(x) \left(\frac{k+1}{k} \right) \left(\frac{p-k+1}{p-k} \right). \tag{3.4}$$

The equality in (3.4) is achieved if and only if $x_i = x_j, \forall i, j \in [p]$.

For a KKT point x^* of ($\mathbf{P}^k$) with associated KKT multipliers $\lambda^{(k)}$ and $\mu^{(k)}$, we will use the following notations:

$$Z_k \coloneqq \left\{ i \mid \mu_i^{(k)} = 0, x_i^* = 0 \right\}; \quad I_k \coloneqq S\left(x^*\right) \cup Z_k = \{ i \mid \mu_i^{(k)} = 0 \}. \tag{3.5}$$

In addition, for a direction d such that $x^* + d$ is a feasible point for ($\mathbf{P}^k$), let

$$Y_k^d \coloneqq S\left(d\right) \setminus I_k = \{ i \mid d_i > 0, \mu_i^{(k)} > 0 \}. \tag{3.6}$$

The following result is a novel bound for the value of a symmetrical polynomial of order k, when constrained by the value of a symmetrical polynomial of order $k - 1$:

Lemma 5. *Consider the following optimization problem for integers $p > k \geq 2$:*

$$\begin{aligned} \textit{minimize} \quad & e_{k,p}(x) \\ \textit{subject to} \quad & e_{k-1,p}(x) = \tbinom{p-1}{k-1}, \\ & x \in [0,1]^p \,, \end{aligned} \tag{3.7}$$

where $e_{k,p}(x)$ the k-th order elementary symmetric polynomial in p variables given by x. Then the optimal value of (3.7) *is $\binom{p-1}{k}$ and is attained at $x = e_p^j$, a p-vector whose j-th entry is 0 and all other entries are 1, for any $j \in [p]$.*

Proof. We treat the cases of $k = 2$ and $k \geq 3$ separately. For $k = 2$ the proof is straightforward, and for $k \geq 3$ we can take advantage of Newton's inequality (3.3).

First, we prove the statement of the lemma for $k = 2$. In this case, the first constraint of (3.7) becomes $\sum_{i=1}^{p} x_i = p - 1$. Hence, the objective function can be rewritten as

$$\frac{1}{2}\sum_{i=1}^{p} x_i(p-1-x_i) = \frac{1}{2}\Big((p-1)^2 - \sum_{i=1}^{p} x_i^2\Big) \geq \frac{1}{2}\big((p-1)^2 - (p-1)\big) = \binom{p-1}{2},$$

with the equality achieved for any binary x, which must have exactly one 0 entry for feasibility.

In the remainder of the proof, we assume that $k \geq 3$. For $x \in [0,1]^p$, let

$$Z(x) := \{i \mid x_i = 0\}, \quad M(x) := \{i \mid 0 < x_i < 1\}, \quad E(x) := \{i \mid x_i = 1\},$$

and

$$e_{k,p}^{S}(x) := \sum_{I \in \binom{[p]\setminus S}{k}} \prod_{i \in I} x_i, \quad k \geq 1.$$

Suppose that x^* is an optimal solution of (3.7). Note that if there is $i \in [p]$ such that $x_i^* = 0$, then $e_{k-1,p}(x^*) = e_{k-1,p}^{\{i\}}(x^*) = \sum_{I \in \binom{[p]\setminus\{i\}}{k-1}} \prod_{j \in I} x_j \leq \binom{p-1}{k-1}$, with equality holding if and only if $x_j^* = 1$ for all $j \neq i$. This implies that $|Z(x^*)| \leq 1$ and the statement of the lemma holds when $|Z(x^*)| = 1$. To complete the proof, we will show that the only remaining case of $|Z(x^*)| = 0$ is impossible. We will use contradiction. Assume that $|Z(x^*)| = 0$, so for all $i \in [p] : x_i^* \neq 0$.

For the equality constraint in (3.7) to hold at x^*, $M(x^*)$ must contain at least two elements. In the remainder of the proof, we will first show that in this case all entries x_i^* corresponding to $i \in M(x^*)$ must be equal to each other; then we will use this observation to obtain a contradiction with optimality of x^*.

Suppose there is a pair $\{i,j\} \subseteq M(x^*)$ such that $x_i^* \neq x_j^*$. It is straightforward to check that the linear independence constraint qualification is satisfied at x^*. Therefore, from the KKT conditions for (3.7), there exists $\lambda \in \mathbb{R}$ such that

$$e_{k-1,p}^{\{i\}}(x^*) = -\lambda e_{k-2,p}^{\{i\}}(x^*), \tag{3.8}$$

$$e_{k-1,p}^{\{j\}}(x^*) = -\lambda e_{k-2,p}^{\{j\}}(x^*). \tag{3.9}$$

The last two equations can be rewritten as

$$x_j^* e_{k-2,p}^{\{i,j\}}(x^*) + e_{k-1,p}^{\{i,j\}}(x^*) = -\lambda\big(x_j^* e_{k-3,p}^{\{i,j\}}(x^*) + e_{k-2,p}^{\{i,j\}}(x^*)\big), \tag{3.10}$$

$$x_i^* e_{k-2,p}^{\{i,j\}}(x^*) + e_{k-1,p}^{\{i,j\}}(x^*) = -\lambda\big(x_i^* e_{k-3,p}^{\{i,j\}}(x^*) + e_{k-2,p}^{\{i,j\}}(x^*)\big). \tag{3.11}$$

By subtracting (3.11) from (3.10) and considering that $x_i^* \neq x_j^*$, we obtain

$$e_{k-2,p}^{\{i,j\}}(x^*) = -\lambda e_{k-3,p}^{\{i,j\}}(x^*), \tag{3.12}$$

which, combined with (3.10) or (3.11), implies that

$$e_{k-1,p}^{\{i,j\}}(x^*) = -\lambda e_{k-2,p}^{\{i,j\}}(x^*). \tag{3.13}$$

Expressing λ from (3.12) and substituting in (3.13) we obtain

$$e_{k-1,p}^{\{i,j\}}(x^*) e_{k-3,p}^{\{i,j\}}(x^*) = \big(e_{k-2,p}^{\{i,j\}}(x^*)\big)^2, \tag{3.14}$$

which contradicts Newton's inequality (3.4). Therefore, x_i^* has to be equal to x_j^*. Hence, each $x_i^*, i \in [p]$ must be equal to either 1 or some constant $t \in (0,1)$, and at least two of the entries must be equal to t. Without loss of generality, we can assume that the first two entries of x^* are equal to t. Denoting the last $p-2$ entries of x^* by $y \in \mathbb{R}^{p-2}$, we can represent x^* as $x^* = (t, t, y)$.

Now let

$$x^{(k)}(\varepsilon) \coloneqq (t+\varepsilon, t_k^*(\varepsilon), y), \tag{3.15}$$

where $\varepsilon < 1-t$ and $t_k^*(\varepsilon)$ is chosen to satisfy the following equation:

$$e_{k+1,p}(x^*) = e_{k+1,p}(x^{(k)}(\varepsilon)). \tag{3.16}$$

Note that

$$e_{k+1,p}(x^{(k)}(\varepsilon)) = e_{k+1,p-2}(y) + (t+\varepsilon)t_k^*(\varepsilon)e_{k-1,p-2}(y) + (t_k^*(\varepsilon)+t+\varepsilon)e_{k,p-2}(y)$$

and

$$e_{k+1,p}(x^*) = e_{k+1,p-2}(y) + t^2 e_{k-1,p-2}(y) + 2te_{k,p-2}(y).$$

Hence, (3.16) is equivalent to

$$(t+\varepsilon)t_k^*(\varepsilon)e_{k-1,p-2}(y) + (t_k^*(\varepsilon)+t+\varepsilon)e_{k,p-2}(y) = t^2 e_{k-1,p-2}(y) + 2te_{k,p-2}(y),$$

which can be rewritten as

$$t_k^*(\varepsilon)\big((t+\varepsilon)e_{k-1,p-2}(y) + e_{k,p-2}(y)\big) = t^2 e_{k-1,p-2}(y) + (t-\varepsilon)e_{k,p-2}(y).$$

We obtain

$$t_k^*(\varepsilon) = \frac{t^2 e_{k-1,p-2}(y) + (t-\varepsilon)e_{k,p-2}(y)}{(t+\varepsilon)e_{k-1,p-2}(y) + e_{k,p-2}(y)}. \tag{3.17}$$

Recall that each entry of y is either 1 or $t \in (0,1)$; hence, $t_k^*(\varepsilon) > 0$ for a sufficiently small ε. Also, it is easy to see that $t_k^*(\varepsilon) < t < 1$. Now observe that $x^{(k-2)}(\varepsilon)$ is a feasible point for (3.7) due to requirement (3.16) and feasibility of x^*. Also, (3.16) implies that $e_{k,p}(x^*) = e_{k,p}(x^{(k-1)}(\varepsilon))$, that is, the objective value of (3.7) is the same at x^* and $x^{(k-1)}(\varepsilon)$. According to (3.15), $x^{(k-1)}(\varepsilon)$ and $x^{(k-2)}(\varepsilon)$ differ only in the second entry. Clearly, if $t_{k-2}^*(\varepsilon) < t_{k-1}^*(\varepsilon)$, this would imply that $e_{k,p}(x^{(k-2)}(\varepsilon)) < e_{k,p}(x^{(k-1)}(\varepsilon)) = e_{k,p}(x^*)$. Hence, showing that $t_{k-2}^*(\varepsilon) < t_{k-1}^*(\varepsilon)$ would yield a contradiction with optimality of x^*, needed to complete the proof. Using (3.17), we can verify that the inequality $t_{k-1}^*(\varepsilon) > t_{k-2}^*(\varepsilon)$ simplifies to

$$\varepsilon^2\big(\left(e_{k-2,p-2}(y)\right)^2 - e_{k-1,p-2}(y)e_{k-3,p-2}(y)\big) > 0,$$

which holds due to Newton's inequality (3.4). This completes the proof. $\square$

Now we are ready to establish the main results of this section.

In the following two lemmata, we assume that x^* is a local maximum of ($\mathbf{P}^k$), the corresponding multipartite clique is given by $S(x^*) = \bigsqcup_{s=1}^p P_s$, where $p \geq k$, and $\lambda^{(k)}$ and $\mu^{(k)}$ are the corresponding KKT multipliers satisfying (2.8)–(2.10). Lemma 6 characterizes the set of vertices outside of the support set of a local maximum that have the corresponding KKT multiplier equal to zero. Lemma 7 further refines this characterization, and is then used in Lemma 8 to show the KKT conditions for ($\mathbf{P}^k$) are satisfied at a point of local maximum of ($\mathbf{P}^{k+1}$).

Lemma 6. *If $Z_k \neq \emptyset$ then for each vertex $u \in Z_k$, $\{u\} \cup S(x^*)$ is a p-partite clique. Moreover, $S(x^*)$ is a maximal p-partite clique if and only if $Z_k = \emptyset$.*

Proof. First, we show that if $u \in Z_k$ has no neighbor in one of the parts P_r, $r \in [p]$, of $S(x^*)$ then $\{u\} \cup S(x^*)$ is a p-partite clique. Suppose there is a vertex in $S(x^*) \setminus P_r$ that is not adjacent to u, then, recalling (1.12), we have the following inequality:

$$\sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) < \sum_{D \in \binom{[p]\setminus\{r\}}{k-1}} \prod_{s \in D} \sum_{v \in P_s} x_v^* = \binom{p-1}{k-1}\frac{1}{p^{k-1}}. \tag{3.18}$$

However, since $\mu_u^{(k)} = 0$, from (2.8) and Corollary 3 we have

$$\sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) = \lambda^{(k)} = \binom{p-1}{k-1} \frac{1}{p^{k-1}}, \tag{3.19}$$

which contradicts (3.18).

Now assume that u is adjacent to at least one vertex in each part of $S(x^*)$. If u is adjacent to every vertex in $S(x^*)$, then x^* is not a local maximum due to Lemma 3. Therefore, there must exist $r \in [p]$ such that some vertex $w \in P_r$ is adjacent to u, while another vertex $v \in P_r$ is not adjacent to u. Consider $d \in \mathbb{R}^n$ defined as

$$d_i \coloneqq \begin{cases} -2, & i = v, \\ 1, & i \in \{u, w\}, \\ 0, & \text{otherwise.} \end{cases}$$

Since $\{u, v\}, \{v, w\} \notin E$ and $x_u^* = 0$, we have:

$$\begin{aligned} f_k(x^* + \varepsilon d) = &\sum_{C \in \mathcal{C}_{k;u,v,w}} \pi_C(x^*) + (x_v^* - 2\varepsilon) \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) + (x_w^* + \varepsilon) \sum_{C \in \mathcal{C}_{k-1;u}^w} \pi_C(x^*) \\ &+ \varepsilon \sum_{C \in \mathcal{C}_{k-1;w}^u} \pi_C(x^*) + \varepsilon (x_w^* + \varepsilon) \sum_{C \in \mathcal{C}_{k-2}^{u,w}} \pi_C(x^*). \end{aligned}$$

Also,

$$f_k(x^*) = \sum_{C \in \mathcal{C}_k} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k;u,v,w}} \pi_C(x^*) + x_v^* \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) + x_w^* \sum_{C \in \mathcal{C}_{k-1;u}^w} \pi_C(x^*).$$

Hence,

$$\begin{aligned} f_k(x^* + \varepsilon d) - f_k(x^*) = &-2\varepsilon \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) + \varepsilon \sum_{C \in \mathcal{C}_{k-1;u}^w} \pi_C(x^*) + \varepsilon \sum_{C \in \mathcal{C}_{k-1;w}^u} \pi_C(x^*) \\ &+ \varepsilon (x_w^* + \varepsilon) \sum_{C \in \mathcal{C}_{k-2}^{u,w}} \pi_C(x^*). \end{aligned} \tag{3.20}$$

Considering that $x_u^* = 0$ and taking into account (2.8), we have

$$\sum_{C \in \mathcal{C}_{k-1;u}^w} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-1}^w} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) = \lambda^{(k)}. \tag{3.21}$$

Also, since $\mu_u^{(k)} = 0$, (2.8) implies that

$$\sum_{C \in \mathcal{C}_{k-1}^u} \pi_C(x^*) = \sum_{C \in \mathcal{C}_{k-1;w}^u} \pi_C(x^*) + x_w^* \sum_{C \in \mathcal{C}_{k-2}^{u,w}} \pi_C(x^*) = \lambda^{(k)}. \tag{3.22}$$

Thus, using (3.21) and (3.22) in (3.20) we obtain

$$f_k(x^* + \varepsilon d) - f_k(x^*) = -2\varepsilon\lambda^{(k)} + \varepsilon\lambda^{(k)} + \varepsilon\lambda^{(k)} + \varepsilon^2 \sum_{C \in \mathcal{C}_{k-2}^{u,w}} \pi_C(x^*) = \varepsilon^2 \sum_{C \in \mathcal{C}_{k-2}^{u,w}} \pi_C(x^*) > 0. \tag{3.23}$$

The last inequality holds since u is adjacent to at least one vertex in each part of $S(x^*)$. Patently, (3.23) implies that d is a feasible direction of improvement for (**P**^{k}) at x^*, which contradicts the assumption that x^* is a local maximum.

To establish the second statement of the lemma, note that from the first statement we have $Z_k \neq \emptyset \Longrightarrow S(x^*)$ is not a maximal p-partite clique. On the other hand, if $S(x^*)$ is not a maximal p-partite clique then there exists $u \in V \setminus S(x^*)$ such that $\{u\} \cup S(x^*)$ is a p-partite clique. From (2.8), $\mu_u^{(k)} = 0$, so $u \in Z_k$ and $Z_k \neq \emptyset$. $\square$

Lemma 7. *Z_k can be represented as a disjoint union of $U_s, s \in [p]$, where for each $s \in [p]$, $U_s \cup S(x^*)$ is a p-partite clique in G, with $U_s \cup P_s$ being one of its p parts. Moreover, the restriction of x^* to $S(x^*) \cup Z_k$ is a global maximum of* (**P**^{k}) *formulated for graph $G[S(x^*) \cup Z_k]$.*

Proof. Given $s \in [p]$, let U_s be the set of vertices from Z_k with no neighbors in P_s. Due to Lemma 6, each $v \in Z_k$ belongs to exactly one among the sets $U_s, s \in [p]$ and forms a multipartite clique together with $S(x^*) \setminus P_s$. To complete the proof, we need to show that U_s is an independent set. Assume otherwise. Then there exist $u, v \in U_s$ such that $\{u, v\} \in E$ and $\{u, v\} \cup S(x^*) \setminus P_s$ forms a $(p+1)$-partite clique. Hence, $S(x^*)$ is not a strongly part-maximal multipartite clique, a contradiction with Theorem 6. Finally, note that to form a clique, we cannot select vertices from both U_s and P_s. This means that a maximum clique in $G\left[S\left(x^*\right) \cup Z_k\right]$ has at most p vertices, while x^* corresponds to a multipartite clique with exactly p parts. Therefore, by Theorems 3 and 5 the restriction of x^* to $S\left(x^*\right) \cup Z_k$ is a global maximum of (**P**^{k}) stated for $G\left[S\left(x^*\right) \cup Z_k\right]$. $\square$

Lemma 8. *Let x^* be a local maximum of* (**P**$^{k+1}$) *for some $k \in \{2, \ldots, \omega-1\}$. Then x^* satisfies the KKT conditions for* (**P**^{k})*. Moreover, if the KKT multiplier $\mu_i^{(k+1)}$ associated with vertex i for* (**P**$^{k+1}$) *is positive, then so is the KKT multiplier $\mu_i^{(k)}$ for* (**P**^{k})*, that is, $I_k \subseteq I_{k+1}$.*

Proof. Assume x^* is a local maximum of (**P**$^{k+1}$) with the corresponding multipartite clique $S\left(x^*\right) = \bigsqcup\limits_{s=1}^{p} P_s$, where $p \geq k+1$, and the KKT multiplier $\lambda^{(k+1)} = \binom{p-1}{k}\frac{1}{p^k}$ (per Corollary 3). Consider any $v \in S\left(x^*\right) \cup Z_{k+1}$. According to Lemma 7, v belongs to some $P_s \cup U_s$, forming a p-partite clique with $P_r, r \in [p] \setminus \{s\}$. Thus, recalling (1.12), we have

$$\sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) = \sum_{D \in \binom{[p]\setminus\{s\}}{k-1}} \prod_{r \in D} \sum_{v \in P_r} x_v^* = \sum_{D \in \binom{[p]\setminus\{s\}}{k-1}} \frac{1}{p^{k-1}} = \binom{p-1}{k-1}\frac{1}{p^{k-1}}.$$

Hence, the KKT condition (2.8) for (**P**^{k}) clearly holds at x^* for all $v \in I_k$ with $\lambda^{(k)} = \binom{p-1}{k-1}\frac{1}{p^{k-1}}$. To complete the proof, we need to show that for any $v \in V \setminus I_{k+1}$:

$$\mu_v^{(k+1)} = \lambda^{(k+1)} - \sum_{C \in \mathcal{C}_k^v} \pi_C(x^*) > 0 \quad \Longrightarrow \quad \mu_v^{(k)} = \lambda^{(k)} - \sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) > 0,$$

or, equivalently,

$$\sum_{C \in \mathcal{C}_{k-1}^v} \pi_C(x^*) \geq \lambda^{(k)} \quad \Longrightarrow \quad \sum_{C \in \mathcal{C}_k^v} \pi_C(x^*) \geq \lambda^{(k+1)}.$$

Let $y^*(v) \in \mathbb{R}^p$ be defined as follows:

$$y_s^*(v) = p \sum_{j \in P_s \cap N_v} x_j^*, \quad s \in [p],$$

where N_v is the set of vertices adjacent to v in G.

Since $\sum_{j \in P_s \cap N_v} x_j^* \leq \sum_{j \in P_s} x_j^* = 1/p$ (by Theorem 5), $y_s^*(v) \in [0,1]^p$.

Note that for $t \in \{0,1\}$ we have:

$$\begin{aligned}\sum_{C \in \mathcal{C}^v_{k-t}} \pi_C(x^*) &= \sum_{D \in \binom{[p]}{k-t}} \prod_{s \in D} \sum_{j \in P_s \cap N_v} x^*_j = \frac{1}{p^{k-t}} \sum_{D \in \binom{[p]}{k-t}} \prod_{s \in D} y^*_s(v) \\ &= \frac{1}{p^{k-t}} e_{k-t,p}(y^*(v)),\end{aligned}$$

where $e_{k-t,p}$ is an elementary symmetric polynomial as defined in (3.2). Now what we want to show becomes

$$e_{k-1,p}(y^*(v)) \geq \binom{p-1}{k-1} \quad \Longrightarrow \quad e_{k,p}(y^*(v)) \geq \binom{p-1}{k}. \tag{3.24}$$

Since $y^*_s(v) \in [0,1]^p$, (3.24) follows from Lemma 5. □

The proof of the main structural result (Theorem 7) will be based on the definition of a local maximum. In addition to the lemmata above, it will use one more technical lemma, established next. Recall the definition of I_k and Y^d_k given in (3.5) and (3.6), respectively.

Lemma 9. *Let x^* be a point satisfying the KKT conditions for* ($\mathbf{P}^k$). *Let*

$$\bar{\varepsilon} := \min\left\{1/(2^n p^{k-2}), 1/(2^{p+1} p^{k-2} n)\right\}. \tag{3.25}$$

Suppose that $\varepsilon \in (0, \bar{\varepsilon}]$ and $d \in \mathbb{R}^n$ is such that $\|d\| < \varepsilon$, $x^* + d$ is feasible for ($\mathbf{P}^k$)*, and $Y^d_k \neq \emptyset$. Then*

$$\sigma' := \sum_{t=2}^{k} \sum_{U \in \mathcal{C}_t(I_k)} \pi_U(d) \sum_{C \in \mathcal{C}^U_{k-t}} \pi_C(x^*) \leq \frac{n}{2} \varepsilon \sum_{i \in Y^d_k} d_i. \tag{3.26}$$

Proof. Since $x^* + d$ is a feasible point,

$$\sum_{i \in S(d)} d_i = 0 \quad \text{and} \quad \sum_{i \in I_k} d_i = -\sum_{i \in Y^d_k} d_i. \tag{3.27}$$

Also, since $\|d\| < \varepsilon$, for $t, q \geq 1$ and any $U \in \mathcal{C}_t(I_k)$, $D \in \mathcal{C}_q(Y_k^d)$ we have

$$|\pi_U(d)| \leq \varepsilon^t \leq \varepsilon, \quad 0 \leq \pi_D(d) \leq \varepsilon^q \leq \varepsilon. \tag{3.28}$$

To derive an upper bound on σ', we first use the multipartite structure of $S(x^*)$ to write

$$\sigma' = \sum_{t=2}^{k} \sum_{U \in \mathcal{C}_t(I_k)} \pi_U(d) \binom{p-t}{k-t} \left(\frac{1}{p}\right)^{k-t} \tag{3.29}$$

$$= \sum_{U \in \mathcal{C}_2(I_k)} \pi_U(d) \sum_{t=0}^{k-2} \sum_{D \in \mathcal{C}_t^U(I_k)} \pi_D(d) \binom{p-t-2}{k-t-2} \left(\frac{1}{p}\right)^{k-t-2}. \tag{3.30}$$

For $u, w \in Z_k$, we have no information on whether the edge $\{u, w\}$ is present in $G[I_k]$ if $u \in U_s$, $w \in U_r$, $s \neq r$. However, we will show that by assuming that every such edge is indeed present, we can obtain a valid upper bound on σ'. Indeed, consider $u \in U_s, w \in U_r, s \neq r$ and let

$$\sigma'[u, w] \coloneqq d_u d_w \sum_{t=0}^{k-2} \sum_{U \in \mathcal{C}_t^{u,w}(I_k)} \pi_U(d) \binom{p-t-2}{k-t-2} \left(\frac{1}{p}\right)^{k-t-2}.$$

Observe that

$$\sigma'[u, w] = d_u d_w \binom{p-2}{k-2} \left(\frac{1}{p}\right)^{k-2} + d_u d_w \sum_{t=1}^{k-2} \sum_{U \in \mathcal{C}_t^{u,w}(I_k)} \pi_U(d) \binom{p-t-2}{k-t-2} \left(\frac{1}{p}\right)^{k-t-2}. \tag{3.31}$$

Since $u, w \in Z_k$, we have $d_u, d_w \geq 0$ due to the feasibility of $x^* + d$, hence

$$d_u d_w \binom{p-2}{k-2} \left(\frac{1}{p}\right)^{k-2} \geq d_u d_w \frac{1}{p^{k-2}}. \tag{3.32}$$

Also, due to (3.28) and Lemma 4,

$$d_u d_w \sum_{t=1}^{k-2} \sum_{U \in \mathcal{C}_t^{u,w}(I_k)} \pi_U(d) \binom{p-t-2}{k-t-2} \left(\frac{1}{p}\right)^{k-t-2} \geq -d_u d_w \sum_{t=1}^{k-2} \sum_{U \in \mathcal{C}_t^{u,w}(I_k)} \varepsilon \geq -d_u d_w 2^n \varepsilon. \tag{3.33}$$

Using (3.32) and (3.33) in (3.31), a lower bound on $\sigma'[u, w]$ can be given as

$$\sigma'[u, w] \geq d_u d_w \frac{1}{p^{k-2}} - d_u d_w 2^n \varepsilon = d_u d_w \left[\frac{1}{p^{k-2}} - 2^n \varepsilon\right] \geq 0, \tag{3.34}$$

assuming

$$\varepsilon \leq \frac{1}{2^n p^{k-2}}. \tag{3.35}$$

Therefore, if the edge $\{u, v\}$ is missing, we cannot decrease the value of $\sigma'[u, w]$ by assuming the edge is present, as long as (3.35) holds. This implies that we can get an upper bound on σ' by assuming $\bigsqcup_{s=1}^{p}(P_s \cup U_s)$ to be a multipartite clique with the parts $P'_s = P_s \cup U_s$. Hence, denoting $d'_s := \sum_{j \in P'_s} d_j$, we can assume that I_k is a multipartite clique in (3.29) to obtain an upper bound

$$\sigma' \leq \sum_{t=2}^{k} \sum_{I \in \binom{[p]}{t}} \prod_{s \in I} \sum_{j \in P'_s} d_j \binom{p-t}{k-t} \left(\frac{1}{p}\right)^{k-t} = \sum_{t=2}^{k} e_{t,p}(d') \binom{p-t}{k-t} \left(\frac{1}{p}\right)^{k-t}, \tag{3.36}$$

where $e_{t,p}(d')$ is an elementary symmetric polynomial as defined in (3.2). Now observe that

$$\sum_{s \in S(d')} d'_s = \sum_{s \in [p]} d'_s = \sum_{s \in [p]} \sum_{j \in P_s \cup U_s} d_j = \sum_{j \in I_k} d_j.$$

Hence, in view of (3.27) we have

$$\sum_{s \in S(d')} d'_s = -\sum_{i \in Y_k^d} d_i. \tag{3.37}$$

Also, $0 \leq d_i \leq \varepsilon \ \forall i \in Y_k^d$ and the definition (3.6) of Y_k^d imply that $0 < \sum_{i \in Y_k^d} d_i \leq n\varepsilon$, thus, we obtain

$$\begin{aligned} 2e_{2,p}(d') &= \sum_{s \in S(d')} d'_s \sum_{r \in S(d') \setminus \{s\}} d'_r = \sum_{s \in S(d')} d'_s \Big(-\sum_{i \in Y_k^d} d_i - d'_s \Big) \\ &= -\Big(\sum_{s \in S(d')} d'_s \Big) \sum_{i \in Y_k^d} d_i - \sum_{s \in S(d')} d_s'^2 = \Big(\sum_{i \in Y_k^d} d_i \Big)^2 - \sum_{s \in S(d')} d_s'^2 \\ &\leq \sum_{i \in Y_k^d} d_i n\varepsilon - \sum_{s \in S(d')} d_s'^2. \end{aligned} \tag{3.38}$$

On the other hand, any term in $e_{t,p}(d')$, where $t > 3$, can be upper bounded by $n\varepsilon \max_{s \in S(d')} d_s'^2$, so using Lemma 4 we have

$$\sum_{t=3}^{k} e_{t,p}(d')\binom{p-t}{k-t}\left(\frac{1}{p}\right)^{k-t} \leq \sum_{t=3}^{k} |e_{t,p}(d')| \leq 2^p n\varepsilon \max_{s\in S(d')} d_s'^2. \tag{3.39}$$

Therefore, using (3.38) and (3.39) in (3.36), we obtain:

$$\sigma' \leq \frac{1}{2}\binom{p-2}{k-2}\left(\frac{1}{p}\right)^{k-2}\Big(\sum_{i\in Y_k^d} d_i n\varepsilon - \sum_{s\in S(d')} d_s'^2\Big) + 2^p n\varepsilon \max_{s\in S(d')} d_s'^2. \tag{3.40}$$

Note that $\max_{s\in S(d')} d_s'^2$ is a part of $\sum_{s\in S(d')} d_s'^2$. Hence,

$$\varepsilon \leq \frac{1}{2^{p+1}p^{k-2}n} \quad \Longrightarrow \quad 2^p n\varepsilon \leq \frac{1}{2}\binom{p-2}{k-2}\left(\frac{1}{p}\right)^{k-2} \tag{3.41}$$

in (3.40) yields the desired upper bound:

$$\sigma' \leq \frac{1}{2}\binom{p-2}{k-2}\left(\frac{1}{p}\right)^{k-2}\sum_{i\in Y_k^d} d_i n\varepsilon \leq \frac{n}{2}\varepsilon\sum_{i\in Y_k^d} d_i. \tag{3.42}$$

□

We are now ready to establish the main structural result.

Theorem 7. *Suppose x^* is a local maximum of* ($\mathbf{P}^{k+1}$) *for some $k \in \{2,\dots,\omega-1\}$. Then x^* is a local maximum of* ($\mathbf{P}^{k}$).

Proof. Since x^* is a local maximum for ($\mathbf{P}^{k+1}$), by Theorem 6, $S(x^*)$ is a strongly part-maximal multipartite clique $S(x^*) = \bigsqcup_{s=1}^{p} P_s$, where $p \geq k+1$. Also, due to Lemma 8, there exist $\lambda^{(k)}$, $\mu^{(k)}$ satisfying KKT conditions for x^* relative to ($\mathbf{P}^{k}$) and $I_k \subseteq I_{k+1}$. We will establish the statement of the theorem by showing that there exists a sufficiently small $\varepsilon > 0$ such that $f_k(x') \leq f_k(x^*)$ for all feasible x' with $\|x' - x^*\| < \varepsilon$, where $\|\cdot\|$ denotes the standard Euclidean norm. First, note that selecting

$$\varepsilon < \min_{i\in S(x^*)} x_i^* \tag{3.43}$$

guarantees that $S(x^*) \subseteq S(x')$. Let us define $d \coloneqq x' - x^*$.

Consider

$$\begin{aligned}
f_k(x') - f_k(x^*) &= \sum_{C \in \mathcal{C}_k} \pi_C(x^* + d) - \sum_{C \in \mathcal{C}_k} \pi_C(x^*) && (3.44)\\
&= \sum_{t=1}^{k} \sum_{D \in \mathcal{C}_t} \pi_D(d) \sum_{C \in \mathcal{C}_{k-t}^D} \pi_C(x^*) && (3.45)\\
&= \sum_{i \in S(d)} d_i \sum_{C \in \mathcal{C}_{k-1}^i} \pi_C(x^*) + \sum_{t=2}^{k} \sum_{D \in \mathcal{C}_t} \pi_D(d) \sum_{C \in \mathcal{C}_{k-t}^D} \pi_C(x^*) && (3.46)\\
&= \sum_{i \in S(d)} d_i(\lambda^{(k)} - \mu_i^{(k)}) + \sum_{t=2}^{k} \sum_{D \in \mathcal{C}_t} \pi_D(d) \sum_{C \in \mathcal{C}_{k-t}^D} \pi_C(x^*) && (3.47)\\
&= \sum_{i \in S(d)} d_i(\lambda^{(k)} - \mu_i^{(k)}) + \sigma, && (3.48)
\end{aligned}$$

where

$$\sigma \coloneqq \sum_{t=2}^{k} \sum_{D \in \mathcal{C}_t} \pi_D(d) \sum_{C \in \mathcal{C}_{k-t}^D} \pi_C(x^*). \tag{3.49}$$

Here (3.47) follows from (2.8), since the KKT conditions hold. Note that $d_i < 0$ implies that $x_i > 0$ and, subsequently, $\mu_i^{(k)} = 0$. Hence, considering (3.27),

$$\sum_{i \in S(d)} d_i(\lambda^{(k)} - \mu_i^{(k)}) = \lambda^{(k)} \sum_{i \in S(d)} d_i - \sum_{i \in Y_k^d} d_i \mu_i^{(k)} = -\sum_{i \in Y_k^d} d_i \mu_i^{(k)} \leq 0. \tag{3.50}$$

The inequality in (3.50) is satisfied at equality if and only if $Y_k^d = \emptyset$. In this case $d_i = 0$ for all i such that $\mu_i^{(k)} > 0$ and hence $S(x') \subseteq I_k$. Due to Lemma 7 applied for ($\mathbf{P}^{k+1}$), any clique in $G[I_{k+1}]$ has at most p vertices. This, along with the fact that $I_k \subseteq I_{k+1}$, implies that $f_k(x') \leq f_k(x^*)$. Hence, in the remainder of the proof we assume that the inequality in (3.50) is strict, i.e., $Y_k^d \neq \emptyset$.

Next we analyze the expression (3.49) for σ, with the aim of proving that the expression in (3.48) is non-positive for a sufficiently small ε. We rewrite the sum in (3.49) by assuming that q of the vertices in a clique D are in Y_k^d for $q = 0, \ldots, k$, and the remaining vertices are in I_k.

We obtain

$$\sigma = \sum_{t=2}^{k} \sum_{D \in \mathcal{C}_t} \pi_D(d) \sum_{C \in \mathcal{C}_{k-t}^D} \pi_C(x^*) = \sigma' + \sigma'' + \sigma''', \tag{3.51}$$

where σ' corresponds to the case where all vertices in D are from I_k, σ'' corresponds to the case where all vertices in D are from Y_k^d, and σ''' describes the case where D contains at least one vertex from I_k and Y_k^d, i.e.,

$$\sigma' \;:=\; \sum_{t=2}^{k} \sum_{U \in \mathcal{C}_t(I_k)} \pi_U(d) \sum_{C \in \mathcal{C}_{k-t}^U} \pi_C(x^*), \tag{3.52}$$

$$\sigma'' \;:=\; \sum_{q=2}^{k} \sum_{D \in \mathcal{C}_q(Y_k^d)} \pi_D(d) \sum_{C \in \mathcal{C}_{k-q}^D} \pi_C(x^*), \tag{3.53}$$

$$\sigma''' \;:=\; \sum_{q=1}^{k-1} \sum_{t=1}^{k-q} \sum_{D \in \mathcal{C}_q(Y_k^d)} \pi_D(d) \sum_{U \in \mathcal{C}_t^D(I_k)} \pi_U(d) \sum_{C \in \mathcal{C}_{k-q-t}^{D \cup U}} \pi_C(x^*). \tag{3.54}$$

By Lemma 9,

$$\sigma' \leq \frac{n}{2} \varepsilon \sum_{i \in Y_k^d} d_i. \tag{3.55}$$

for a sufficiently small $\varepsilon > 0$. Next, we establish upper bounds on σ'' and σ''' defined in (3.53) and (3.54), respectively. Note that since $0 \leq d_i \leq \varepsilon \; \forall i \in Y_k^d$, we have:

$$\pi_D(d) \leq \sum_{i \in Y_k^d} d_i, \quad \forall D \in \mathcal{C}_q(Y_k^d), \; q \geq 1. \tag{3.56}$$

Using (3.28) and (3.56), we obtain the following bounds on σ'' and σ''', respectively:

$$
\begin{aligned}
\sigma'' &= \sum_{q=2}^{k} \sum_{D\in\mathcal{C}_q(Y_k^d)} \pi_D(d) \sum_{C\in\mathcal{C}_{k-q}^{D}} \pi_C(x^*) \\
&\le \sum_{i\in Y_k^d} d_i \Big(\sum_{q=1}^{k-1} \sum_{D\in\mathcal{C}_q^i(Y_k^d)} \pi_D(d) \sum_{C\in\mathcal{C}_{k-q}^{\{i\}\cup D}} \pi_C(x^*) \Big) \\
&\le \sum_{q=1}^{k-1} \sum_{i\in Y_k^d} d_i \sum_{D\in\mathcal{C}_q^i(Y_k^d)} \varepsilon \sum_{C\in\mathcal{C}_{k-q}^{\{i\}\cup D}} \pi_C(x^*) \\
&\le \varepsilon \sum_{q=1}^{k-1} \sum_{i\in Y_k^d} d_i \sum_{D\in\mathcal{C}_q(Y_k^d)} \sum_{C\in\mathcal{C}_{k-q}^{D}} \pi_C(x^*) \\
&= \varepsilon \sum_{q=1}^{k-1} \sum_{t=0}^{0} \sum_{D\in\mathcal{C}_q(Y_k^d)} \sum_{i\in Y_k^d} d_i \sum_{U\in\mathcal{C}_t^D(I_k)} \sum_{C\in\mathcal{C}_{k-q}^{D\cup U}} \pi_C(x^*),
\end{aligned}
$$

$$
\begin{aligned}
\sigma''' &= \sum_{q=1}^{k-1} \sum_{t=1}^{k-q} \sum_{D\in\mathcal{C}_q(Y_k^d)} \pi_D(d) \sum_{U\in\mathcal{C}_t^D(I_k)} \pi_U(d) \sum_{C\in\mathcal{C}_{k-q-t}^{D\cup U}} \pi_C(x^*) \\
&\le \sum_{q=1}^{k-1} \sum_{t=1}^{k-q} \sum_{D\in\mathcal{C}_q(Y_k^d)} \pi_D(d) \sum_{U\in\mathcal{C}_t^D(I_k)} \varepsilon \sum_{C\in\mathcal{C}_{k-q-t}^{D\cup U}} \pi_C(x^*) \\
&\le \varepsilon \sum_{q=1}^{k-1} \sum_{t=1}^{k-q} \sum_{D\in\mathcal{C}_q(Y_k^d)} \sum_{i\in Y_k^d} d_i \sum_{U\in\mathcal{C}_t^D(I_k)} \sum_{C\in\mathcal{C}_{k-q-t}^{D\cup U}} \pi_C(x^*).
\end{aligned}
$$

Hence,

$$
\sigma'' + \sigma''' \le \varepsilon \sum_{q=1}^{k-1} \sum_{t=0}^{k-q} \sum_{D\in\mathcal{C}_q(Y_k^d)} \sum_{i\in Y_k^d} d_i \sum_{U\in\mathcal{C}_t^D(I_k)} \sum_{C\in\mathcal{C}_{k-q-t}^{D\cup U}} \pi_C(x^*) \tag{3.57}
$$

Also, due to Lemma 4, and Theorem 5 we have

$$
\sum_{C\in\mathcal{C}_{k-q-t}^{D\cup U}} \pi_C(x^*) \le \binom{p-q-t}{k-q-t} \left(\frac{1}{p}\right)^{k-q-t} \le 1. \tag{3.58}
$$

Using (3.58) in (3.57) and considering that the number of different subsets of the set of n nodes is bounded from above by 2^n, we obtain

$$\begin{aligned}\sigma'' + \sigma''' &\leq \varepsilon \sum_{i \in Y_k^d} d_i \sum_{q=1}^{k-1} \sum_{D \in \mathcal{C}_q(Y_k^d)} \sum_{t=0}^{k-q} \sum_{U \in \mathcal{C}_t^D(I_k)} 1 \\ &\leq \varepsilon \sum_{i \in Y_k^d} d_i \sum_{q=1}^{k-1} \sum_{D \in \mathcal{C}_q(Y_k^d)} 2^n \leq 4^n \varepsilon \sum_{i \in Y_k^d} d_i.\end{aligned} \tag{3.59}$$

From (3.51), (3.55), and (3.59) we obtain the following upper bound on σ:

$$\sigma \leq \left(\frac{n}{2} + 4^n\right) \varepsilon \sum_{i \in Y_k^d} d_i. \tag{3.60}$$

Therefore, considering (3.48) and (3.50),

$$f_k(x') - f_k(x^*) \leq -\sum_{i \in Y_k^d} d_i \mu_i^{(k)} + \left(\frac{n}{2} + 4^n\right) \varepsilon \sum_{i \in Y_k^d} d_i = -\sum_{i \in Y_k^d} d_i \left(\mu_i^{(k)} - \left(4^n + \frac{n}{2}\right) \varepsilon\right),$$

which is guaranteed to be negative by choosing ε such that

$$\mu_i^{(k)} > \varepsilon \left(4^n + \frac{n}{2}\right) \quad \forall i \in Y_k^d \Longleftrightarrow \varepsilon < \min_{i \in V \setminus I_k} \frac{\mu_i^{(k)}}{4^n + n/2}. \tag{3.61}$$

Finally, by combining all the conditions for ε (i.e., (3.43), (3.35), (3.41), (3.61)), for

$$\varepsilon < \min \left\{ \min_{i \in S(x^*)} x_i^*, \frac{1}{2^n p^{k-2}}, \frac{1}{2^{p+1} p^{k-2} n}, \min_{i \in V \setminus I_k} \frac{\mu_i^{(k)}}{4^n + n/2} \right\},$$

x^* satisfies the definition of a local maximum for (**P**^{k}). □

4. REGULARIZED POLYNOMIAL FORMULATIONS FOR MAXCLIQUE PROBLEM

4.1 Background and research questions

As discussed in previous section, a characteristic vector x^C of a maximum clique C in a graph G is a global maximum of the MSQP. However, the converse is not true, as the MSQP is known to allow "spurious" local and global maxima, whose support is not a clique in the graph [15, 63]. Analogous claim holds for MSPP, as strongly supported by the result of Theorem 4, which only guarantees that a local (global) maximum is necessarily a p-partite multi-clique. It can be observed that given a Turán's graph $T(m\omega, \omega) = (V, E)$, both x^V and x^C, where C consists of a single vertex taken from each part, are global maxima of MSPP (see Figure 2.1 for a $T(4, 2)$ example).

For MSQP, this was viewed as a drawback of the formulation, which was addressed by introducing regularizations, ensuring a one-to-one correspondence between the local maxima of a regularized formulation and the (characteristic vectors of) maximal cliques in the graph. The first such regularization was proposed by Bomze [38] and consisted of adding diagonal terms to the Hessian matrix of the objective function of the MSQP:

$$\begin{aligned} \text{maximize} \quad & f^{\gamma}(x) = \sum_{\{i,j\} \in E} x_i x_j + \gamma \sum_{v \in V} x_v^2, \\ \text{subject to} \quad & x \in \Delta^{|V|}. \end{aligned} \tag{BR}$$

Initially in [38], parameter γ of BR was limited to $\frac{1}{2}$, but in latter works ([64]) it was generalized to allow for $\gamma \in \left(0, \frac{1}{2}\right]$. Later, Hungerford and Rinaldi [41] established general conditions on a class of regularization terms that ensure the desired correspondence. Let $\Phi : X \to \mathbb{R}$ be a twice continuously differentiable function defined on some open set $X \supset \Delta_n$, such that

(i) $\nabla^2 \Phi(x)$ is positive definite $\forall x \in \Delta_n$;

(ii) $\|\nabla^2 \Phi(x)\|_2 < 1 \; \forall x \in \Delta_n$;

(iii) Φ is constant on the set $\{\bar{x} \in \Delta_n : \exists \sigma \in \mathcal{S}_n$ such that $\bar{x}_i = x_{\sigma(i)} \; \forall i \in [n]\}$, where $\mathcal{S}_n$ is the set of permutations of $[n]$.

Hungerford and Rinaldi [41] proved that a point $x \in \Delta_n$ is a local maximizer of the problem

$$\max_{x \in \Delta^n} \sum_{\{i,j\} \in E} x_i x_j + \Phi(x) \tag{GR}$$

if and only if x is the characteristic vector of some maximal clique in G. They compared the performance of three different regularizations satisfying the conditions, including Bomze's regularization and two non-quadratic (in fact, non-polynomial) examples, computationally.

Note that BR is a special case of GR, as

$$\Phi(x) = \gamma \sum_{v \in V} x_v^2$$

clearly satisfies the conditions (1)–(3) for $\gamma \in (0, \frac{1}{2}]$.

Existence of such regularizations for MSQP raises the question if an analogous result can be established for MSPP.

4.2 Results on Regularized Formulations

Before we can proceed, we need to establish some set of properties for the regularization to satisfy. Based on the properties of the regularizations introduced in [38] and [41], we propose the following three basic requirements for a regularization to be considered "proper":

Req. 1 The regularized formulation of order k must guarantee that for any local maximum x^*, $S(x^*)$ corresponds to a clique of a size at least $k-1$.

Req. 2 Any local maximum x^* must be of form $x^{S(x^*)}$.

Req. 3 If the regularization is parametrized (e.g., with a parameter γ in BR), parameters must not depend on the specific parameters of the input graph, such as the number of nodes or edges. Note that it might depend on the order of the formulation.

To further simplify some of the expressions, we introduce the notation

$$\sigma_{k;W}^{U}(x^*) \coloneqq \sigma_{k;w_1,\ldots,w_t}^{u_1,\ldots,u_p}(x^*) \coloneqq \sum_{C \in \mathcal{C}_{k;W}^{U}} \pi_C(x^*).$$

We will drop the argument x^* when it is clear from the context. Note that for a pair of adjacent vertices u and v, $\sigma_k^u(x^*)$ can be equivalently expressed as

$$\sigma_k^u(x^*) = \sigma_{k;v}^u(x^*) + x_v^* \sigma_{k-1}^{u,v}(x^*). \tag{4.1}$$

In our derivations, we will often deal with $\sigma_{k-i;W}^U$ for some clique U and a positive integer i. Note that for $i \geq k$, we have $\sigma_{k-i,W}^U = 1$ if $i = k$ and $\sigma_{k-i,W}^U = 0$ if $i > k$.

4.2.1 Quadratic Regularization

In this section, we will attempt to apply Bomze's regularization for MSQP to higher-order formulations. First, we consider an example demonstrating that the quadratic regularization may introduce undesirable local optima, even when applied to the classical MSQP.

Example 1. *Let us consider a regularized quadratic formulation as given by [38] for a graph $G = (\{1,2,3\},\{\{2,3\}\})$, i.e., for a $\bar{P}_3$ graph. We will show that $x^* = (1,0,0)$ is a strict local maximum for any $\gamma \in \left(0, \frac{1}{2}\right)$. Note that x^* is clearly not a local maximum for $\gamma = 0$. The optimization problem for this graph G is*

$$\begin{aligned} \textit{maximize} \quad & f(x) = x_2x_3 + \gamma\left(x_1^2 + x_2^2 + x_3^2\right), \\ \textit{subject to} \quad & x_1 + x_2 + x_3 = 1. \end{aligned}$$

Consider a point $x' = x^* + d = (1 + d_1, d_2, d_3)$ for a feasible direction $d \neq 0$, where $d_1 =$

$-d_2 - d_3$ *and* $d_2, d_3 \geq 0$. *Then*

$$
\begin{aligned}
f(x') - f(x^*) &= d_2 d_3 + \gamma \left[(1 - (d_2 + d_3))^2 + d_2^2 + d_3^2 \right] - \gamma \\
&= d_2 d_3 + \gamma \left[-2(d_2 + d_3) + (d_2 + d_3)^2 + d_2^2 + d_3^2 \right] \\
&= d_2 d_3 + 2\gamma(d_2^2 + d_3^2) - 2\gamma(d_2 + d_3) + 2\gamma d_2 d_3 \\
&= (1 - 2\gamma) d_2 d_3 + 2\gamma(d_2^2 + 2d_2 d_3 + d_3^2) - 2\gamma(d_2 + d_3) \\
&= (1 - 2\gamma) d_2 d_3 + 2\gamma(d_2 + d_3) \left[d_2 + d_3 - 1 \right].
\end{aligned}
\tag{4.2}
$$

Let $d_2 < \gamma$, $d_3 < \gamma$. *Then from* (4.2)

$$
\begin{aligned}
f(x') - f(x^*) &< (1 - 2\gamma) d_2 d_3 + 2\gamma(d_2 + d_3)\left(2\gamma - 1\right) \\
&= (1 - 2\gamma)(d_2 d_3 - 2\gamma d_2 - 2\gamma d_3) \\
&= (1 - 2\gamma) \left[d_2 \left(\frac{1}{2} d_3 - 2\gamma \right) + d_3 \left(\frac{1}{2} d_2 - 2\gamma \right) \right] < 0,
\end{aligned}
\tag{4.3}
$$

and hence x^* *is a local maximum for any* $\gamma \in \left(0, \frac{1}{2}\right)$.

Note that in the example above the considered local maximum corresponds to a maximal clique consisting of an isolated vertex. The one-to-one correspondence between local maxima of a formulation and maximal cliques in the graph is a remarkable mathematical property imposed by the quadratic regularization. However, from a practical perspective of solving the maximum clique problem, this example shows that the regularization given in [38] may introduce undesirable single-vertex local maxima. While technically $S\left(x^*\right)$ is a maximal clique, we would like to avoid such cases.

Now, let us consider a regularized problem similar in structure to the Bomze's regularization of MSQP. Specifically, let

$$
f_k^\gamma(x) \coloneqq f_k(x) + \gamma \sum_{v \in V} x_v^2, \tag{4.4}
$$

where $\gamma \in (0, 1/2)$. Consider an optimization problem

$$\begin{aligned} \text{maximize} \quad & f_k^\gamma(x), \\ \text{subject to} \quad & x \in \Delta^{|V|}. \end{aligned} \tag{QR}$$

We can show that the attempt for quadratic regularization in the form of (QR) does not satisfy the requirements we established for the proper regularization. Moreover, the following example demonstrates that for $k \geq 3$ we can have local maxima that correspond to one-vertex cliques that are not maximal.

Example 2. *Consider a complete graph $G = (V, E)$ on three vertices. For $k = 3$, $x^* = (1, 0, 0)$ is a local maximum for* (QR).

Proof. Consider $x' = x^* + d$, where $d_1 = -d_2 - d_3$ and $0 \leq d_1, d_2 < \gamma$. Following the derivations in (4.2) and (4.3), we have

$$\begin{aligned} f(x') - f(x^*) &< d_1 d_2 d_3 + (1 - 2\gamma)\left[d_2\left(\frac{1}{2}d_3 - 2\gamma\right) + d_3\left(\frac{1}{2}d_2 - 2\gamma\right)\right] \\ &= -(d_2 + d_3)d_2 d_3 + (1 - 2\gamma)\left[d_2\left(\frac{1}{2}d_3 - 2\gamma\right) + d_3\left(\frac{1}{2}d_2 - 2\gamma\right)\right] < 0, \end{aligned}$$

and, hence, x^* is a strict local maximum corresponding to a one-vertex clique that is not maximal in G. □

Next we show that a quadratic regularization can still be useful for computing cliques in higher-order formulations. We will use the first order optimality conditions in our proof. Clearly, (QR) satisfies the linearity constraint qualification regularity conditions. Therefore, any local maximum x^* of (QR) must satisfy Karush-Kuhn-Tucker (KKT) first order necessary conditions for some $\lambda^* \in \mathbb{R}$ and $\mu^* \in \mathbb{R}_+^n$. Specifically, the following must hold:

- Stationarity:

$$\sigma_{k-1}^v + 2\gamma x_v^* + \mu_v^* = \lambda^*, \quad \forall v \in V. \tag{4.5}$$

- Primal feasibility:

$$\sum_{v\in V} x_v^* = 1; \quad x_v^* \geq 0, \quad \forall v \in V. \tag{4.6}$$

- Dual feasibility and complimentary slackness:

$$x_v^* \mu_v^* = 0, \quad \mu_v^* \geq 0, \quad \forall v \in V. \tag{4.7}$$

Theorem 8. *If x^* is a local maximum of* (QR)*, then $S(x^*)$ is a clique in G such that either $|S(x^*)| = 1$ or $|S(x^*)| \geq k$.*

Proof. If $|S(x^*)| = 1$, then the only vertex in $S(x^*)$ forms a clique.

Let us assume that $S(x^*)$ is not a clique. Then $|S(x^*)| \geq 2$ and there exist two vertices, $v, u \in S(x^*)$ such that u is not adjacent to v. Since x^* is a local maximum, from the KKT stationarity condition,

$$\sigma_{k-1}^v + 2\gamma x_v^* = \sigma_{k-1}^u + 2\gamma x_u^*. \tag{4.8}$$

Consider a direction given as $d = d_u - d_v$:

$$\begin{aligned} f_k^\gamma(x^* + \varepsilon d) &= \sigma_{k;u,v} + (x_u^* + \varepsilon)\sigma_{k-1}^u + (x_v^* - \varepsilon)\sigma_{k-1}^v + \gamma(x_u^* + \varepsilon)^2 + \gamma(x_v^* - \varepsilon)^2 + \gamma \sum_{w \in S(x^*)\setminus\{u,v\}} (x_w^*)^2 \\ &= f_k^\gamma(x^*) + \varepsilon(\sigma_{k-1}^u + 2\gamma x_u^* - \sigma_{k-1}^v - 2\gamma x_v^*) + 2\gamma\varepsilon^2 \\ &= f_k^\gamma(x^*) + 2\gamma\varepsilon^2. \end{aligned} \tag{4.9}$$

Clearly, d is a direction of improvement, hence x^* is not a local maximum, which contradicts the initial assumption.

Finally, if $1 < |S(x^*)| < k$ then $f_k(x^*) = 0$ and (4.8) implies that $x_v^* = x_u^*$ for all $v, u \in S(x^*)$. For the same direction $d = d_u - d_v$ as before, we obtain $f_k^\gamma(x^* + \varepsilon d) \geq f_k^\gamma(x^*) + 2\gamma\varepsilon^2$, which again contradicts the local maximality of x^*. □

4.2.2 Polynomial Regularization

As it can be observed in the previous section, the attempt at quadratic regularization fails due to the regularization's quadratic term strictly dominating the cubic (or higher order) terms of the original objective function for small enough ε. One way to overcome this is by guaranteeing that the quadratic interaction occurs only if there are enough non-zero elements in x^* so that the linear increment dominates the quadratic one. This can be achieved by considering the following polynomial of degree $k \in \{2, 3, \ldots, \omega\}$ over the standard simplex:

$$f_k^\gamma(x) \coloneqq f_k(x) + \gamma \sum_{v \in V} x_v^2 \sigma_{k-2}^v, \tag{4.10}$$

with a corresponding optimization problem

$$\begin{aligned} \text{maximize} \quad & f_k^\gamma(x), \\ \text{subject to} \quad & x \in \Delta^{|V|}. \end{aligned} \tag{PR}$$

where $\gamma \in \left(0, \frac{1}{2}\right)$. For $k = 2$, this formulation coincides with Bomze's regularization (QR) of Motzkin-Straus formulation [38]. We will show that x^* is a local maximum of (PR) if and only if $S\left(x^*\right)$ is a maximal clique of cardinality at least $k - 1$ in G.

Clearly, any local maximum x^* of (PR) must satisfy the KKT stationarity conditions

$$\sigma_{k-1}^v + 2\gamma x_v^* \sigma_{k-2}^v + \gamma \sum_{u \in \mathrm{N}(v)} (x_u^*)^2 \sigma_{k-3}^{v,u} + \mu_v^* = \lambda^*, \quad \forall v \in V \tag{4.11}$$

for some $\lambda^* \in \mathbb{R}$ and $\mu^* \in \mathbb{R}_+^n$, in addition to the primal feasibility (4.6) as well as dual feasibility and complimentary slackness conditions (4.7).

For $U \subset V$, let $\mathcal{C}_k(U)$ denote the set of all cliques of cardinality k in $G[U]$. First, we observe that every vertex from the support of a local maximum x^* of (PR) belongs to at least one $(k-1)$-vertex clique from the support of x^*:

Lemma 10. *If x^* is a local maximum of* (PR) *for a given $k \in \{2, 3, \ldots, \omega\}$, then any $v \in S\left(x^*\right)$*

belongs to some clique $C \in \mathcal{C}_{k-1}(S(x^*))$.

Proof. If v does not belong to any clique in $\mathcal{C}_{k-1}(S(x^*))$, then $f_k(x^*) = f_k(x^* - e_v x_v^*)$. Since $k \leq \omega(G)$, there exists a clique $C \in \mathcal{C}_k$. Clearly, $d = x^{C\setminus\{v\}} - e_v$ is a feasible direction of improvement. $\square$

Theorem 9. *If x^* is a local maximum of* (PR)*, then $S(x^*)$ is a clique of cardinality $|S(x^*)| \geq k-1$.*

Proof. If $|S(x^*)| < k-1$ then $f_k^\gamma(x^*) = 0$ and x^* cannot be a local maximum (a direction of improvement can be easily established using a clique of cardinality $k = 1$). Now assume $S(x^*)$ is not a clique. This implies that there exist two vertices, u and v such that $u, v \in S(x^*)$ and $\{u, v\} \notin E$. Consider a direction $d \in \mathbb{R}^{|V|}$ given as $d := e_u - e_v$. Then, due to Lemma 10 and the stationarity condition (4.11),

$$
\begin{aligned}
f_k^\gamma(x^* + \varepsilon d) &= (x_v^* - \varepsilon)\sigma_{k-1}^v + (x_u^* + \varepsilon)\sigma_{k-1}^u + \sigma_{k;u,v} + \gamma(x_v^* - \varepsilon)^2\sigma_{k-2}^v + \gamma(x_u^* + \varepsilon)^2\sigma_{k-2}^u \\
&\quad + \gamma(x_u^* + \varepsilon)\sum_{w\in \mathrm{N}(u)}(x_w^*)^2\sigma_{k-3}^{w,u} + \gamma(x_v^* - \varepsilon)\sum_{w\in \mathrm{N}(v)}(x_w^*)^2\sigma_{k-3}^{w,v} \\
&= f_k^\gamma(x^*) + \varepsilon^2(\sigma_{k-2}^u + \sigma_{k-2}^v) + \varepsilon\Big(\sigma_{k-1}^u + 2\gamma x_u^*\sigma_{k-2}^u + \gamma\sum_{w\in \mathrm{N}(u)}(x_w^*)^2\sigma_{k-3}^{w,u}\Big) \\
&\quad - \varepsilon\Big(\sigma_{k-1}^v - 2\gamma x_v^*\sigma_{k-2}^v - \gamma\sum_{w\in \mathrm{N}(v)}(x_w^*)^2\sigma_{k-3}^{w,v}\Big) \\
&= f_k^\gamma(x^*) + \varepsilon^2(\sigma_{k-2}^u + \sigma_{k-2}^v) > f_k^\gamma(x^*)
\end{aligned}
\tag{4.12}
$$

$\square$

Theorem 10. *If $S(x^*)$ is a clique and KKT conditions* (2.8)–(4.7) *hold for* (PR)*, then $x^* = x^{S(x^*)}$. In particular, this holds for a local maximum.*

Proof. For any two vertices $u, v \in S(x^*)$, we apply representation (4.1) to σ_{k-1}^v, σ_{k-2}^v, and $\sigma_{k-3}^{u,v}$ in the stationarity condition (2.8) to obtain

$$
\lambda^* = \sigma_{k-1;u}^v + x_u^*\sigma_{k-2}^{u,v} + 2\gamma x_v^*\big(\sigma_{k-2;u}^v + x_u^*\sigma_{k-3}^{u,v}\big) + \gamma(x_u^*)^2\sigma_{k-3}^{u,v} + \gamma\sum_{w\in S(x^*)\setminus\{u,v\}}(x_w^*)^2\big(\sigma_{k-3;u}^{v,w} + x_u^*\sigma_{k-4}^{w,u,v}\big)
\tag{4.13}
$$

Since $S(x^*)$ is a clique, $\sigma^u_{k-1;v} = \sigma^v_{k-1;u}$, $\sigma^u_{k-2;v} = \sigma^v_{k-2;u} = \sigma^{u,v}_{k-2}$, and $\sigma^{u,j}_{k-3;v} = \sigma^{v,j}_{k-3;u}$ for any $j \in S(x^*)$. Thus, by subtracting equation (4.13) above from the analogous equation for λ^*, with u and v swapped, we obtain

$$\begin{aligned} 0 &= (x^*_v - x^*_u)\sigma^{u,v}_{k-2} + 2\gamma(x^*_u - x^*_v)\sigma^{u,v}_{k-2} + \gamma(x^*_v - x^*_u)(x^*_v + x^*_u)\sigma^{u,v}_{k-3} \\ &+ \gamma(x^*_v - x^*_u)\sum_{w \in S(x^*)\setminus\{u,v\}} (x^*_w)^2 \sigma^{w,u,v}_{k-4} \\ &= (x^*_v - x^*_u)\Big[(1-2\gamma)\sigma^{u,v}_{k-2} + \gamma(x^*_v + x^*_u)\sigma^{u,v}_{k-3} + \gamma\sum_{w \in S(x^*)\setminus\{u,v\}} (x^*_w)^2 \sigma^{w,u,v}_{k-4}\Big] \end{aligned} \tag{4.14}$$

The term in the square brackets is positive since $\gamma \in (0, 1/2)$, $\sigma^{u,v}_{k-2} \geq 0$, $\sigma^{u,v}_{k-3} > 0$ (due to Lemma 10) and $\sigma^{w,u,v}_{k-4} \geq 0$. Therefore, x^*_v must be equal to x^*_u for the equality to hold. This implies that $x^*_u = \frac{1}{|S(x^*)|}$ for any $u \in S(x^*)$. □

Corollary 7. *If x^* is a KKT point for* (PR) *and $S(x^*)$ is a clique, then, assuming $p = |S(x^*)|$,*

$$\lambda^* = \binom{p-1}{k-1}\left(\frac{1}{p}\right)^{k-1} + 2\gamma\binom{p-1}{k-2}\left(\frac{1}{p}\right)^{k-1} + (p-1)\gamma\binom{p-2}{k-3}\left(\frac{1}{p}\right)^{k-1}. \tag{4.15}$$

Proof. Straightforward from (2.8). □

Lemma 11. *If x^* is a local maximum for* (PR)*, then for any $v \in V$ either $\mu^*_v = 0$ or $x^*_v = 0$, but not both.*

Proof. If one of μ^*_v, x^*_v is positive, then the other one must be zero by complementary slackness. Suppose $\mu^*_v = x^*_v = 0$ for some $v \in V$. Note that $S(x^*)$ is a clique due to Theorem 9. Let $p := |S(x^*)|$ and $p' := |\mathrm{N}(v) \cap S(x^*)|$. Then (2.8) for vertex v becomes:

$$\lambda^* = \sigma^v_{k-1} + \gamma\sum_{w \in \mathrm{N}(v)} (x^*_w)^2 \sigma^{v,w}_{k-3} = \binom{p'}{k-1}\left(\frac{1}{p}\right)^{k-1} + p'\gamma\binom{p'-1}{k-3}\left(\frac{1}{p}\right)^{k-1}. \tag{4.16}$$

Clearly, if $p' \leq p-1$, (4.16) contradicts (4.15). Let us consider the remaining possible case of $p' = p$. Multiplying both sides of (4.15) and (4.16) by p^{k-1} and subtracting the resulting equations, we obtain

$$\begin{aligned} 0 &= \binom{p-1}{k-1} + 2\gamma\binom{p-1}{k-2} + (p-1)\,\gamma\binom{p-2}{k-3} - \binom{p}{k-1} - p\gamma\binom{p-1}{k-3} \\ &= (2\gamma-1)\binom{p-1}{k-2} - \gamma\binom{p-2}{k-3} - p\gamma\binom{p-2}{k-4}. \end{aligned} \tag{4.17}$$

Since $\gamma \in \left(0, \frac{1}{2}\right)$, the last equation can hold only if $p < k-2$. This contradicts Theorem 9, according to which $p \geq k-1$. □

Theorem 11. *If x^* is a local maximum of* (PR)*, then $S\left(x^*\right)$ is a maximal clique of cardinality $\left|S\left(x^*\right)\right| \geq k-1$.*

Proof. From Theorem 9, $S\left(x^*\right)$ is a clique of cardinality $\left|S\left(x^*\right)\right| \geq k-1$. Suppose $S\left(x^*\right)$ is not a maximal clique. Then there exists a vertex $v \in V \setminus S\left(x^*\right)$ such that v is adjacent to every vertex in $S\left(x^*\right)$, while $x_v^* = 0$. But this is exactly the second case considered in Lemma 11 when $p = p'$, which violates the KKT conditions as long as $\gamma \in \left(0, \frac{1}{2}\right)$.

□

Theorem 12. (PR) *achieves its global maximum at point x^*, such that $S\left(x^*\right)$ is a maximum clique. The optimal value of* (PR) *is*

$$f_k^\gamma(G) := \left(\frac{1}{\omega}\right)^k \left(\binom{w}{k} + \gamma\omega\binom{\omega-1}{k-2}\right). \tag{4.18}$$

Proof. Due to the results of Theorem 11, the support of a global maximum x^* of (PR) is necessarily a maximal clique. Moreover, $x_i^* = x_j^*$ for any $i, j \in S\left(x^*\right)$ due to Theorem 10. As before, let $p = \left|S\left(x^*\right)\right|$ and let $g(p) : \mathbb{Z}_+ \to \mathbb{R}_{\geq 0}$ be the value of $f_k^\gamma(x^*)$ as a function of p. Then

$$g(p) = f_k^\gamma(x^*) = \sum_{C \in \mathcal{C}_k} \pi_C(x^*) + \gamma \sum_{i \in V} \left(x_i^*\right)^2 \sum_{C \in \mathcal{C}_{k-2}^i} \pi_C(x^*) = \binom{p}{k}\left(\frac{1}{p}\right)^k + \gamma p \left(\frac{1}{p}\right)^k \binom{p-1}{k-2}.$$

Consider a complete graph G on p vertices. Clearly, G has a single maximal and maximum clique. Due to Theorem 11, it follows that $g(p) > g(p-1)$ as long as $\gamma \in \left(0, \frac{1}{2}\right)$. Since the value of g

only depends on $G[S(x^*)]$, which is always a clique, due to Theorem 9, the result follows. Then, (4.18) is exactly $g(\omega)$. □

Theorem 13. *C is a maximal clique of cardinality $p \geq k-1$ in G if and only if $x^* := x^C$ is a strict local maximum for* (PR).

Proof. The "if" direction is the result of Theorem 11. For the "only if" direction, we will use the second order sufficient condition to prove the claim of the theorem. First, we show that the KKT conditions hold at x^* for some λ^* and μ^*. Indeed, let

$$\lambda^* = \binom{p-1}{k-1} p^{-k+1} + 2\gamma \binom{p-1}{k-2} p^{-k+1} + (p-1)\gamma \binom{p-2}{k-3} p^{-k+1}.$$

Clearly, for any $v \in S(x^*)$, μ_v^* must be equal to 0. For any $u \notin S(x^*)$, there exists at least one vertex w in $S(x^*)$ that is not adjacent to u. Therefore

$$\mu_u^* = \lambda^* - \sigma_{k-1}^u - \gamma \sum_{v \in \mathrm{N}(u)} (x_v^*)^2 \sigma_{k-3}^{u,v} \geq \lambda^* - \binom{p-1}{k-1} p^{-k+1} - \gamma \sum_{v \in S(x^*) \setminus \{w\}} \binom{p-2}{k-3} p^{-k+1} > 0.$$

and the KKT conditions are satisfied, while strict complementarity holds for every non-negativity constraint. Now we will use the second order optimality conditions for maximum. According to the second order sufficient condition (SOSC), x^* is a strict local maximum if

$$\sum_{i \in C} s_i^2 \frac{\partial^2 f_k^\gamma(x^*)}{(\partial x_i)^2} + \sum_{\{i,j\} \in \binom{C}{2}} 2 s_i s_j \frac{\partial^2 f_k^\gamma(x^*)}{\partial x_i \partial x_j} < 0 \quad \forall s \in T(x^*), \tag{4.19}$$

where $T(x^*) := \{s \in \mathbb{R}^n \mid \sum_{i \in C} s_i = 0; \;\; s_i = 0, \forall i \in V \setminus C\}$. By taking derivatives and plugging in values for x^*, we obtain

$$\rho_1 := \frac{\partial^2 f_k^\gamma(x^*)}{(\partial x_i)^2} = 2\gamma \binom{p-1}{k-2} p^{-k+2} = 2\gamma \binom{p-2}{k-2} p^{-k+2} + 2\gamma \binom{p-2}{k-3} p^{-k+2},$$

$$\frac{\partial^2 f_k^\gamma(x^*)}{\partial x_i \partial x_j} = \binom{p-2}{k-2} p^{-k+2} + 4\gamma \binom{p-2}{k-3} p^{-k+2} + \gamma(p-2) \binom{p-3}{k-4} p^{-k+2} = \rho_1 + \rho_2,$$

where $\rho_2 := (1-2\gamma)\binom{p-2}{k-2}p^{-k+2} + 2\gamma\binom{p-2}{k-3}p^{-k+2} + \gamma(p-2)\binom{p-3}{k-4}p^{-k+2}$. So, the expression in (4.19) becomes

$$\begin{aligned}
\sum_{i\in C} s_i^2 \frac{\partial^2 f_k^\gamma(x^*)}{(\partial x_i)^2} + \sum_{\{i,j\}\in\binom{C}{2}} 2s_is_j \frac{\partial^2 f_k^\gamma(x^*)}{\partial x_i \partial x_j} &= \rho_1 \sum_{i\in C} s_i^2 + \rho_1 \sum_{\{i,j\}\in\binom{C}{2}} 2s_is_j + \rho_2 \sum_{\{i,j\}\in\binom{C}{2}} 2s_is_j \\
&= \rho_1 \left(\sum_{i\in C} s_i\right)^2 + 2\rho_2 \sum_{\{i,j\}\in\binom{C}{2}} s_is_j \\
&= \rho_2 \sum_{i\in C} s_i \sum_{j\in C\setminus\{i\}} s_j \\
&= -\rho_2 \sum_{i\in C} s_i^2 < 0, \quad \forall s \neq 0,
\end{aligned}$$

since $\rho_2 > 0$ for $\gamma \in \left(0, \frac{1}{2}\right)$. Thus, the SOSC is satisfied and x^* is a strict local maximum. □

Corollary 8. *Let* ($\mathbf{P}^{k,\gamma}$) *be* (PR) *formulated for order k with parameter γ. Suppose x^* is a local maximum of* ($\mathbf{P}^{k+1,\gamma}$) *for some $k \in \{2,\ldots,\omega-1\}$. Then x^* is a local maximum of* ($\mathbf{P}^{k,\gamma}$).

Proof. Since x^* is a local maximum for ($\mathbf{P}^{k+1,\gamma}$), $S(x^*)$ is a maximal clique of size at least $k+1$. Therefore, due to Theorem 13, x^* is a local maximum for ($\mathbf{P}^{k,\gamma}$). □

The following example demonstrates that the KKT conditions for (PR) can hold for a feasible point x such that $S(x)$ is not a clique and not a local maximum.

Example 3. *Consider the graph given in Figure 4.1. Let $S(x) = \{1,2,3,4\}$, and therefore*

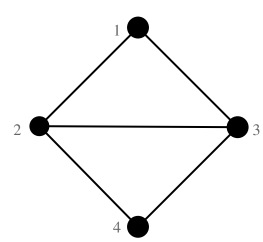

Figure 4.1: A graph on 4 nodes used in Example 3.

$\mu^* = (0,0,0,0)$. *The objective function of* (PR) *for* $k=3$ *is*

$$f_k^{\gamma}(x) = x_1x_2x_3 + x_2x_3x_4 + \gamma\left(x_1^2(x_2+x_3) + x_2^2(x_1+x_3+x_4) + x_3^2(x_1+x_2+x_4) + x_4^2(x_2+x_3)\right).$$

The KKT stationarity condition written for vertices 1 and 2, by setting $x_1 = x_4$ *and* $x_2 = x_3$, *becomes*

$$\begin{aligned}
\lambda &= x_2x_3 + \gamma(2x_1(x_2+x_3) + x_2^2 + x_3^2) = x_2^2 + \gamma(4x_1x_2 + 2x_2^2),\\
\lambda &= x_1x_3 + x_3x_4 + \gamma(x_1^2 + 2x_2(x_1+x_3+x_4) + x_3^2 + x_4^2) = 2x_1x_2 + \gamma(2x_1^2 + 4x_1x_2 + 3x_2^2).
\end{aligned}$$

Since $2x_1 + 2x_2 = 1$, *it follows that* $x_2 = 1/2 - x_1$. *Then, subtracting the two equations above,*

$$3x_2^2 - x_2 - \gamma(1/2 - 2x_2 + 3x_2^2) = 0.$$

By letting $\gamma = \frac{1}{3}$, *we obtain*

$$12x_2^2 - 2x_2 - 1 = 0 \Rightarrow x_2 = \frac{1+\sqrt{13}}{12}, x_1 = 1/2 - x_2.$$

Hence, the KKT *conditions hold for* $x = (1/2 - x_2, x_2, x_2, 1/2 - x_2)$, *but* $d = (1,0,0,-1)$ *is a feasible direction of improvement at this point.*

4.3 General Regularized Formulations

Let $\Phi : \mathbb{R}^n \to \mathbb{R}$ be a twice-differentiable function, and let $\Phi_{u,v}$ denote a restriction of Φ to $\mathbb{R}^2$ induced by assuming all variables except x_u and x_v are fixed. Let us consider a formulation

$$f_k^{\Phi}(G) = \max_{x\in\Delta^n} \sum_{C\in\mathcal{C}_k} \prod_{i\in C} x_i + \Phi(x) = \sigma_k + \Phi(x), \tag{$\mathbf{P}^{k,\Phi}$}$$

where $\Phi : \mathbb{R}^n \to \mathbb{R}$ is a twice-differentiable function that satisfies the following set of conditions.

$$\text{If } \mathcal{C}_{k-1}(S(x^*)) = \emptyset \text{ then } \Phi(x^*) = \min_{x\in\Delta^n} \Phi(x). \tag{\textbf{C1}}$$

$$\text{If } u, v \in S(x^*), u \in C \in \mathcal{C}_{k-1}(S(x^*)),\ \text{and } \{u,v\} \notin E \text{ then } d^T \nabla^2 \Phi_{u,v}(x^*) d > 0 \text{ for any } d = (d_1, d_2)^T \neq (0,0)^T \text{ such that } d_1 + d_2 = 0. \quad \textbf{(C2)}$$

$$\text{If } S(x^*) \in \mathcal{C}_k,\ u, v \in S(x^*), \text{ and } (x_u^* - x_v^*)\sigma_{k-2}^{u,v} = \frac{\partial \Phi(x^*)}{\partial x_u^*} - \frac{\partial \Phi(x^*)}{\partial x_v^*} \text{ then } x_v = x_u. \quad \textbf{(C3)}$$

$$\forall C \subseteq V,\ \forall v \in C,\ \forall u \in V \setminus C:\ \frac{\partial \Phi(x^C)}{\partial x_v} - \frac{\partial \Phi(x^C)}{\partial x_u} < \binom{|C|-1}{k-2}\left(\frac{1}{|C|}\right)^{k-1}. \quad \textbf{(C4)}$$

Condition (**C1**) ensures that adding the regularization term $\Phi(x)$ does not introduce local maxima that do not correspond to cliques of cardinality less than $k-1$. Requirement (**C2**) is used to eliminate local maxima that do not correspond to a clique. Conditions (**C3**) and (**C4**) are additional technical requirements used to establish the correspondence of a local maximum of (**P**$^{k,\Phi}$) to the characteristic vectors of a clique. It is worth noting that any bounded-variation twice-differentiable function over the standard simplex can be adjusted by a scaled factor to satisfy (**C4**), as long as (**C3**) is maintained. In fact, γ in (PR) is such a scaling factor, as demonstrated in the following example.

Example 4. *Consider the polynomial regularization term $\Phi_\gamma(x) := \gamma \sum_{v\in V} x_v^2 \sigma_{k-2}^v$. We will verify that $\Phi(x) = \Phi_\gamma(x)$ satisfies conditions* (**C1**)–(**C4**).

First, note that $\Phi(x) \geq 0$ over Δ^n. If $S(x^*)$ contains no clique of size $k-1$, $\Phi(x^*) = 0$, hence (**C1**) *is satisfied.*

Second, let us notice that

$$\frac{\partial \Phi(x)}{\partial x_v} = 2\gamma x_v \sigma_{k-2}^v + \gamma \sum_{w \in V\setminus\{v\}} x_w^2 \sigma_{k-3}^{w,v}, \tag{4.20}$$

$$\frac{\partial^2 \Phi(x)}{\partial x_v^2} = 2\gamma\sigma_{k-2}^v, \quad \frac{\partial^2 \Phi(x)}{\partial x_v \partial x_u} = 0 \quad \forall v, u \in V, \{u,v\} \notin E. \tag{4.21}$$

As v and u are independent, it follows that

$$\nabla^2 \Phi_{v,u}(x) = \gamma \begin{pmatrix} 2\sigma_{k-2}^v & 0 \\ 0 & 2\sigma_{k-2}^u \end{pmatrix}.$$

Hence, for $d = (d_1, d_2)^T \neq (0,0)^T$ *such that* $d_1 + d_2 = 0$*, we have:*

$$d^T \nabla^2 \Phi_{v,u}(x) d = 2\sigma_{k-2}^v d_1^2 + 2\sigma_{k-2}^u d_2^2 > 0$$

as v *belongs to at least one* $C \in \mathcal{C}_{k-1}(S(x))$ *and* $d_1 \neq 0$*.*

For (**C3**)*:*

$$\begin{aligned}(x_u - x_v)\sigma_{k-2}^{u,v} &= \gamma \left[2x_u \sigma_{k-2}^u + \sum_{w \in V\setminus\{u\}} x_w^2 \sigma_{k-3}^{w,u} - 2x_v \sigma_{k-2}^v - \sum_{w\in V\setminus\{v\}} x_w^2 \sigma_{k-3}^{w,v} \right] \\ &= \gamma \left[2(x_u - x_v)\sigma_{k-2}^{v,u} + (x_v - x_u)(x_u + x_v)\sigma_{k-3}^{u,v} + (x_v - x_u) \sum_{w\in V\setminus\{u,v\}} x_w^2 \sigma_{k-4}^{u,v,w} \right].\end{aligned} \tag{4.22}$$

Now, assuming $x_u \neq x_v$*, we obtain*

$$0 = (2\gamma - 1)\sigma_{k-2}^{v,u} - (x_u + x_v)\sigma_{k-3}^{u,v} - \sum_{w\in V\setminus\{u,v\}} x_w^2 \sigma_{k-4}^{u,v,w}, \tag{4.23}$$

however, the right-hand side of (4.23) *is negative as long as* $\gamma < 1/2$*; a contradiction.*

Finally, to verify (**C4**)*, assume that* $|C| = p$ *and* $x = x^C$*. Since* $u \in V \setminus C$*,* $x_u = 0$ *and*

$$\begin{aligned}\frac{\partial \Phi(x)}{\partial x_v} - \frac{\partial \Phi(x)}{\partial x_u} &= 2x_v \sigma_{k-2}^v + \sum_{w\in V\setminus\{v\}} x_w^2 \sigma_{k-3}^{v,w} - \sum_{w\in V\setminus\{u\}} x_w^2 \sigma_{k-3}^{u,w} \\ &= 2x_v \sigma_{k-2}^v + \sum_{w\in V\setminus\{v,u\}} x_w^2 \sigma_{k-3}^{u,v,w} - x_v^2 \sigma_{k-3}^{u,v} - \sum_{w\in V\setminus\{v,u\}} x_w^2 (\sigma_{k-3}^{u,w,v} + x_v \sigma_{k-4}^{u,w,v}) \\ &= 2x_v \sigma_{k-2}^v - x_v^2 \sigma_{k-3}^{u,v} - x_v \sum_{w\in V\setminus\{v,u\}} x_w^2 \sigma_{k-4}^{u,w,v} \\ &= \left(\frac{1}{p}\right)^{k-1} \left[\binom{p-1}{k-2} - \binom{p-1}{k-3} - (p-1)\binom{p-2}{k-4} \right] \\ &\leq \left(\frac{1}{p}\right)^{k-1} \binom{p-1}{k-2}.\end{aligned} \tag{4.24}$$

As before, any local maximum for ($\mathbf{P}^{k,\Phi}$) must satisfy the KKT conditions, hence, the following stationarity condition holds:

$$\sigma_{k-1}^{v} + \frac{\partial \Phi(x^*)}{\partial x_v} + \mu_v^* = \lambda^*, \quad \forall v \in V. \tag{4.25}$$

In addition, the primal feasibility (4.6) as well as the dual feasibility and complementary slackness conditions (4.7) must hold at x^*.

Theorem 14. *If x^* is a local maximum of ($\mathbf{P}^{k,\Phi}$), then $S\left(x^*\right)$ is a maximal clique of cardinality at least $k-1$ and $x^* = x^{S(x^*)}$.*

Proof. First, let us assume that $S\left(x^*\right)$ does not contain any clique of size $k-1$. Let $v \in S\left(x^*\right)$ and $C \in \mathcal{C}_{k-1}$. Let $d = x^{C\setminus\{v\}} - e_v$. Then, due to (**C1**),

$$f_k^{\Phi}(x^* + \varepsilon d) - f_k^{\Phi}(x^*) = \prod_{u \in C}(x_u^* + \varepsilon d_u) + \Phi(x^* + \varepsilon d) - \Phi(x^*) > 0, \tag{4.26}$$

as the first term is strictly positive and $\Phi(x^* + \varepsilon d) - \Phi(x^*) \geq 0$. Hence, there must exist a clique $C \in \mathcal{C}_{k-1}\left(S\left(x^*\right)\right)$. Next, assume that $u \in S\left(x^*\right)$ such that $C \cup \{u\} \notin \mathcal{C}_k(S\left(x^*\right))$. There must exist a vertex $w \in C$ such that $\{u, w\} \notin E$. Consider a direction $d \in \mathbb{R}^{|V|}$ given as $d = e_w - e_u$. Then, for any $\varepsilon \in (-x_w^*, x_u^*)$

$$f_k^{\Phi}(x^* + \varepsilon d) = (x_u^* - \varepsilon)\sigma_{k-1}^{u} + (x_w^* + \varepsilon)\sigma_{k-1}^{w} + \sigma_{k;u,w} + \Phi(x^* + \varepsilon d). \tag{4.27}$$

From the Taylor series expansion for Φ, which is a twice-differentiable function, we have

$$\begin{aligned} \Phi(x^* + \varepsilon d) &= \Phi(x^*) + \varepsilon \sum_{i=1}^{n} d_i \frac{\partial \Phi(x^*)}{\partial x_i} + \frac{\varepsilon^2}{2} d^T \nabla \Phi(\xi) d \\ &= \Phi(x^*) + \varepsilon \left(\frac{\partial \Phi(x^*)}{\partial x_u} + \frac{\partial \Phi(x^*)}{\partial x_w} \right) + \frac{\varepsilon^2}{2} d^T \nabla \Phi_{w,u}(\xi) d, \end{aligned} \tag{4.28}$$

where $\xi = x^* + \rho\varepsilon d$ for some $\rho \in [0, 1]$. Substituting the expression(4.28) for Φ in (4.27) and using (4.25) and (**C2**), we obtain

$$f_k^{\Phi}(x^* + \varepsilon d) - f_k^{\Phi}(x^*) = \varepsilon\left(\sigma_{k-1}^{w} + \frac{\partial\Phi(x^*)}{\partial x_w} - \sigma_{k-1}^{u} - \frac{\partial\Phi(x^*)}{\partial x_u}\right) + \frac{\varepsilon^2}{2} d^T \nabla^2 \Phi_{w,u}(\xi) d$$
$$= \frac{\varepsilon^2}{2} d^T \nabla^2 \Phi_{w,u}(\xi) d > 0.$$

(Note that (**C2**) applies at ξ since $S(\xi) = S(x^*)$.) This proves that $S(x^*)$ is a clique of cardinality at least $k-1$.

To show that $x^* = x^{S(x^*)}$, consider the KKT stationarity condition (4.25) for $u, v \in S(x^*)$. Since both u and v are in $S(x^*)$, if follows that $\mu_v^* = \mu_u^* = 0$. Therefore,

$$\sigma_{k-1}^{u} + \frac{\partial\Phi(x^*)}{\partial x_u} = \sigma_{k-1}^{v} + \frac{\partial\Phi(x^*)}{\partial x_v}. \tag{4.29}$$

Since $S(x^*)$ is a clique, it follows that $\sigma_{k-1}^{u} = \sigma_{k-1;v}^{u} + x_v^* \sigma_{k-2}^{v,u}$ and, symmetrically, $\sigma_{k-1}^{v} = \sigma_{k-1;u}^{v} + x_u^* \sigma_{k-2}^{v,u}$, while $\sigma_{k-1;v}^{u} = \sigma_{k-1;u}^{v}$. Therefore, (4.29) yields

$$(x_u^* - x_v^*)\sigma_{k-2}^{u,v} = \frac{\partial\Phi(x^*)}{\partial x_u} - \frac{\partial\Phi(x^*)}{\partial x_v}. \tag{4.30}$$

Finally, due to (**C3**), it necessarily holds that $x_v^* = x_u^*$, and, subsequently, $x^* = x^{S(x^*)}$.

To complete the proof, we need to show that $S(x^*)$ is a maximal clique. By contradiction, let us assume that $S(x^*)$ is not a maximal clique. This implies that there exists a vertex $v \in V \setminus S(x^*)$ such that $S(x^*) \subseteq \mathrm{N}(v)$.

Let us consider the KKT stationarity condition for some vertex $u \in S(x^*)$ and v:

$$\begin{cases} \lambda^* = \sigma_{k-1}^{u} + \frac{\partial\Phi(x^*)}{\partial x_u} \\ \lambda^* = \sigma_{k-1}^{v} + \frac{\partial\Phi(x^*)}{\partial x_v} + \mu_v^* \end{cases} \Rightarrow \mu_v^* = \sigma_{k-1}^{u} - \sigma_{k-1}^{v} + \frac{\partial\Phi(x^*)}{\partial x_u} - \frac{\partial\Phi(x^*)}{\partial x_v}. \tag{4.31}$$

Last expression can be rewritten, by noticing that $\sigma_{k-1}^{v} = \sigma_{k-1}^{u,v} + x_u^* \sigma_{k-2}^{u,v}$, hence (4.31) implies that

$$\mu_v^* = \frac{\partial \Phi(x^*)}{\partial x_u} - \frac{\partial \Phi(x^*)}{\partial x_v} - x_u^* \sigma_{k-2}^{u,v} = \frac{\partial \Phi(x^*)}{\partial x_u} - \frac{\partial \Phi(x^*)}{\partial x_v} - \binom{|C|-1}{k-2} \left(\frac{1}{|C|}\right)^{k-1},$$

and applying (**C4**), it follows that $\mu_v^* < 0$. Since KKT dual feasibility condition is violated, x^* is not a local maximum, a contradiction. □

Theorem 15. *If C is a maximal clique in G of size greater than $k-1$, then $x^* = x^C$ is a strict local maximum of* ($\mathbf{P}^{k,\Phi}$).

Proof. Let λ^* and μ^* be the corresponding KKT multipliers. Let $u \in V \setminus C$. Since C is a maximal clique, there must exist $v \in C$ such that $\{v, u\} \notin E$. Let $\lambda^* = \frac{\partial \Phi(x^*)}{\partial x_v} + \sigma_{k-1}^{v}$. Then, for μ_u, from (4.25):

$$\begin{aligned} \mu_u^* &= \sigma_{k-1}^{v} + \frac{\partial \Phi(x^*)}{\partial x_v} - \sigma_{k-1}^{u} - \frac{\partial \Phi(x^*)}{\partial x_u} \\ &= \left[\binom{|C|-1}{k-1} - \binom{|C \cap N[u]|}{k-1}\right] \left(\frac{1}{|C|}\right)^{k-1} + \left[\frac{\partial \Phi(x^*)}{\partial x_v} - \frac{\partial \Phi(x^*)}{\partial x_u}\right] \end{aligned} \tag{4.32}$$

□

4.4 Computational Study

In this section we evaluate the performance of both the original standard polynomial programming formulations ($\mathbf{P}^k$) and their polynomial regularizations (PR) using the CONOPT solver [61], which aims to compute a local optimum satisfying the KKT optimality conditions. We focus on the cases of $k = 2, \ldots, 5$, since the time required to formulate and solve the considered models is rather large for higher values of k, making the approach impractical at this point. The solutions obtained using CONOPT are evaluated in terms of the cardinality of cliques they guarantee. According to Theorem 11, $S(x^*)$ is a maximal clique for any local maximum x^* of a regularized formulation (PR). This makes extracting of a maximal clique corresponding to a local maximum found by CONOPT a trivial task. It is possible, however, for the solver to output a KKT point that does not correspond to a clique (see Example 3). If this is the case, an extra post-processing effort is required to obtain a clique using a KKT point returned by the solver. Nevertheless, such a situation is unlikely to occur in practice, as was observed from the results of numerical experiments, which allows one to take advantage of the correspondence of local maxima to maximal cliques. As for the case of the original formulations ($\mathbf{P}^k$), the need for post-processing is rather expected, since the local maxima are known to correspond to strongly part-maximal multipartite cliques, which include but are not limited to maximal cliques. On a positive note, the multi-linear structure of the objective function in ($\mathbf{P}^k$) makes it easy to convert a KKT point into a clique. It is interesting to investigate how the two approaches (based on ($\mathbf{P}^k$) and (PR)) compare in practice, which is the main motivation of this computational study.

The first set of experiments, for $k \in \{2, \ldots, 5\}$, uses 24 sparse graphs arising in social networks [65], with the number of nodes ranging between 19 and 232, as described Table 4.1. In this table, the column "Graph" contains the name of each instance used. The next six columns give the number of vertices ($|V|$), edges ($|E|$), cliques of cardinality k ($|\mathcal{C}_k|$) for $k = 3, 4,$ and 5, respectively, and the clique number (ω) of the graph.

The second set of experiments is based on the instances from the Second DIMACS Implementation Challenge [66], shown in Table 4.2, for $k = 2$ and 3. The graphs in this set are considerably denser compared to the first set. Since the performance of a local solver strongly depends on the choice of the initial point, we used 100 random starting points for each instance in both sets of experiments. For fairness of comparison of the performance of different formulations, the same 100 random starting points generated for a given instance were used for all formulations we ran for that instance (non-regularized and regularized, with different k values).

The experiments were conducted on a MacBook Pro notebook with 8 GB 1600 MHz DDR3 RAM, 2.6 GHz Quad-Core Intel Core i7 processor, running macOS Catalina Version 10.15.7. The formulations were implemented in AMPL, with the CONOPT 3.17A solver used to obtain the reported solutions.

4.4.1 First set of experiments: Social networks

Summary of the results obtained in the first set of experiments are presented in Tables 4.3–4.6 for $k = 2, 3, 4$, and 5, respectively. More specifically, for both non-regularized and regularized formulations, the tables report the best and average solution value obtained over 100 runs (columns "Best" and "Mean", respectively), as well as the corresponding standard deviation ("St.D.") and average time per run ("Time"). Whenever one of the two formulations (non-regularized/regularized) beats the other in terms of the best or mean solution value, the better of the two values is shown in bold.

Notably, both non-regularized and regularized formulations managed to produce optimal solutions over the course of execution in almost all considered cases. The only exceptions were two instances for $k = 2$ ("strike" and "prison") and one instance for $k = 3$ ("lindenstrasse"). In these three cases, the best solution found using the regularized formulation had value $\omega - 1$. Remarkably, the best solution found using the non-regularized formulation was optimal for every single instance and for all considered k values. Non-regularized formulation also consistently outperforms its regularized counterpart in terms of the mean solution value. In fact, the regularized formulation beats the non-regularized one in terms of the average solution quality only on two instances ("jean" and "santafe"), both for $k = 3$, and matches it on one more instance ("anna" for $k = 5$). In all remaining cases the non-regularized formulation yields a strictly better average. The inferior performance of the regularized formulation can be explained by the fact that the regularization introduces local maxima corresponding to cliques of cardinality $k - 1$, whereas ($\mathbf{P}^k$) cannot have a local maximum yielding a clique with less than k vertices. In particular, for $k = \omega$ regularization introduces local maxima that are not global. The "lindenstrasse" instance for $k = 3$ provides a vivid illustration of this effect: Every single run for the regularized formulation yielded a clique on two vertices, whereas $\omega = 3$. This is in contrast to the non-regularized formulation, which produces a globally optimal solution on each run for this instance, as prescribed by theory.

Table 4.1: Basic characteristics of the social networks used in the first set of experiments.

Graph	$\|V\|$	$\|E\|$	$\|\mathcal{C}_3\|$	$\|\mathcal{C}_4\|$	$\|\mathcal{C}_5\|$	ω
monkeys5	19	60	78	54	22	6
taro	22	39	10	0	0	3
strike	24	38	12	1	0	4
dining	26	42	5	0	0	3
high-tech	33	91	77	29	7	6
korea1	33	68	44	12	2	5
karate	34	78	45	11	2	5
korea2	35	84	62	22	2	5
mexican	35	117	101	24	2	5
sawmill	36	62	18	0	0	3
tailorT1	39	158	201	119	42	6
tailorT2	39	223	451	448	234	7
flying	48	170	151	50	10	6
attiro	59	128	36	2	0	4
dolphins	62	159	95	27	3	5
terrorist	62	153	133	68	21	6
prison	67	142	58	14	1	5
huck	69	297	672	1013	1093	11
sanjuansur	74	144	44	3	0	4
jean	77	254	467	639	644	10
david	87	406	957	1457	1574	11
santa fe	118	200	113	35	5	5
anna	138	493	942	1243	1181	11
lindenstrasse	232	303	12	0	0	3

4.4.2 Second set of experiments: DIMACS instances.

DIMACS instances used in the second set of experiments are much more challenging than the graphs used in the first set of experiments. In particular, as can be seen in Table 4.2 the number of cliques in $\mathcal{C}_3$ is in the order of tens of millions for some of the instances, making the methods studied in this paper impractical in such cases. As a consequence, in this set of experiments we only consider $k = 2$ (for all 50 instances) and $k = 3$ (for 37 out of 50 instances that have $|\mathcal{C}_3| < 4 \times 10^6$). The results we obtained for $k = 2$ and 3 are summarized in Tables 4.7 and 4.8, respectively. Once again, the non-regularized formulation yields better overall results, albeit the advantage over the regularization is not as clear-cut as in the first set of experiments. Specifically, ($\mathbf{P}^k$) has an edge over (PR) in terms of the number of instances solved to optimality, the number of instances with higher best solution valuefound, and the number of instances with higher mean solution value, for both $k = 2$ and 3:

	$k = 2$		$k = 3$	
The number of instances	($\mathbf{P}^k$)	(PR)	($\mathbf{P}^k$)	(PR)
– solved to optimality	24	20	23	19
– with higher best solution value	11	9	8	4
– with higher mean solution value	33	15	19	12

Comparing the quality of the solutions obtained for the same formulation with different k value, we observe that ($\mathbf{P}^3$) beats ($\mathbf{P}^2$) on 5 and 20 instances in terms of the best and mean solution value found respectively, while ($\mathbf{P}^2$) outperforms ($\mathbf{P}^3$) in terms of the same criteria on 2 and 11 instances, respectively. Somewhat surprisingly, (PR) performs slightly better for $k = 2$ than for $k = 3$: It wins by the scores of 4-2 and 19-15 in terms of the best and mean solution value, respectively.

Finally, we observe that while the CPU time taken to solve the non-regularized and regularized formulations for the same k value is comparable, it is considerably higher for $k = 3$ than for $k = 2$.

Table 4.2: Description of DIMACS graphs used in the second set of experiments.

Graph	$\lvert V\rvert$	$\lvert E\rvert$	$\lvert\mathcal{C}_3\rvert$	ω
brock200_1	200	14834	543700	21
brock200_2	200	9876	159896	12
brock200_3	200	12048	291129	15
brock200_4	200	13089	373436	17
brock400_1	400	59723	4437011	27
brock400_2	400	59786	4450091	29
brock400_3	400	59681	4427156	31
brock400_4	400	59765	4445905	33
c-fat200-1	200	1534	5410	12
c-fat200-2	200	3235	25586	24
c-fat200-5	200	8473	182084	58
c-fat500-1	500	4459	18568	14
c-fat500-2	500	9139	82336	26
c-fat500-5	500	23191	546654	64
c-fat500-10	500	46627	2232248	126
hamming6-2	64	1824	30720	32
hamming6-4	64	704	960	4
hamming8-2	256	31616	2510592	128
hamming8-4	256	20864	672000	16
hamming10-2	1024	518656	173246464	512
hamming10-4	1024	434176	100624384	40
johnson8-2-4	28	210	420	4
johnson8-4-4	70	1855	23940	14
johnson16-2-4	120	5460	120120	8
johnson32-2-4	496	107880	13592880	16
keller4	171	9435	216597	11
keller5	776	225990	32681210	27
MANN_a9	45	918	11244	16
MANN_a27	378	70551	8669466	126
MANN_a45	1035	533115	182218740	345
p_hat300-1	300	10933	82394	8
p_hat300-2	300	21928	651470	25
p_hat300-3	300	33390	1888207	36
p_hat500-1	500	31569	419094	9
p_hat500-2	500	62946	3319308	36
p_hat500-3	500	93800	9053351	50
p_hat700-1	700	60999	1114944	11
p_hat700-2	700	121728	8885543	44
p_hat700-3	700	183010	24536683	62
san200_07_1	200	13930	466912	30
san200_07_2	200	13930	484808	18
san200_09_1	200	17910	960241	70
san200_09_2	200	17910	957904	60
san200_09_3	200	17910	957003	44
san400_0.5_1	400	39900	1741832	13
san400_0.7_1	400	55860	3796314	40
san400_0.7_2	400	55860	3760033	30
san400_0.7_3	400	55860	3723922	22
sanr200_07	200	13868	444234	18
sanr200_09	200	17863	950096	42

Table 4.3: Results of experiments with social networks for $k = 2$ using 100 starting points. The higher of best and mean solution values found among the two approaches are shown in bold.

Graph	Non-regularized				Regularized			
	Best	Mean	St.D.	Time	Best	Mean	St.D.	Time
monkeys5	6	**5.84**	0.367	0.005	6	5.76	0.450	0.005
taro	3	**2.98**	0.140	0.005	3	2.93	0.255	0.005
strike	**4**	**2.98**	0.316	0.005	3	2.75	0.433	0.005
dining	3	**2.81**	0.392	0.005	3	2.66	0.474	0.005
high-tech	6	**5.78**	0.715	0.005	6	5.30	1.153	0.005
korea1	5	**4.95**	0.218	0.005	5	4.75	0.517	0.005
karate	5	**4.35**	0.606	0.005	5	4.25	0.698	0.005
korea2	5	**4.78**	0.481	0.005	5	4.50	0.520	0.005
mexican	5	**4.69**	0.595	0.005	5	4.41	0.680	0.005
sawmill	3	**3.00**	0.000	0.005	3	2.97	0.171	0.005
tailorT1	6	**5.62**	0.485	0.005	6	5.42	0.764	0.005
tailorT2	7	**6.85**	0.357	0.005	7	6.57	0.587	0.005
flying	6	**4.88**	0.828	0.005	6	4.60	0.748	0.005
attiro	4	**3.09**	0.449	0.005	4	3.04	0.677	0.005
dolphins	5	**3.73**	0.705	0.005	5	3.56	0.697	0.005
terrorist	6	**5.78**	0.687	0.005	6	5.27	1.240	0.005
prison	**5**	**3.15**	0.536	0.005	4	2.97	0.538	0.005
huck	11	**9.89**	1.489	0.005	11	9.20	1.685	0.005
sanjuansur	4	**3.18**	0.384	0.005	4	2.89	0.371	0.005
jean	10	**9.66**	1.051	0.005	10	9.58	1.298	0.006
david	11	**10.60**	1.105	0.006	11	10.19	1.521	0.006
santafe	5	**4.86**	0.425	0.006	5	4.57	0.667	0.006
anna	11	**9.86**	1.020	0.006	11	8.69	0.731	0.007
lindenstrasse	3	**2.07**	0.255	0.006	3	2.01	0.099	0.007

Table 4.4: Results of experiments with social networks for $k = 3$ using 100 starting points. The higher of best and mean solution values found among the two approaches are shown in bold.

Graph	Non-regularized				Regularized			
	Best	Mean	St.D.	Time	Best	Mean	St.D.	Time
monkeys5	6	**5.84**	0.367	0.005	6	5.76	0.492	0.006
taro	3	**3.00**	0.000	0.005	3	2.99	0.099	0.005
strike	4	**3.45**	0.497	0.005	4	3.23	0.444	0.005
dining	3	**3.00**	0.000	0.005	3	2.77	0.421	0.005
high-tech	6	**5.98**	0.199	0.005	6	5.59	0.971	0.006
korea1	5	**4.90**	0.300	0.005	5	4.68	0.564	0.005
karate	5	**4.96**	0.196	0.005	5	4.31	0.611	0.005
korea2	5	**4.98**	0.140	0.005	5	4.71	0.454	0.006
mexican	5	**4.90**	0.300	0.005	5	4.50	0.557	0.006
sawmill	3	3.00	0.000	0.005	3	3.00	0.000	0.005
tailorT1	6	**5.86**	0.347	0.006	6	5.67	0.617	0.007
tailorT2	7	**6.62**	0.485	0.007	7	6.43	0.515	0.008
flying	6	**5.38**	0.675	0.005	6	4.87	0.611	0.007
attiro	4	**3.56**	0.496	0.005	4	3.15	0.477	0.006
dolphins	5	**4.73**	0.444	0.006	5	3.86	0.825	0.007
terrorist	6	**5.98**	0.140	0.006	6	5.76	0.776	0.007
prison	5	**4.34**	0.514	0.006	5	3.52	0.624	0.006
huck	11	**10.67**	1.059	0.008	11	10.21	1.169	0.010
sanjuansur	4	**3.58**	0.494	0.005	4	3.09	0.286	0.006
jean	10	9.29	1.089	0.007	10	**9.93**	0.534	0.009
david	11	**10.92**	0.462	0.009	11	10.13	1.467	0.012
santafe	5	4.11	0.313	0.006	5	**4.65**	0.638	0.008
anna	11	**10.96**	0.280	0.009	11	9.00	0.883	0.013
lindenstrasse	**3**	**3.00**	0.000	0.006	2	2.00	0.000	0.007

Table 4.5: Results of experiments with social networks for $k = 4$ using 100 starting points. The higher of best and mean solution values found among the two approaches are shown in bold.

Graph	Non-regularized				Regularized			
	Best	Mean	St.D.	Time	Best	Mean	St.D.	Time
monkeys5	6	**5.92**	0.271	0.005	6	5.83	0.376	0.006
strike	4	**4.00**	0.000	0.005	4	3.41	0.492	0.005
high-tech	6	**6.00**	0.000	0.005	6	5.75	0.654	0.006
korea1	5	**4.91**	0.286	0.005	5	4.75	0.456	0.005
karate	5	**4.97**	0.171	0.005	5	4.89	0.371	0.005
korea2	5	**5.00**	0.000	0.005	5	4.93	0.255	0.006
mexican	5	**4.91**	0.286	0.005	5	4.67	0.491	0.006
tailorT1	6	**5.99**	0.099	0.006	6	5.88	0.431	0.007
tailorT2	7	**6.42**	0.494	0.007	7	6.37	0.483	0.010
flying	6	**5.89**	0.343	0.005	6	5.13	0.673	0.006
attiro	4	**4.00**	0.000	0.005	4	3.41	0.492	0.006
dolphins	5	**4.91**	0.286	0.005	5	4.62	0.562	0.006
terrorist	6	**6.00**	0.000	0.005	6	5.99	0.099	0.007
prison	5	**4.67**	0.470	0.005	5	4.35	0.536	0.006
huck	11	**10.75**	0.622	0.011	11	10.71	0.931	0.016
sanjuansur	4	**4.00**	0.000	0.005	4	3.50	0.500	0.006
jean	10	**9.69**	0.744	0.008	10	9.20	1.342	0.012
david	11	**10.91**	0.531	0.013	11	10.66	1.032	0.019
santafe	5	**4.37**	0.483	0.006	5	4.10	0.300	0.007
anna	11	**11.00**	0.000	0.012	11	10.88	0.637	0.019

Table 4.6: Results of experiments with social networks for $k = 5$ using 100 starting points. The higher of best and mean solution values found among the two approaches are shown in bold.

Graph	Non-regularized				Regularized			
	Best	Mean	St.D.	Time	Best	Mean	St.D.	Time
monkeys5	6	**5.98**	0.140	0.005	6	5.86	0.347	0.006
high-tech	6	**6.00**	0.000	0.005	6	5.90	0.436	0.005
korea1	5	**5.00**	0.000	0.005	5	4.85	0.357	0.005
korea2	5	**5.00**	0.000	0.005	5	4.97	0.171	0.005
karate	5	**5.00**	0.000	0.005	5	4.94	0.237	0.005
mexican	5	**5.00**	0.000	0.005	5	4.88	0.325	0.005
tailorT1	6	**6.00**	0.000	0.005	6	5.99	0.099	0.007
tailorT2	7	**6.55**	0.497	0.007	7	6.36	0.480	0.012
flying	6	**5.92**	0.271	0.005	6	5.81	0.504	0.006
dolphins	5	**5.00**	0.000	0.005	5	4.76	0.427	0.006
terrorist	6	**6.00**	0.000	0.005	6	6.00	0.000	0.006
prison	5	**5.00**	0.000	0.005	5	4.54	0.498	0.005
huck	11	**10.74**	0.577	0.013	11	10.73	0.676	0.026
jean	10	**9.69**	0.744	0.009	10	9.59	0.861	0.017
david	11	**10.97**	0.298	0.016	11	10.81	0.717	0.035
santafe	5	**5.00**	0.000	0.005	5	4.41	0.492	0.006
anna	11	11.00	0.000	0.013	11	11.00	0.000	0.032

Table 4.7: Results of experiments with DIMACS instances for $k = 2$ using 100 starting points. The higher of best and mean solution values found among the two approaches are shown in bold. Optimal values are underlined.

0.95 Graph	Non-regularized				Regularized			
	Best	Mean	St.D.	Time	Best	Mean	St.D.	Time
brock200_1	**20**	**18.16**	0.997	0.053	19	17.42	1.124	0.043
brock200_2	10	**8.83**	0.762	0.031	10	8.65	0.684	0.028
brock200_3	13	**11.48**	0.818	0.039	13	11.08	0.924	0.034
brock200_4	**16**	**13.49**	0.877	0.045	15	12.94	0.915	0.038
brock400_1	**24**	**20.41**	1.150	0.276	23	19.43	1.290	0.208
brock400_2	23	**20.82**	1.126	0.267	23	20.10	1.221	0.206
brock400_3	23	**20.52**	1.162	0.268	23	19.41	1.141	0.200
brock400_4	24	**21.10**	1.162	0.280	24	20.00	1.371	0.210
c-fat200-1	12	11.98	0.140	0.009	12	11.98	0.140	0.009
c-fat200-2	24	**22.93**	0.852	0.012	24	22.91	0.814	0.013
c-fat200-5	58	**57.49**	0.671	0.023	58	57.48	0.655	0.023
c-fat500-1	14	**13.98**	0.140	0.018	14	13.73	1.094	0.019
c-fat500-2	26	**25.85**	0.357	0.028	26	25.82	0.384	0.028
c-fat500-5	64	63.25	0.753	0.062	64	**63.37**	0.744	0.065
c-fat500-10	126	125.42	0.751	0.122	126	**125.46**	0.727	0.123
hamming6-2	32	**29.38**	4.381	0.010	32	26.09	5.406	0.009
hamming6-4	4	**3.99**	0.099	0.007	4	3.98	0.140	0.007
hamming8-2	128	**107.47**	16.823	0.204	128	89.82	14.167	0.132
hamming8-4	16	**15.69**	0.935	0.073	16	14.99	1.847	0.062
hamming10-2	**512**	**403.50**	58.342	5.948	490	345.74	47.341	4.483
hamming10-4	**35**	**31.63**	1.978	4.289	34	30.74	1.346	2.575
johnson8-2-4	4	3.98	0.140	0.005	4	**4.00**	0.000	0.005
johnson8-4-4	14	**13.46**	1.276	0.009	14	12.39	2.009	0.009
johnson16-2-4	8	**7.98**	0.140	0.028	8	7.97	0.171	0.020
johnson32-2-4	16	**15.99**	0.099	1.409	16	15.56	0.554	0.662
keller4	**11**	**8.68**	0.747	0.034	10	8.34	0.651	0.030
keller5	20	17.52	1.144	1.477	20	**17.59**	0.928	1.137
MANN_a9	16	14.90	0.656	0.008	16	**15.10**	0.714	0.007
MANN_a27	117	117.00	0.000	0.255	**119**	**117.24**	0.531	0.635
MANN_a45	330	330.00	0.000	2.445	**331**	**330.01**	0.099	4.909
p_hat300-1	8	**6.86**	0.633	0.032	8	6.51	0.557	0.031
p_hat300-2	25	**22.97**	1.396	0.084	25	21.92	1.917	0.072
p_hat300-3	**36**	**32.47**	1.118	0.151	34	31.60	1.000	0.119
p_hat500-1	9	**7.33**	0.708	0.105	9	7.20	0.632	0.099
p_hat500-2	36	**33.52**	1.786	0.283	36	32.45	1.526	0.230
p_hat500-3	**49**	**46.90**	0.943	0.493	48	46.04	1.199	0.380
p_hat700-1	**10**	**7.86**	0.762	0.215	9	7.48	0.608	0.198
p_hat700-2	**44**	**41.19**	2.129	0.658	43	38.54	2.071	0.495
p_hat700-3	**61**	**58.16**	0.946	1.027	60	56.77	1.630	0.861
san200_0.7_1	15	15.00	0.000	0.039	**16**	**15.19**	0.392	0.064
san200_0.7_2	12	12.00	0.000	0.036	**13**	**12.02**	0.140	0.073
san200_0.9_1	45	45.00	0.000	0.051	**47**	**45.22**	0.481	0.087
san200_0.9_2	39	36.15	1.260	0.068	**40**	**37.25**	1.299	0.074
san200_0.9_3	35	30.51	2.729	0.082	35	**31.13**	1.724	0.068
san400_0.5_1	7	7.00	0.000	0.115	7	7.00	0.000	0.265
san400_0.7_1	20	20.00	0.000	0.178	**21**	**20.02**	0.140	0.398
san400_0.7_2	16	15.01	0.099	0.187	**17**	**15.06**	0.276	0.408
san400_0.7_3	13	12.01	0.099	0.161	**14**	**12.18**	0.409	0.410
sanr200_0.7	17	**15.11**	0.968	0.050	17	14.66	0.951	0.042
sanr200_0.9	**41**	**37.58**	1.550	0.084	39	36.12	1.505	0.062

Table 4.8: Results of experiments with DIMACS instances for $k = 3$ using 100 starting points. The higher of best and mean solution values found among the two approaches are shown in bold. Optimal values are underlined.

Graph	Non-regularized				Regularized			
	Best	Mean	St.D.	Time	Best	Mean	St.D.	Time
brock200_1	20	**18.14**	0.980	3.896	20	17.62	1.047	3.555
brock200_2	**11**	**9.05**	0.876	0.985	10	8.57	0.752	1.006
brock200_3	13	**11.64**	0.843	1.844	13	11.33	0.895	1.858
brock200_4	**16**	**13.78**	0.878	2.457	15	13.14	0.959	2.400
c-fat200-1	12	11.99	0.099	0.027	12	11.99	0.099	0.041
c-fat200-2	24	22.89	0.882	0.128	24	**22.95**	0.841	0.160
c-fat200-5	58	57.55	0.638	0.946	58	**57.58**	0.635	1.015
c-fat500-1	14	13.99	0.099	0.102	14	**14.00**	0.000	0.150
c-fat500-2	26	**25.89**	0.313	0.491	26	25.77	0.421	0.568
c-fat500-5	64	63.29	0.791	2.931	64	**63.35**	0.779	3.200
c-fat500-10	126	125.43	0.711	13.512	126	**125.44**	0.697	13.542
hamming6-2	32	**29.61**	4.326	0.160	32	26.33	5.521	0.151
hamming6-4	4	4.00	0.000	0.009	4	4.00	0.000	0.014
hamming8-2	128	**106.39**	16.817	33.652	128	90.14	14.215	21.353
hamming8-4	16	**15.90**	0.574	4.931	16	14.72	2.025	4.478
johnson8-2-4	4	4.00	0.000	0.007	4	4.00	0.000	0.008
johnson8-4-4	14	**13.87**	0.770	0.121	14	12.81	1.683	0.128
johnson16-2-4	8	**8.00**	0.000	0.942	8	7.94	0.237	0.706
keller4	**11**	**8.63**	0.673	1.354	10	8.48	0.640	1.392
MANN_a9	16	14.99	0.640	0.057	16	**15.09**	0.694	0.064
p_hat300-1	8	**6.92**	0.643	0.483	8	6.59	0.585	0.584
p_hat300-2	25	**22.87**	1.527	5.095	25	21.69	1.927	4.463
p_hat300-3	**36**	**32.47**	1.144	15.443	34	31.59	0.939	13.161
p_hat500-1	9	**7.69**	0.595	2.735	9	7.07	0.725	2.955
p_hat500-2	36	**33.43**	1.756	29.067	36	32.55	1.621	25.776
p_hat700-1	**11**	**8.09**	0.826	7.991	9	7.55	0.712	8.159
san200_0.7_1	15	15.00	0.000	2.267	**16**	**15.09**	0.286	4.249
san200_0.7_2	12	12.00	0.000	2.174	12	12.00	0.000	4.941
san200_0.9_1	45	45.00	0.000	5.413	**47**	**45.21**	0.496	8.682
san200_0.9_2	40	36.02	1.175	6.565	40	**37.18**	1.276	7.592
san200_0.9_3	**36**	30.47	2.907	7.848	34	**30.86**	1.761	6.899
san400_0.5_1	7	7.00	0.000	9.059	7	7.00	0.000	22.209
san400_0.7_1	20	20.00	0.000	22.468	20	20.00	0.000	49.743
san400_0.7_2	15	15.00	0.000	21.683	**16**	**15.02**	0.140	48.226
san400_0.7_3	12	12.00	0.000	20.077	**14**	**12.10**	0.332	50.096
sanr200_0.7	**18**	**15.21**	1.070	3.067	17	14.66	0.992	2.885
sanr200_0.9	**41**	**37.43**	1.512	8.278	40	36.04	1.483	6.653

5. CONCLUSIONS AND FUTURE WORK

In this dissertation, we discussed applications of continuous optimization methods for discrete problems, focusing on a NP-hard problem of finding a maximum clique in a given graph. In the following, we give a summary of obtained results and provide some insights into possible future research ideas.

5.1 Conclusions

We introduced a hierarchy of standard polynomial programming formulations for the maximum clique problem. Specifically, for a given graph $G = (V, E)$ and $k \in \{2, \ldots, \omega\}$, where ω is the clique number of the graph, the maximum clique problem is formulated as a problem ($\mathbf{P}^k$) of maximizing a multilinear polynomial of degree k over the standard simplex $\Delta^{|V|}$ in $\mathbb{R}^{|V|}$. We have shown that the support of a local maximum of each formulation corresponds to a strongly part-maximal multipartite clique in G. This gives the most complete characterization of the local maxima structure for MSQP and MSPP problems.

Moreover, we have demonstrated the hierarchical aspect of the formulations, where the local maximality of a point for ($\mathbf{P}^{k+1}$) implies its local maximality for ($\mathbf{P}^k$), leading to every local maximum of ($\mathbf{P}^\omega$) being global.

Following the framework developed for quadratic formulations, we have developed multiple families of regularized formulations, which guarantee one-to-one correspondence between local maxima of the formulation and maximal cliques in the given graph. While the lack of correspondence of local maxima to cliques in the given graph was considered a major drawback of a non-regularized formulation, we have argued that corresponding cliques can be efficiently extracted from any local maximum point and hence non-regularized formulation can be used just as efficiently as regularized one. We have additionally shown that both regularized and non-regularized formulations can be used as a set of benchmarks for polynomial programming solvers.

We have also developed a novel bound on a value of elementary symmetrical polynomial of order k over p variables when constrained by a symmetric polynomial of order $k-1$ over the same set of variables.

5.2 Future Work

Given the scope of this work, we have identified a set of possible directions for future work. A natural direction of exploration would be the study of formulations for clique relaxations models. As it was mentioned, extensions of MSQP were formulated for s-plex and s-defective clique, which suggests that it would be possible to formulate analogous extensions using MSPP.

Another possible direction lies in the study of higher-order formulations for elementary structures different from clique. In MSPP formulation of order k, we relied on a set $\mathcal{C}_k$ of cliques of size k in a given graph G. Of course, for MSQP, the only other option would be the sets of two independent vertices, which is equivalent to formulating MSQP for a complement graph $\bar{G}$. On the other hand, for MSPP, we have exponentially more options as k grows. For example, what would be the combinatorial structure of maxima for a maximization problem formulated over the set of open triangles $\mathcal{T}_3$ of G as

$$g(G) \coloneqq \max_{x\in\Delta^n} \sum_{T\in\mathcal{T}_3} \prod_{i\in T} x_i = \max_{x\in\Delta^n} \sum_{T\in\mathcal{T}_3} \pi_T(x). \tag{5.1}$$

It is of interest to formulate optimization problems for finding maximum structures related to clique relaxations or generalizations in continuous terms. Such structures might possibly be s-cliques (distance-based relaxation, where for any two vertices in S, v and w, there must exist a path in G of length at most s from v to w), independent unions of cliques, or s-clubs (where the diameter of $G[S]$ is at most s).

Another question related to the previous one is if it is possible to formulate a general condition for a subgraph property Π that would mean there there is a corresponding continuous formulation for maximum Π problem. One possible direction of attack for this question is from the viewpoint of forbidden subgraph characterizations.

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