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Continuous Characterizations of the Maximum Clique Problem

by

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ABSTRACT

Given a graph G whose adjacency matrix is A, the Motzkin-Strauss formulation of the Maximum-Clique Problem is the quadratic program $\max\{x^T Ax | x^T e = 1, x \geq 0\}$. It is well known that the global optimum value of this QP is $(1 - 1/\omega(G))$, where $\omega(G)$ is the clique number of G. Here, we characterize the following: 1) first order optimality 2) second order optimality 3) local optimality 4) strict local. These characterizations reveal interesting underlying discrete structures, and are polynomial time verifiable. A parametrization of the Motzkin-Strauss QP is then introduced and its properties are investigated. Finally, an extension of the Motzkin-Strauss formulation is provided for the weighted clique number of a graph and this is used to derive a maximin characterization of perfect graphs.

1 Introduction

1.1 The Problem of Interest

Let A be the adjacency matrix of a graph G. Consider the *Motzkin-Strauss formulation* (also called the *Motzkin-Strauss QP*) of the Maximum Clique Problem:

$$\boxed{\begin{array}{lll} \max & : & x^T Ax/2 \\ \text{s.t.} & & e^T x = 1 \\ & & x \geq 0. \end{array}} \tag{\textbf{P}}$$

The following well known result is due to Motzkin and Strauss[13].

Proposition 1 *The global optimal value of* $\mathbf{P}$ *is given by*

$$f^* = 1/2(1 - 1/\omega(G)),$$

where $\omega(G)$ *is the clique number of* G.

In this paper, characterizations and polynomial time recognition algorithms are presented for the feasible solutions of $\mathbf{P}$ that:

1. satisfy first order necessary conditions for optimality.
2. satisfy second order necessary conditions for optimality.
3. are locally optimal for $\mathbf{P}$.
4. are strictly locally optimal for $\mathbf{P}$.

These characterizations reveal interesting graph theoretic structure underlying these properties. In §6, a parametrization of $\mathbf{P}$ is introduced and its properties are explored. Then, in §7, a weighted extension of the Motzkin-Strauss formulation is established.

1.2 Notation

A graph is denoted by $G = (V, E)$, where $V = \{1, \ldots, n\}$ is the vertex set, and E is the edge set. We write $u \sim v$ if u and v are adjacent, and $u \not\sim v$ otherwise. The neighborhood of a node v, denoted by $\partial(v)$, is the set of nodes adjacent to v. The characteristic vector of a subset C of the node set V will be denoted by $\chi(C)$. For any nonnegative vector $x \in \Re^V_+$, $S(x)$ will be the support of x, i.e. $S(x) = \{u | x_u > 0\}$, and $Z(x)$ will denote the complement of $S(x)$.

A *clique* (resp. *stable set*) in a graph is a pairwise adjacent (resp. nonadjacent) subset of the nodeset. A clique C is said to be *maximal*, if it is not contained in any larger clique. A maximal clique will be called *strictly maximal* if no single vertex in C can be exchanged with some vertex outside C to obtain a clique.

The maximum size of a clique in G is called the *clique number* of G and will be denoted by $\omega(G)$ (simply by ω when no confusion is likely to arise). If w_u for $u \in V$ are given node weightes, then the *weigthed clique number* $\omega(w, G)$ is the largest of $\sum_{u \in C} w_u$ among all cliques C of G. Note that the weights are all ones, then we recover $\omega(G)$. The *chromatic number* of a graph is the least number of colors required to "color" the vertices of G such that no two adjacent vertices are given the same color; it is denoted by $\chi(G)$.

A *complete l-partite* graph is one whose vertex set can be partitioned as $V = S_1 \cup S_2 \cup \ldots S_l$, where each of the S_i induce a stable set and every pair of vertices in different parts are adjacent. A graph is called *complete multipartite*, if it is complete l-partite for some l.

A symmetric matrix A is said to be:

Positive Semidefinite: If $y^T Ay \geq 0 \ \forall \ y$.
Negative Semidefinite: If $y^T Ay \leq 0 \ \forall \ y$.
Almost Negative Semidefinite: If $y^T Ay \leq 0$ for every y such that $e^T y = 0$.
Co-Positive: If $y^T Ay \geq 0 \ \forall \ y \geq 0$.

The simplex of feasible solutions of $\mathbf{P}$ is denoted by Δ_n. We will denote by e the vector of all ones, by J the matrix of all ones, and I is the identity matrix.

1.3 Optimality and Related Conditions

Consider an optimization problem $\max\{f(x) | x \in \Delta_n\}$. A solution $\bar{x} \in \Delta_n$ is *globally maximal* if $f(x) \leq f(\bar{x}) \ \forall \ x \in \Delta_n$, and it is *locally maximal*, if there exists an $\alpha > 0$, such that $f(x) \leq f(\bar{x}) \ \forall \ x \in \Delta_n \cap B(\bar{x}, \alpha)$, where $B(\bar{x}, \alpha) = \{x | \parallel x - \bar{x} \parallel_\infty \leq \alpha\}$; i.e. , in a neighborhood around itself, $\bar{x}$ has the largest function value. A locally optimal solution $\bar{x}$ is said to be *strictly locally optimal* if $f(x) < f(\bar{x})$ for every x in a neigborhood of $\bar{x}$. The solution $\bar{x}$ is an *isolated local optimum* if it is the only local maximum solution in some neighborhood. It is not hard to show that every isolated local optimum is a strict local optimum, while the converse is not true in general. The optimal value of an optimization problem $\mathbf{Q}$ will be denoted by $v(\mathbf{Q})$.

Stated below are the first and second order necessary conditions for optimality (of $\bar{x}$ for $\mathbf{P}$) (see Luenberger[12], chapter 10):

First Order (KKT) Conditions:

$$\begin{aligned} -A\bar{x} + \lambda e - \mu &= 0 \\ \bar{x}^T e &= 1 \\ \bar{x} &\geq 0 \\ \mu &\geq 0 \\ \mu_u \bar{x}_u &= 0 \ \forall \ u. \end{aligned} \tag{1OC}$$

Second Order Conditions: Let $Z(\bar{x}) = \{u | \bar{x}_u = 0\}$.

$$-y^T Ay \geq 0, \ \forall \ y \text{ s.t. } y^T e = 0, y_u = 0 \ \forall \ u \in Z(\bar{x}). \tag{2OC}$$

We say that a feasible solution $\bar{x}$ to $\mathbf{P}$ is a *first order point*, if there exist λ and μ such that the conditions (1OC) are satisfied. A first order point is said to be *second order point*, if (2OC) holds. Since the constraints of $\mathbf{P}$ are simplex constraints, regularity conditions always hold, and hence both (1OC) and (2OC) are necessary for a solution to be locally (or globally) optimal. Therefore, for the nonlinear program $\mathbf{P}$, the following chain of inclusions is evident:

$$\begin{aligned} \text{global optimal solutions} &\subset \text{local optimal solutions} \\ &\subset \text{second order points} \\ &\subset \text{first order points} \end{aligned}$$

While it is easily shown that the recognition of global optima is NP-Hard, it follows from the results of this paper that the recognition of the remaining three classes of solutions can be accomplished in polynomial time.

1.4 Outline of the Paper

In §2, we derive a technical lemma which gives a combinatorial characterization of certain semidefiniteness propertis of the adjacency matrix. In §3, we characterize the first order and second order points, the latter by an application of the technical lemma. Another application of the same will result in a characterization of local optima of **P**. This is then applied to show that strict local maxima and isolated local optima are one and the same for the problem **P**, and that these points are in a one-to-one correspondence with the (discrete) strictly maximal cliques. Recognition complexity results are presented in §5.

A parametrization of the Motzkin-Strauss QP is introduced in §6. We derive some results concerning the optimal value function of this parametrization, and develop an expression for the optimal solution sets. A one-to-one correspondence between the maximum cliques of G and the global solutions of the parametrized problem is then established.

Finally, in §7, the Motzkin-Strauss formulation is extended to the weighted case. More specifically, for any positive weight vector $w > 0$, a class of quadratic programs is given, all of whose optimum values are $\omega(w, G)$.

2 A Key Semidefiniteness Lemma

The following lemma concerns the negative semidefiniteness of the quadratic form $y^T Ay$, with A being the adjacency matrix A of a graph G, over a polyhedral cone associated with a partition $S \cup T$ of V. The lemma will be critically employed in the analysis to follow.

Lemma 1 *Let $G = (V, E)$ be a graph whose adjacency matrix is A. Let $S \subset V$, $T = V \backslash S$, and define the polyhedral cone:*

$$Y = \{y | y^T e = 0, y_v \geq 0 \ \forall \ v \in T\}.$$

Then the following are equivalent.

1. *A is negative semidefinite over the cone Y, i.e. $y^T Ay \leq 0 \ \forall \ y \in Y$.*
2. *If $u, v, w \in V, u \not\sim v, u \not\sim w, v \sim w$, then either $u, v \in T$ or $u, w \in T$.*
3. *The node sets S, T can be partitioned as:*

$$S = S_1 \cup S_2 \cup \ldots S_l, T = T_0 \cup T_1 \cup \ldots T_l,$$

such that

   (a) *Each S_i is nonempty.*
   (b) *$S_i \cup T_i$ is an independent set for every $i = 1, .., l$.*
   (c) *For all $i \neq j$, every vertex in $S_i \cup T_i$ is adjacent to every vertex in S_j.*
   (d) *Every node of T_0 is adjacent to every node in S.*

Proof:
Given distinct nodes u, v, w, we say that the triplet $\{u, v, w\}$ violates *2*, if $u, v, w \in V, u \not\sim v, u \not\sim w, v \sim w$, and neither $u, v \in T$ nor $u, w \in T$. Note that such a triplet must satisfy: either $u \in T$ and $v, w \in S$ (called Case 1), or $u \in S$ (Case 2).

1 ⇒2
Let u, v, w be a triplet violating *2*. Put $y_u = \delta, y_v = -\delta/2, y_w = -\delta/2$, where $\delta = 1$ if $u \in T$ (case 1) and -1 if $u \in S$ (case 2). It is then seen that $y \in Y$, and $y^T Ay = 1/2$, which violates *1*.

2 ⇒3
The proof of this implication will be given by induction on n. The base case of $n = 1$ is trivial.

Let us assume that condition *2* is satisfied. If $S = \emptyset$, then it suffices to set $l = 0, T_0 = V = T$. Suppose that S is not empty, and let u be any vertex in S. Define the sets:

$$S_1 = \{v \in S | v \not\sim u\} \text{ and } T_1 = \{v \in T | v \not\sim u\},$$

and note that S_1 is nonempty.

It is claimed that $S_1 \cup T_1$ is an independent set. If this is not the case, let $v, w \in S_1 \cup T_1, v \sim w$. From the definition of S_1 and T_1, we observe that v and w are distinct from u, and neither of these nodes is adjacent to u. This implies that $\{u, v, w\}$ is a triplet violating *2* (case 2).

Clearly u is adjacent to every node outside $S_1 \cup T_1$. We claim that every node in S_1 is adjacent to every node outside $S_1 \cup T_1$: Suppose not, and let $v \in S_1 \backslash \{u\}$ and $w \in V \backslash (S_1 \cup T_1)$ with $w \not\sim v$; since $u \not\sim v, u \sim w$, $\{v, u, w\}$ is a triplet violating *2* (case 2), a contradiction. It will now be shown that every node in T_1 is adjacent to every node in $S \backslash S_1$. If not, then there exist $v \in T_1$, and $w \in S \backslash S_1$ such that $v \not\sim w$. But we have $u \not\sim v$ and $u \sim w$, and hence the triplet $\{v, u, w\}$ violates *2* (case 1).

Let $V' = V \backslash (S_1 \cup T_1), S' = V' \cap S, T' = V' \cap T$. Then, by the induction hypothesis, one can partition V' as

$$V' = T_0 \cup (S_2 \cup T_2) \cup \dots (S_l \cup T_l),$$

such that the properties described in *3* hold. Adding $S_1 \cup T_1$ to this partition gives the desired partition of V.

3 ⇒1
Let $y \in Y$, and consider

$$\begin{aligned} y^T Ay &= (y^T e)^2 - \textstyle\sum_{u \in T_0} y_u^2 - \sum_{i=1}^{l} (\sum_{u \in S_i \cup T_i} y_u)^2 \\ &\quad -2 \textstyle\sum \{y_u y_v | u, v \in T_0, u \not\sim v\} \\ &\quad -2 \textstyle\sum \{y_u y_v | u \in T_i, v \in T_j, u \not\sim v, 0 \le i < j \le l\}. \end{aligned}$$

Since $y^T e = 0$, and $y_u \ge 0 \ \forall \ u \in T$, $y^T Ay \le 0$. □

The corollary below specializes the above result to the case in which $T = \emptyset$.

Corollary 1 *Let $G = (V, E)$ be a graph with adjacency matrix A. Then the following are equivalent.*

1. *A is almost negative semidefinite (i.e. $y^T e = 0 \Rightarrow y^T Ay \le 0$).*
2. *There do not exist distinct vertices u, v, w such that $u \not\sim v, u \not\sim w, v \sim w$.*
3. *G is complete multipartite.*

The condition of *2* says that the almost negative semidefiniteness of the adjacency matrix of a graph is characterized by the nonexistence of $K_1 + K_2$ as an induced subgraph (K_n is the complete subgraph on n vertices).

3 Necessary Conditions for Local Optimality

3.1 First Order Solutions

Given a (feasible) solution $\bar{x} \in \Delta_n$, it is quite easy to characterize whether there exist $\mu \in \Re^n, \lambda \in \Re$ such that conditions (1OC) are satisfied (i.e. whether $\bar{x}$ is a first order point).

Note that if $(\bar{x}, \mu, \lambda)$ satisfies (1OC), then we must have

$$0 = \bar{x}^T(\lambda e - A\bar{x} - \mu) = \lambda - \bar{x}^T A\bar{x} - \bar{x}^T\mu = \lambda - \bar{x}^T A\bar{x}.$$

The lemma below follows quite easily.

Lemma 2 *Let $\bar{x} \in \Delta_n$, and $S(\bar{x}) = \{u|\bar{x}_u > 0\}$. Then $\bar{x}$ is a first order point if and only if the vector*

$$\mu := (\bar{x}^T A\bar{x})e - A\bar{x}$$

satisfies

$$\mu \geq 0 \text{ and } \mu_u = 0 \; \forall \; u \in S(\bar{x}).$$

3.2 Second Order Solutions

In this section a characterization of second order points of **P** is established. The result is a strengthening of a result in [6] (also [5]) where it was proven that the conditions which are shown here to be necessary and sufficient for second order optimality, are necessary for global optimality.

In contrast with Lemma 2, which characterizes the first order points, one notes that the following result brings out the underlying combinatorial structure of the conditions. One manifestation of this is that, the Lagrange multiplier associated with the constraint $e^T x = 1$ is required to be among the discrete set of values $(1 - 1/l)$, where l is a positive integer.

Theorem 1 *Let $\bar{x}$ be a feasible solution to* **P**, *and let H be the induced subgraph of G indexed on $S(\bar{x})$, the support of $\bar{x}$. Then $\bar{x}$ is a second order point if and only if the following hold:*

1. *H is a complete l-partite graph (for some l), with the partition $S(\bar{x}) = S_1 \cup \ldots \cup S_l$, with each S_i being nonempty.*
2. $\sum_{u \in S_j} \bar{x}_u = 1/l \; \forall \; j = 1, .., l.$
3. $A\bar{x} \leq (1 - 1/l)e.$

Also, if $\bar{x}$ is a second order point, then $f(\bar{x})$ is $(1/2)(1 - 1/l)$, and $\lambda = 1 - 1/l$, where λ is the Lagrange multiplier associated with the constraint $e^T x = 1$ in **P**.

Proof:

Suppose that $\bar{x}$ satisfies (1OC) and (2OC) for a certain set of multipliers λ and $\mu \geq 0$. Let H be the graph induced by the nonempty support $S(\bar{x})$ of $\bar{x}$, and let B be the adjacency matrix of H. Then, (2OC) reduces to

$$y^T By \leq 0 \ \forall \ y \text{ s.t. } y^T e = 0.$$

An application of Corollary 1 gives that H must be a complete l-partite graph. Let $S(\bar{x}) = S_1 \cup S_2 \cup \ldots S_l$ be the partition. By complementary slackness, $\mu_u = 0 \ \forall \ u \in S(\bar{x})$, hence

$$(A\bar{x})_u = \lambda \ \forall \ u \in S(\bar{x}). \tag{1}$$

Let

$$\rho_j = \sum_{u \in S_j} \bar{x}_u.$$

Then, we have

- $\sum_{j' \neq j} \rho_{j'} = \lambda \ \forall \ j = 1, .., l$ (from (1)).
- $\sum_j \rho_j = 1$ (since $\bar{x}^T e = 1$)

The above clearly imples that $\rho_j = 1/l \ \forall \ j$, and we must also have $\lambda = (1 - 1/l)$. Since

$$A\bar{x} = \lambda e - \mu \leq \lambda e,$$

the necessity follows.

Sufficiency is trivially established by setting $\lambda = (1 - 1/l)$, $\mu = \lambda e - A\bar{x}$ and making another application of Corollary 1.

The last part of the theorem concerning the optimal value and the Lagrange multiplier of a second order point is quite evident. □

4 Local Optimality

The following theorem characterizes local optimality in the Motzkin-Strauss QP formulation. Throughout this section, $f(x)$ will denote the function $x^T Ax/2$.

Theorem 2 *Let $\bar{x} \in \Delta_n$. Then $\bar{x}$ is a local maximum of* **P** *if and only if there exists an integer l such that, with*

$$\lambda := 1 - 1/l, S := \{u | \bar{x}_u > 0\}, T := \{u | \bar{x}_u = 0, (A\bar{x})_u = \lambda\},$$

we have

1. *$A\bar{x} \leq \lambda e$.*
2. *$(A\bar{x})_u = \lambda \ \forall \ u \in S$.*

3. *We can partition S and T as*

$$S = S_1 \cup \ldots \cup S_l, T = T_1 \cup \ldots \cup T_l,$$

such that

(a) $S_i \neq \emptyset \ \forall \ i = 1, .., l.$

(b) $S_i \cup T_i$ *is independent for every* i.

(c) $i \neq j, u \in S_i \cup T_i, v \in S_j \Rightarrow u \sim v.$

Proof:
Define the node set

$$U := V \backslash (S \cup T) = \{u | \bar{x}_u = 0, (A\bar{x})_u < \lambda\},$$

and the polyhderal cone

$$Y = \{y \in \Re^n | y^T e = 0, y_u \geq 0 \ \forall \ u \in T \cup U\}.$$

Observe that Y is the tangent cone to the feasible region, i.e. the simplex Δ_n, at the $\bar{x}$.

Sufficiency: It suffices to show that there exists $\alpha > 0$ such that $\forall \ y \in Y$, $\| y \|_\infty \leq \alpha$,

$$\theta := f(\bar{x} + y) - f(\bar{x}) \leq 0.$$

Upon expansion,

$$2\theta = y^T Ay + 2y^T A\bar{x}.$$

We will first dispose of the situation when $U = \emptyset$. In this case, $A\bar{x} = \lambda e$, and so when $y \in Y$,

$$2\theta = y^T Ay + 2\lambda y^T e = y^T Ay.$$

By an application of Lemma 1 it follows that $\theta \leq 0$. (In fact, since Y contains Δ_n, it actually follows that $\bar{x}$ is a global optimum for the problem $\mathbf{P}$ in this case).

Let us now assume that $U \neq \emptyset$, and define the quantities:

$$\begin{array}{rcl} \hat{\lambda} & := & \min_{u \in U}(\lambda - (A\bar{x})_u) > 0 \\ \alpha & := & \frac{\hat{\lambda}}{n}. \end{array}$$

Let $y \in Y, \| y \|_\infty \leq \alpha$, and split y into two vectors

$$y = y_1 + y_2,$$

where the support of y_1 is contained in $S \cup T$ and that of y_2 is contained in U.

We have the following equality/inequality chain, with ensuing explanation, which establishes that $\theta \leq 0$:

$$\begin{array}{rcl} 2\theta & = & (y_1 + y_2)^T A(y_1 + y_2) + 2(y_1 + y_2)^T A\bar{x} \\ & = & y_1^T Ay_1 + y_2^T Ay_2 + 2y_1^T Ay_2 + 2y_1^T A\bar{x} + 2y_2^T A\bar{x} \\ & \leq & y_2^T Ay_2 + 2y_1^T Ay_2 + 2y_1^T A\bar{x} + 2y_2^T A\bar{x} \\ & = & y_2^T Ay_2 + 2y_1^T Ay_2 + 2\lambda y_1^T e + 2y_2^T A\bar{x} \\ & = & y_2^T Ay_2 + 2y_1^T Ay_2 + 2y_2^T (A\bar{x} - \lambda e) \\ & \leq & y_2^T Ay_2 + 2y_1^T Ay_2 - 2y_2^T e\hat{\lambda} \\ & \leq & \alpha |U| y_2^T e + 2\alpha |S \cup T| y_2^T e - 2y_2^T e\hat{\lambda} \\ & = & y_2^T e(\alpha(|U| + 2|S \cup T|) - 2\hat{\lambda}) \\ & \leq & y_2^T e(2\alpha n - 2\hat{\lambda}) \\ & = & 0. \end{array}$$

Explanation: The graph induced by $S \cup T$ satisfies the decomposition of condition *3* of Lemma 1 (with $T_0 = \emptyset$), and therefore $y_1^T A y_1 \le 0$, implying the first inequality in the above. The following equality is from $(A\bar{x})_u = \lambda \ \forall \ u \in S \cup T$, and $(y_1)_u = 0$ for $u \notin S \cup T$, and so $y_1^T A\bar{x} = \lambda y_1^T e$, and the succeding equality uses $y_1^T e = -y_2^T e$. The second inequality is from the definition $\hat{\lambda}$. Since $Ay_1 \le \alpha|S \cup T|e$ and $y_2 \ge 0$, $y_2^T A y_1 \le \alpha |S \cup T| y_2^T e$, and similarly, $y_2^T A y_2 \le \alpha |U| y_2^T e$, and the third inequlity follows.

Necessity: Let $\bar{x}$ be a local maximum for $\mathbf{P}$. It is clear that $\bar{x}$ must be a second order point. Let λ, μ be such that (1OC) and (2OC) hold. Define

$$S := \{u | \bar{x}_u > 0\} \text{ and } T := \{u | \bar{x}_u = 0, (A\bar{x})_u = \lambda\}.$$

Let H' be the subgraph induced by $S \cup T$.

Let y be such that $y^T e = 0$. Then,

$$\begin{aligned} \theta &= (\bar{x}+y)^T A(\bar{x}+y) - \bar{x}^T A\bar{x} \\ &= y^T Ay + 2y^T A\bar{x} \\ &= y^T Ay + 2y^T(A\bar{x} - \lambda e) + 2\lambda y^T e \\ &= y^T Ay + 2\textstyle\sum_{v \in U} y_v((A\bar{x})_v - \lambda) \end{aligned}$$

Hence, if $y_v = 0 \ \forall \ v \in U$, then we must have $y^T Ay \le 0$. Therefore, we can apply Lemma 1 (for the graph H'), to conclude that the partitions

$$S = S_1' \cup \ldots \cup S_{l'}', T = T_0 \cup \ldots \cup T_l,$$

with appropriate properties exist.

In our present case, $T_0 = \emptyset$; this is so since if $v \in T_0$, then

$$\sum_{u \in \partial(v)} \bar{x}_u = \sum_{u \in S} \bar{x} = 1,$$

which violates $(A\bar{x})_v \le \lambda$, as

$$\lambda = \bar{x}^T A\bar{x} = 1 - 1/l.$$

The theorem now follows. □

The following corollary shows that every maximal clique in G gives rise to a local maximum of $\mathbf{P}$.

Corollary 2 *Let C be a maximal clique in G. Then $\chi(C)/|C|$ is a local maximum of* $\mathbf{P}$.

Proof: Let $C = \{u_1, u_2, \ldots, u_l\}$ be a maximal clique, and let $\bar{x} = \chi(C)/|C|, l = |C|$ and $\lambda = 1 - 1/l$. Then T as defined in the statement of Theorem 2 is precisely the set of nodes in $V \backslash C$ that are adjacent to exactly $l-1$ nodes in C. Letting $S_i = \{u_i\}$ and T_i be the set of nodes in T that are not adjacent to u_i, we will obtain a partition satisfying the required properties. It follows that $\bar{x}$ is a local optimum. □

The corollary below relates local optimality to the chromatic number of G.

Corollary 3 *Let $\bar{x}$ be a local optimum of G, and let l, U be as given by Theorem 2. Then the chromatic number of G is at most l plus the chromatic number of the subgraph induced by U.*

The proof is evident from the fact that we can first optimally color U, and then color each of the independent sets $S_i \cup T_i$ with a new color.

4.1 Strict and Isolated Local Maximality

By an application of Theorem 2 and its proof, we obtain the result that the strict local optima and the isolated local optima of $\mathbf{P}$ are jointly equal to the set of vectors of the form $\chi(C)/|C|$, where C is a strictly maximal clique (i.e. every node u not in C is nonadjacent to at least two nodes of C). From the definitions, every isolated local optimum is also strictly locally optimal.

Theorem 3 *For any $\bar{x} \in \Delta_n$, the following are equivalent:*

1. *$\bar{x}$ is strictly locally optimal for $\mathbf{P}$.*
2. *there exists a strictly maximal clique C such that $\bar{x} = \chi(C)/|C|$.*
3. *$\bar{x}$ is an isolated local optimum of $\mathbf{P}$.*

Proof:

1 $\Rightarrow$ 2

Suppose that $\bar{x}$ is a strict local maximum. We make an application of Theorem 2 (since $\bar{x}$ is a local maximum), and let l, λ, S, T be as given by the theorem. Define the polytope

$$X := \{x \in \Delta_n | \sum_{u \in S_1 \cup T_1} x_u = 1/l, x_u = \bar{x}_u \; \forall \; u \notin S_1 \cup T_1\}.$$

Clearly, $\bar{x} \in X$, and it is easily shown that for any $x \in X$, $f(x) = f(\bar{x}) = 1/2(1 - 1/l)$. If $S_1 \cup T_1$ is not a singleton, then X contains points other than $\bar{x}$, which means that $\bar{x}$ is not a strict local maximum. Hence $|S_1 \cup T_1| = 1$, and similarly

$$|S_i \cup T_i| = 1 \; \forall \; i = 1, .., l.$$

This must imply that for every i, S_i is a singleton and T_i is empty. Therefore, $C := S(\bar{x})$ is a clique in G. Now, if there is a vertex u not in C which is adjacent to at least $l-1$ nodes in C, then $(A\bar{x})_u \geq (l-1)/l$, which implies that $u \in T$, a contradiction. Hence C is a strictly maximal clique.

2 $\Rightarrow$ 3

Let $\bar{x} = \chi(C)/|C|$ for some strictly maximal clique C. By Corollary 2, $\bar{x}$ is a local maximum of $\mathbf{P}$, and for the sake of contradiction, suppose that $\bar{x}$ is not an isolated local maximum. Then, there exists a sequence $\{x^k\} \subset \Delta_n$ of local optimal solutions, each member of which is different from $\bar{x}$, that converges to $\bar{x}$. Let S^k be the support of x^k. Since there are only finitely many subsets of V, by passing to a subsequence, we may assume that $S^k = S \; \forall \; k$ for some fixed set S. Since the sequence $\{x^k\}$ converges to $\bar{x}$, $C \subset S$. Let us now make an application of Theorem 1, and conclude firstly that S induces a complete-l-partite subgraph in G, with the partition $S = S_1 \cup \ldots S_l$, and secondly that $f(x^k) = (1/2)(1 - 1/l) \; \forall \; k$. Since the x^k converge to $\bar{x}$ and since $f(\bar{x}) = (1/2)(1 - 1/|C|)$, it follows that $l = |C|$. Since each of the S_j is independent, it must be that each node of C is contained in exactly one of the S_i. Consequently, if any of the $S_i, i = 1, .., l$ is not a singleton, then we clearly have a violation to the strict maximality of the clique C. Hence we conclude that $S = C$. By an application of *2* of Theorem 1, we conclude that $x_u^k = 1/l = 1/|C| \; \forall \; u \in S = C$. It follows that $x^k = \bar{x} \; \forall \; k$, which is a contradiction. Hence $\bar{x}$ is an isolated local maximum of $\mathbf{P}$.

The theorem now follows. □

Recently, Pelillo and Jalota [18] independently proved the implication *1* $\Leftrightarrow$ *2* by employing second order sufficiency conditions of nonlinear programming.

5 Recognition Complexity

In this section, we will address the issue of verifying whether a given feasible solution $\bar{x}$ is a first order point, second order point, or a local maximum. The main result is that the recognition of all these three types of points is polynomial time solvable. This is interesting due to the fact that the detection of local optimality in quadratic programs in NP-Hard. In fact, for a very simple modification of the Motzkin-Strauss formulation, the recognition of local optimality turns NP-Hard, as we will show in the subsection to follow.

5.1 On Local Maximality Recognition

Let a graph G and an integer k be given. By Proposition 1, we have the following.

$$\begin{aligned} \omega(G) \le k \quad &\Leftrightarrow \quad \max\{x^T A x | x \in \Delta_n\} \le 1 - 1/k \\ &\Leftrightarrow \quad \max\{x^T (A - (1 - 1/k)J) x | x \in \Delta_n\} \le 0, \end{aligned}$$

where J is the matrix of all ones (the last implication is from $x^T J x = (x^T e)^2$). Let us define $Q := kA - (k-1)J$, and consider the homogeneous QP:

$$\max\{x^T Q x | x \ge 0\}. \qquad (\mathbf{HP})$$

The following lemma was suggested by Lovász in a personal communication.

Lemma 3 *The following are equivalent.*

1. $\omega(G) \le k$
2. $x^T Q x \le 0 \ \forall \ x \ge 0$, *i.e.* $-Q$ *is Co-Positive.*
3. 0 *is a local maximum of* **HP**.
4. 0 *is a global maximum of* **HP**.

Proof: The equivalence of *1,2* and *4* is clear. Now, if 0 is a local maximum, then from the homogeneity of the objective function, and since the feasible region is conical, the global maximality follows. □

Thus, in general, detecting local maximality is a difficult problem (that local optimality detection in quadratic programs is NP-Hard was originally established by Kabadi and Murty [10]). See [17] for related results. It will be shown in the following that for the Motzkin-Strauss QP, one can check local maximality of any feasible solution in polynomial time.

5.2 Local Maximality Recognition in Motzkin-Strauss

Given $\bar{x} \in \Delta_n$, whose local optimality status needs to be assessed, we perform the following sequence of steps.

1. Let $S = \{u | \bar{x}_u > 0\}$, $\lambda = \bar{x}^T A \bar{x}$, and $\mu = (\bar{x}^T A \bar{x})e - A\bar{x}$.

2. Check if $\mu \geq 0$, and $\mu_u = 0 \ \forall \ u \in S$. If so, then $\bar{x}$ is a first order point, and proceed to next step. Otherwise, $\bar{x}$ is not a first order point, and hence terminate.

3. Now, check if S induces a complete multipartite graph in G (see below for a $O(n^2)$ algorithm). If so, then $\bar{x}$ is a second order point, and proceed to next step. Otherwise, stop.

4. Let $T = \{u | (A\bar{x})_u = \lambda\}$. Now we determine ($O(n^2)$) if $S \cup T$ can be partitioned as depicted in Theorem 2. This will now be explained in detail.

Given a graph G' whose vertex set is $S \cup T$ for two disjoint sets S and T, the following scheme determines a partition (if such a partition does not exist, this fact will be indicated):

$$S = S_1 \cup \ldots \cup S_l, T = T_1 \cup \ldots \cup T_l,$$

such that,

- $S_j \cup T_j$ is independent for every j, and
- for $i \neq j, u \in S_i \cup T_i, v \in S_j$, we have $u \sim v$.

By using condition *2* of Lemma 1, one can readily obtain a $O(n^3)$ for verifying this condition. However, we improve the complexity to $O(n^2)$ by using the following algorithm. (Note also that by setting $T = \emptyset$, one can check if G' is complete multipartite, as required in Step 3 of the algorithm for checking local maximality.)

1. Pick any node u in S, and let $S' = S \backslash \partial(u)$, and $T' = T \backslash \partial(u)$. Add S' and T' as the next elements of the partition.

2. Delete S' from S and T' from T. If S is now empty but T is not empty, then the partition as required does not exist. So terminate.

3. Repeat Steps 1 and 2 until S is empty.

4. Now, check to see if the incidence as depicted in the conditions above is satisfied. If yes, we have the desired partition, and otherwise, no such partition exists.

The correctness of the method is quite easy to show, and the complexity is $O(n^2)$.

6 A Parametrization of Motzkin-Strauss

From the Motzkin-Strauss formulation, observe that if G has a maximum clique C of size ω, then for $x = \chi(C)/\omega$, we have $x^T x = 1/\omega$. Hence, every global solution of the optimization problem

$$\begin{array}{lll} \max & : & x^T A x/2 \\ \text{s.t.} & & x^T e = 1 \\ & & x^T x = 1/\omega \\ & & x \geq 0 \end{array}$$

is also a global solution of $\mathbf{P}$. As before, $f(x)$ will denote $x^T A x/2$.

Since the value of ω is not known a priori, we consider the **Parametrized Motzkin-Strauss** problem $\mathbf{P}(s)$:

$$\boxed{\begin{array}{lll} \max & : & f(x) := x^T Ax/2 \\ \text{s.t.} & & x^T e = 1 \\ & & x^T x = 1/s \\ & & x \geq 0, \end{array}} \qquad (\mathbf{P}(s))$$

wherein the parameter s is a *real* number in the interval $[1, n]$. Observe that this is precisely the range for which $\mathbf{P}(s)$ is feasible. Let the optimal value of this program be denoted by $v(s)$.

The following result (Theorem 4) relates $v(s)$ to the maximal clique size $\omega(G)$. But first let us define the following set of solutions for a given subset C of V, and a real number $s \in [1, n]$:

$$X(s, C) := \{x | x^T e = 1, x^T x = 1/s, x \geq 0, x_u = 0 \ \forall \ u \notin C\}.$$

The following lemma is easy to establish.

Lemma 4 *The set $X(s, C)$ is nonempty if and only if $1 \leq s \leq |C|$. For $s = |C|$, $X(s, C)$ consists simply of the vector $\chi(C)/|C|$.*

In the theorem below, we will establish some properties of the optimal value function $v(s)$ and the set of optimal solutions of $\mathbf{P}(s)$.

Theorem 4 *Let G be a graph with maximum clique size ω. Then the following hold:*

1. *$v(s) = 1/2(1 - 1/s)$ whenever $1 \leq s \leq \omega$.*
2. *$v(s) \leq 1/2(1 - 1/\omega) < 1/2(1 - 1/s)$ for every $\omega < s \leq n$.*
3. *$v(s) = 1/2(1 - 1/s)$ if and only if $s \leq \omega$.*
4. *$v(\mathbf{P}) = \max_{1 \leq s \leq n} v(s) = 1/2(1 - 1/\omega)$*
5. *For $s \leq \omega$, the set of global optimal solutions of $\mathbf{P}(s)$ is given by*

   $$\cup\{X(s, C) | C \text{ is a clique, and } s \leq |C|\}.$$

6. *The set of global optimal solutions of $P(\omega)$ is precisely vectors of the form $\chi(C)/\omega$, where C is an (optimal) ω-clique. Hence there is a one-to-one correspondence between the global optimal solutions of $\mathbf{P}(\omega)$ and the optimal cliques in G.*

Proof:

<u>Proof of *1*</u>
Let $s \leq \omega$. Let $\bar{A}$ be the adjacency matrix of the complement graph $\bar{G}$ (i.e. $\bar{A} = J - I - A$), and let x be any solution feasible to $\mathbf{P}$(s). We then have,

$$\begin{aligned} f(x) &= 1/2 x^T Ax \\ &= 1/2(x^T Jx - x^T x - x^T \bar{A}x) \\ &= 1/2((x^T e)^2 - x^T x - x^T \bar{A}x) \\ &= 1/2(1 - 1/s) - (1/2)x^T \bar{A}x \\ &\leq 1/2(1 - 1/s) \text{ (Since } \bar{A} \geq 0, x \geq 0). \end{aligned}$$

Hence $v(s) \leq 1/2(1-1/s)$. Let C be a clique of size S in G for some $S \geq s$ (note that s is not assumed to be integral), and note that $X(s,C)$ is not empty. Now, for an arbitrary $x \in X(s,C)$,

$$\begin{aligned} f(x) &= (1/2)\sum\{x_u x_v | u, v \in C, u \neq v\} \\ &= (1/2)((\textstyle\sum_{u \in C} x_u)^2 - (\sum_{u \in C} x_u^2)) = (1/2)(1-1/s). \end{aligned} \tag{2}$$

Therefore, $v(s) = 1/2(1-1/s)$ whenever $s \leq \omega$.

Proof of *2*
Let $s > \omega$. Since any x that is feasible for $\mathbf{P}(s)$ is also feasible for $\mathbf{P}$, and since $v(\mathbf{P}) = 1/2(1-1/\omega)$, we can conclude that

$$v(s) \leq 1/2(1-1/\omega) < 1/2(1-1/s).\square$$

Proof of *3*
Since $1/2(1-1/s)$ is an increasing function of s, *1* and *2* together imply *3*.

Proof of *4*
The feasible region of $\mathbf{P}$ is the union of the feasible regions of $\mathbf{P}(s)$ for s in the range $[1,n]$. This, coupled with *1* and *2* implies *4*.

Proof of *5*
By equation (2), every $x \in X(s,C)$, where C is a clique of size at least s, satisfies

$$f(x) = (1/2)(1-1/s),$$

and hence is globally optimal.

On the other hand, for an arbitrary feasible solution x of $\mathbf{P}(s)$, with $\bar{A}$ being the adjacency matrix of the complement graph $\bar{G}$, we have

$$f(x) = 1/2(1-1/s - x^T\bar{A}x).$$

Hence, if $f(x) = 1/2(1-1/s)$, then $x^T\bar{A}x = 0$, since $x \geq 0$ and $A \geq 0$, this happens if and only if:

$$x_i x_j = 0 \text{ whenever } \bar{A}_{ij} = 1,$$

implying that the support $S(x)$ of x forms a stable set in $\bar{G}$, and hence a clique in G; let C be this clique. Clearly, $x \in X(s,C)$, which by Lemma 4 implies that $s \leq |C|$.

Proof of *6* follows from an application of *5* and Lemma 4. The proof of the theorem is now complete. $\square$.

7 A Weigthed extension of Motzkin-Strauss

Given a nonnegative weight (node weights) vector w, for any subset C of the vertex set, $w(C)$ denotes the sum of the weights of nodes in C. The weighted clique number $\omega(w;G)$ is the maximum of $w(C)$ over all cliques C of G. Note that $\omega(e,G)$ is the usual clique number $\omega(G)$ of the graph.

In this section, a weighted extension of the Motzkin-Strauss Theorem will be given, more specifically, a quadratic programming formulation is given for the weighted clique number $\omega(w;G)$, where w is assumed to be a positive weight vector. First, let us consider the following reformulation of Proposition 1.

Proposition 2 *For a graph G with edge set E, and a positive node weight vector w, we have:*

$$1/\omega(w,G) = \min\{x^T(I+\bar{A})x | e^Tx = 1, x \geq 0\},$$

where $\bar{A}$ is the adjacency matrix of the complement graph $\bar{G}$.

Proof: By Proposition 1,

$$\begin{aligned}
1/\omega(G) &= 1-\max\{x^TAx|e^Tx=1, x\geq 0\}\\
&= \min\{1-x^TAx|e^Tx=1, x\geq 0\}\\
&= \min\{x^T(J-A)x|e^Tx=1, x\geq 0\}\\
&= \min\{x^T(I+\bar{A})x|e^Tx=1, x\geq 0\}.\square
\end{aligned}$$

Given a positive weight vector w, define the following set of matrices:

$$\mathcal{M}(w,G) := \{B|B_{ii}=1/w_i\ \forall\ i, B_{ij}+B_{ji}\geq(1/w_i+1/w_j)\ \forall\ ij\in\bar{E}, B_{ij}=0\ \forall\ ij\in E\},$$

and observe that $I+\bar{A}\in\mathcal{M}(e,G)$. And hence the following theorem is a generalization of Proposition 2. The proof technique is similar to one employed in [11].

Theorem 5 *For any positive weight vector w, and $B\in\mathcal{M}(w)$, we have:*

$$1/\omega(w,G)=\min\{x^TBx|e^Tx=1, x\geq 0\}. \qquad \textbf{(WP)}$$

Proof:

The first part of the proof is to show that there exists a global optimum to the problem **(WP)** whose support S induces a clique in G. The second part shows that the optimal value for this solution equals $1/w(S)$, and then the theorem will follow.

Let $\bar{x}$ be global optimum solution whose support S does not induce a clique in G, i.e. , there exist two nodes u,v such that $\bar{x}_u,\bar{x}_v>0$, but $u\not\sim v$.

Consider the parametrized line segment $x(\nu)$ given by $x(\nu)_u=\bar{x}_u+\nu, x(\nu)_v=\bar{x}-\nu, x(\nu)_w=\bar{x}_w\ \forall\ w\neq u,v$. In the range $-\bar{x}_u\leq\nu\leq\bar{x}_v$, $x(\nu)$ is feasible for **(WP)**. Consider the value of the objective function on this segment. It is not difficult to show that

$$f(x(\nu))=\nu^2(1/w_i+1/w_j-B_{ij}-B_{ji})+\text{ a linear term in }\nu.$$

Since $B_{ij}+B_{ji}\geq(1/w_i+1/w_j)$, the above quadratic function is concave. Therefore, the minimum of $f(x(\nu))$ over $-\bar{x}_u\leq\nu\leq\bar{x}_v$ occurs at either extreme $\nu=-\bar{x}_u$ or $\nu=\bar{x}_v$. Let ν^* be such an optimal ν. Clearly $x(\nu^*)$ has either the ith or jth component is zero, and hence the support of $x(\nu^*)$ is smaller than that of $\bar{x}$. Since $\bar{x}$ is global optimal for **(WP)**, it must be that so is $x(\nu^*)$. By repeating this argument, with $\bar{x}$ being replaced by $x(\nu^*)$, it can be deduced that there exists a global optimal solution $\bar{x}$, whose support S induces a clique in G.

When the support of x in **(WP)** is restricted to a clique S in G, then the objective function value is

$$x^TBx=\sum_{i\in S}x_i^2/w_i,$$

and its minimum over the simplex can easily be shown to be at

$$\begin{aligned}
x_i &= w_i/(\textstyle\sum_{i\in S}w_i)=w_i/w(S)\ \forall\ i\in S\\
&= 0\ \forall\ i\notin S,
\end{aligned}$$

and substitution yields that the optimal value is $1/w(S)$. For the solution $\bar{x}$ to be global optimal, $w(S)$ must be the maximum weighted clique in G, and the proof is complete.$\square$

From the proof, it is clear that if B is chosen to be in the relative interior of $\mathcal{M}(w,G)$, i.e. if $B_{ij}+B_{ji} > 1/w_i + 1/w_j$ for every $ij \notin E$, then the support of every global optimal solution induces a clique in G. Thus, there is a direct correpondence between the maximum weighted cliques and the global solutions for such a choice of B.

7.1 A Continuous Characterization of Perfect Graphs

In this section, we state without proof a characterization of perfect graphs. It can be derived from Theorem 5. For the necessary background on perfect graphs, the reader is referred to Chapter 9 of [8] and the edited volume [2].

A graph G is said to be *perfect*, if for every induced subgraph H of G, the clique number $\omega(H)$ equals the chromatic number $\chi(H)$. The fascination surrounding perfect graphs stems from, among others, the following aspects relating to them:

1. For general graphs, the problems of finding the clique number, coloring number and the like is NP-Hard. But, when a graph is perfect, these problems can be solved in polynomial time, as demonstrated in the book [8].
2. Among the most celebrated conjectures in graph theory is the *Strong Perfect Graph Conjecture (SPGC)*. This conjecture, made by Claude Berge in 1960, states that a graph G is perfect if and only if neither G nor $\bar{G}$ (complement of G) contains an induced odd cycle. This conjecuture remains unsettled.
3. Perfect graphs have many interesting geometric and combinatorial features and intriguing connections with semidefinite programming.

Much of the notation employed here is taken from [8]. Briefly, $\alpha(w,G), \omega(w,G)$ and $\chi(w,G)$ denote the weighted stability number, clique number and the chromatic number, respectively. For a positive vector w, w^{-1} denotes the vector whose ith component is $1/w_i$. For two vectors u, v, $u \oplus v$ is the matrix whose ijth entry is $u_i + v_j$, $A \circ B$ for two matrics A and B is the *Hadamard product*, i.e. , $(A \circ B)_{ij} = A_{ij}B_{ij}$.

Theorem 6 *The following are equivalent:*

1. *G is perfect.*
2. *For every induced subgraph H of G, $\omega(H)\alpha(H) \geq |H|$.*
3. *For every $w \geq 0$,*
$$\omega(w,G)\alpha(w,G) \geq w^T w.$$
4. *For every $w > 0$,*
$$\omega(w,G)\alpha(w,G) \geq w^T w.$$
5. *The following maximin condition holds:*
$$\sup_{w>0} \min_{x,y \in \Delta_n} (w^T w) x^T Rx . y^T Sy \leq 1,$$

where

$$\begin{aligned} R &= (w^{-1} \oplus w^{-1}) \circ (I + \bar{A}) \\ S &= (w^{-1} \oplus w^{-1}) \circ (I + A). \end{aligned}$$

An interesting act is that, the following multiquadratic system is feasible if and only if G is imperfect. First, let $\mathcal{C}$ and $\mathcal{S}$ denote respectively the collections of maximal cliques and stable sets of G, and $\phi(.)$ denotes the characteristic vector of a subset of V.

$$\begin{aligned} \phi(C)^T w . \phi(S)^T w &< 1 \ \forall \ C \in \mathcal{C}, S \in \mathcal{S} \\ w^T w &= 1 \\ w &\geq 0. \end{aligned}$$

8 Concluding Remarks

In this paper, we have investigated several aspects of the Motzkin-Strauss QP formulation of the Maximum Clique Problem. Here are some related issues that seem worth investigating.

- Characterize the second order, and locally optimal solutions for the parametrized and weighted versions of Motzkin-Strauss formulations introduced in this paper.
- We have seen that local maximality detection in the Motzkin-Strauss quadratic program (**P**) has polynomial complexity and that in the homogeneous version (**HP**) is NP-Hard. Are there broad classes of quadratic programs for which local optimality is polynomial time solvable?

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