Journal of Global Optimization (2006) 35: 405–421
DOI 10.1007/s10898-005-5185-6

On a Polynomial Fractional Formulation for Independence Number of a Graph

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(Received 14 September 2004; accepted in revised form 15 November 2005)

Abstract. In this paper we characterize the local maxima of a continuous global optimization formulation for finding the independence number of a graph. Classical Karush-Kuhn-Tucker conditions and simple combinatorial arguments are found sufficient to deduce several interesting properties of the local and global maxima. These properties can be utilized in developing new approaches to the maximum independent set problem.

Key words: Global optimization, Maximum independent set, Polynomial fractional programming

1. Introduction

Many important discrete optimization problems such as maximum clique, maximum independent set, MAX CUT, quadratic assignment and others can be formulated as continuous global optimization problems (Pardalos, 1996). The standard quadratic programming formulation due to Motzkin and Straus (1965), continuous formulation due to Gibbons et al. (1996) and other formulations (Harant, 1998; Harant et al., 1999; Harant, 2000) have led to the development of effective heuristics for maximum clique and maximum independent set problems (Bomze, 1997; Abello et al., 2001; Burer et al., 2002; Busygin et al., 2002; de Angelis et al., 2004). Gibbons et al. (1997) also characterize maximal cliques in terms of local solutions to the Motzkin-Straus formulation. Efficient approximation algorithms due to Goemans and Williamson for MAX CUT problem, using semidefinite programming can be found in (Goemans and Williamson, 1995). Burer et al. have also developed heuristics for MAX CUT problem in (Burer et al., 2001).

With the development of powerful global optimization algorithms and software packages, it is essential to study the characteristics of continuous formulations of discrete problems, to identify special properties that can be exploited in order to adapt and improve the performance of these algorithms and build effective heuristics. Thus, successful numerical methods developed for special types of global optimization problems, such as polynomial fractional programming (Tuy et al., 2004), can be utilized for solving properly formulated discrete optimization problems. In this paper, we consider a polynomial fractional formulation for the maximum independent set problem and study its local and global maximum properties. We first characterize the local maxima of this formulation and then obtain a modified formulation which has one-to-one correspondence between maximal independent sets and local maxima. The two formulations are further compared in terms of numerical results obtained using a simple local search algorithm and the standard constrained optimization function available in MATLAB® Optimization Toolbox.

The paper is organized as follows. After introducing the required definitions and the notations used in this paper, we provide the formulation for independence number in Section 3. In Section 4, we study the properties of its local maxima in the continuous and binary neighborhoods. In Section 5, we modify this formulation so that the local maxima of the newly obtained formulation correspond to maximal independent sets. In Section 6, we present some computational test results and then conclude.

2. Definitions and Notations

Let $G=(V,E)$ be a simple undirected graph with vertex set $V=\{1,\dots,n\}$ and edge set $E\subseteq V\times V$. For $i\in V$, let $N(i)$ and d_i denote the set of neighbors and degree of vertex i in G, respectively. The *complement graph* of G is the graph $\bar{G}=(V,\bar{E})$, where $\bar{E}=\{(i,j)\in V\times V : i\neq j, (i,j)\notin E\}$. For a subset $W\subseteq V$ let $G(W)$ denote the subgraph induced by W on G, $G(W)=(W, E\cap(W\times W))$.

A dominating set $D\subseteq V$ is a set of vertices such that every vertex in the graph is either in this set or has a neighbor in this set. A set of vertices $I\subseteq V$ is called an independent set if for every $i,j\in I$, $(i,j)\notin E$, *i.e.*, the graph $G(I)$ is edgeless. An independent set is *maximal* if it is not a subset of any larger independent set, and *maximum* if there are no larger independent sets in the graph. The maximum cardinality of an independent set of G is called the *independence number* of the graph G and is denoted by $\alpha(G)$. A *clique* C is a subset of V such that the subgraph $G(C)$ induced by C on G is complete. The maximum clique problem is to find a clique of maximum cardinality. The *clique number* $\omega(G)$ is the cardinality of a maximum clique in G.

Clearly, I is a maximum independent set of G if and only if I is a maximum clique of $\bar{G}$. Computation of $\alpha(G)$ and $\omega(G)$ for general graphs is difficult as the maximum independent set and the maximum clique problems are NP-hard (Garey and Johnson, 1979). These problems are very important due to a wide range of their practical applications (Bomze et al., 1999). For any graph, Wei's lower bound (Wei, 1981; Caro and Tuza, 1991) on the independence number is given by,

$$\alpha(G) \geq \sum_{i \in V(G)} \frac{1}{1+d_i} \tag{1}$$

Finally, for a given vector $x \in \{0, 1\}^n$, its binary neighborhood consists of all the binary vectors that are at Hamming distance 1 from x. That is, the set of all binary vectors that can be obtained from x by changing the value of one of its components to the opposite.

3. Continuous Global Optimization Formulation

The following formulation of the maximum independent set problem was proposed in (Balasundaram and Butenko, 2005a).

THEOREM 1. *The independence number $\alpha(G)$ satisfies the continuous global optimization formulation:*

$$\alpha(G) = \max_{x \in [0,1]^n} \sum_{i \in V(G)} \frac{x_i}{1 + \sum_{j \in N(i)} x_j} \tag{2}$$

The proof of this result in (Balasundaram and Butenko, 2005) also shows that every local maximum of (2) is a 0-1 vector. Denote by $x^* \equiv I^*$, the equivalence of a binary vector to a subset of vertices constructed as $I^* = \{i \in V : x_i^* = 1\}$. We will say that a 0-1 solution x^* of (2) corresponds to a set of vertices $I^* \subseteq V$. Even though all local maximizers of (2) are binary vectors, they do not necessarily correspond to independent sets. In fact, it was found in (Balasundaram and Butenko, 2005) that, if x^* is a global maximizer of (2) then V^* induces a graph whose components are cliques. That is, V^* is such that Wei's lower bound is sharp on the graph $G(V^*)$. Further in this paper we will use term *independent union of cliques* (IUC) for a graph whose connected components are cliques. Figure 1 shows a graph that has independence number 2 with maximum independent sets {1, 5}, {2, 5}, {3, 5} and {1, 4}. But the objective function attains optimum for {1, 2, 3, 5} also, which is an IUC with two clique components {1, 2, 3} and {5}.

4. Local Maxima

We now identify some properties of local maxima of the above formulation. Note that since any local maximum of (2) is a 0-1 vector, it corresponds to a subset of vertices of the graph (denoted by $x \equiv I$). We now set up the

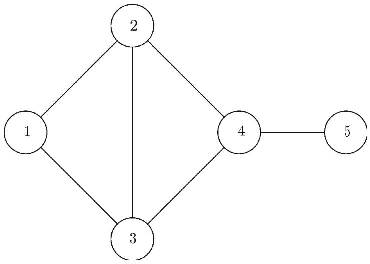

Figure 1. An example of a graph for which an optimal solution to (2) does not correspond to an independent set.

Karush-Kuhn-Tucker (KKT) conditions for this formulation and a simple lemma that will be used subsequently.

Denote by $f(x)$ the objective function of (2):

$$f(x)=\sum_{i\in V}\frac{x_i}{1+\sum_{j\in N(i)} x_j}. \tag{3}$$

We apply the first order necessary conditions (FONC) to problem (2) written as follows,

$$\max f(x)$$

subject to:

$$\begin{aligned} x_i-1\le 0 \quad &\forall\ i\in V \quad :\lambda_i;\\ -x_i\le 0 \quad &\forall\ i\in V \quad :\mu_i. \end{aligned}$$

Recall that all local maximizers of (2) are binary vectors. And it is easy to check that the Jacobian of all active constraints has full rank at any binary vector, therefore all feasible binary vectors are regular points for problem (2). Thus, any local maximizer x^o of (2) satisfies the KKT conditions. This implies that there exist λ^o, μ^o such that the following conditions are satisfied,

$$\begin{aligned} \forall\ k\in V:\ \left.\frac{\partial f}{\partial x_k}\right|_{x=x^o} &=\lambda_k^o-\mu_k^o;\\ \lambda_k^o(x_k^o-1) &=0;\\ \mu_k^o(-x_k^o) &=0;\\ \lambda_k^o &\ge 0;\\ \mu_k^o &\ge 0; \end{aligned}$$

where

$$\left.\frac{\partial f}{\partial x_k}\right|_{x=x^o} = \frac{1}{1+\sum_{j\in N(k)} x_j^o} - \sum_{i\in N(k)} \frac{x_i^o}{(x_k^o + 1 + \sum_{j\in N(i)\setminus\{k\}} x_j^o)^2}.$$

Consider $I^o \subseteq V$, where $x^o \equiv I^o$. Then $\forall\ k\in I^o,\ x_k^o = 1$ and from the KKT conditions above we have,

$$\begin{aligned}
\mu_k^o &= 0;\\
\lambda_k^o &= \frac{1}{1+\sum_{j\in N(k)} x_j^o} - \sum_{i\in N(k)} \frac{x_i^o}{(x_k^o + 1 + \sum_{j\in N(i)\setminus\{k\}} x_j^o)^2}\\
&= \frac{1}{1+|N(k)\cap I^o|} - \sum_{i\in N(k)\cap I^o} \frac{1}{(1+|N(i)\cap I^o|)^2}.
\end{aligned}$$

On the other hand, if $k\in V\setminus I^o$ then $x_k^o = 0$ and the KKT conditions yield,

$$\begin{aligned}
\lambda_k^o &= 0;\\
\mu_k^o &= \sum_{i\in N(k)} \frac{x_i^o}{(x_k^o + 1 + \sum_{j\in N(i)\setminus\{k\}} x_j^o)^2} - \frac{1}{1+\sum_{j\in N(k)} x_j^o}\\
&= \sum_{i\in N(k)\cap I^o} \frac{1}{(1+|N(i)\cap I^o|)^2} - \frac{1}{1+|N(k)\cap I^o|}.
\end{aligned}$$

Next we prove a trivial lemma that will be used in further discussion.

LEMMA 1. *Consider the problem*

$$\begin{aligned}
&\text{maximize } f(x)\\
&\text{s.t.} \qquad Ax \le b,
\end{aligned}$$

where $f:\Re^n \to \Re$ *is a continuously differentiable function,* $A\in\Re^{m\times n}, m>n$. *Assume that a regular point* x^* *satisfies the FONC so that* n *constraints are active in* x^* *and strict complementarity holds, i.e., there exists* $\mu \ge 0$ *such that*

$$\nabla f(x^*) = A^T \mu \tag{4}$$

and the components of μ *corresponding to active constraints in* x^* *are positive. Then* x^* *is a local maximizer of the considered problem.*

Proof. Denote by $\bar{A} \in \Re^{n\times n}$ the submatrix of A consisting of rows corresponding to the constraints that are active in x^* and by $\bar{\mu}\in\Re^n$ the corresponding Lagrange multipliers; $\bar{\mu} > 0$. Then

$$\nabla f(x^*) = \bar{A}^T \bar{\mu}. \tag{5}$$

Consider any feasible direction d in x^*. Then $\bar{A}(x^*+d) \leq \bar{b}$, where $\bar{b} \in \Re^n$ is the vector of components of b corresponding to the active constraints. Since $\bar{A}x^* = \bar{b}$, we have $\bar{A}d \leq 0$. Moreover, since x^* is regular, $\bar{A}x = \bar{b}$ has a unique solution (given by x^*), thus if $d \neq 0$ then at least one of the components of $\bar{A}d$ has to be negative. Thus, using (5) we have

$$\nabla f(x^*)^T d = \mu^T \bar{A} d < 0.$$

So, d is a descent direction. Since d is an arbitrary feasible direction, x^* is a local maximizer. □

THEOREM 2. *If x^o is a point of local maximum of* (2) *and $x^o \equiv I^o$, then I^o is a dominating set.*

Proof. Suppose that I^o is not a dominating set, then there exists $x_i^o = 0$ such that $N(i) \cap I^o = \emptyset$. Construct x', such that

$$x'_j = \begin{cases} \epsilon > 0, & \text{if } j = i; \\ x_j^o, & \text{if } j \in V \setminus \{i\}. \end{cases}$$

Then we have, $f(x') = f(x^o) + \epsilon$, which contradicts the fact that x^o is a local maximum. Hence, I^o must be a dominating set. □

COROLLARY 1. *If x^o is a local maximizer of* (2) *with $x^o \equiv I^o$ and I^o is an independent set, then it is maximal and there exist unique λ^o, μ^o such that (x^o, λ^o, μ^o) solves KKT-FONC given by*

$$\lambda_k^o = \begin{cases} 1, & \text{if } k \in I^o; \\ 0, & \text{if } k \in V \setminus I^o; \end{cases}$$

$$\mu_k^o = \begin{cases} 0, & \text{if } k \in I^o; \\ |N(k) \cap I^o| - \frac{1}{1+|N(k) \cap I^o|}, & \text{if } k \in V \setminus I^o. \end{cases}$$

□

REMARK. The conclusion that a local maximum corresponds to a dominating set is only a necessary condition and the converse is obviously not true. For example, consider the graph G_1 in Figure 2 with $\alpha(G_1) = 2$. The set of vertices $I = \{1, 2, 3\}$ is a dominating set. Since we already know that a global maximum corresponds to an independent union of cliques with maximum number of components, we can also consider maximal by inclusion IUC (*i.e.*, such that it is not a subset of IUC with larger number of components) to be candidates for local maxima. Note that I is a maximal clique and there does not exist a strict superset which induces an IUC with 2 or more components making this a maximal IUC. However,

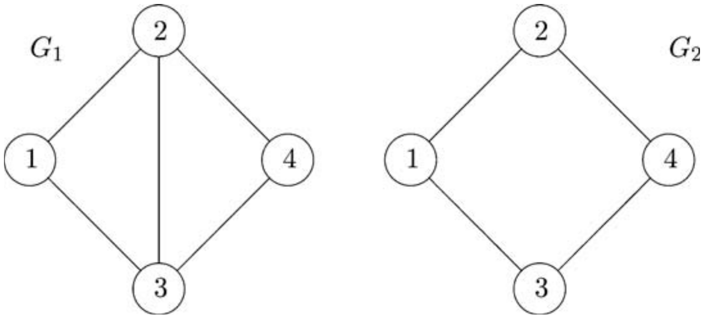

Figure 2. Graphs to illustrate non-local-optimality of a dominating set and a maximal independent union of cliques and local optimality of a vector not corresponding to an IUC.

$x=[1,1,1,0]^T \equiv I$ is not a local maximum. Let $x'=[1,1,1,\epsilon]^T$, where $\epsilon>0$. Then $f(x')=1+\frac{\epsilon(1+\epsilon)}{3(3+\epsilon)}>f(x)=1$ for any $\epsilon>0$. So, even a maximal IUC may not correspond to a local maximizer.

Next example shows that even though a global maximizer always corresponds to an IUC, a local maximizer may not have the same property. Consider the graph G_2 with $\alpha(G_2)=2$. The sets $\{1,4\}$ and $\{2,3\}$ are maximal, as well as maximum independent sets. But it can be verified that the point $x=[1,1,1,1]^T \equiv V(G_2)$ is also a local maximum with multipliers $\lambda_k=\frac{1}{9}$ and $\mu_k=0$ for all $k\in V(G_2)$. So, a local maximizer may correspond to a set that is not an independent set or even IUC. The following theorem establishes the converse for a special case when the set is a maximal independent set.

THEOREM 3. *If I^o is a maximal independent set and $x^o \equiv I^o$ then x^o is a local maximizer of* (2).

Proof. As before x^o is a regular point. FONC are satisfied in x^o as the KKT system has the following unique solution

$$\lambda_k^o=\begin{cases}1, & \text{if } k\in I^o;\\ 0, & \text{if } k\in V\setminus I^o;\end{cases}$$
$$\mu_k^o=\begin{cases}0, & \text{if } k\in I^o;\\ |N(k)\cap I^o|-\frac{1}{1+|N(k)\cap I^o|}, & \text{if } k\in V\setminus I^o;\end{cases}$$

and $\mu_k^o>0$ as $|N(k)\cap I^o|\geq 1$ for all $k\in V\setminus I^o$ since I^o is a maximal independent set.

Problem (2) and $x^*=x^o$ satisfy all conditions of Lemma 1, where $m=2n$ and exactly n constraints are active in x^o. Hence, x^o is a local maximizer of (2). □

We now look at local maximum properties of (2) in the binary neighborhood. The results are similar to the continuous case.

THEOREM 4. *If x^o is a point of local maximum of* (2) *in the binary neighborhood and $x^o \equiv I^o$, then I^o is a dominating set.*

Proof. Consider x^o, a local maximizer in the binary neighborhood with $x^o \equiv I^o$. Let $k \in V \setminus I^o$, then $x^o_k = 0$. Construct a neighbor of x^o as follows,

$$x''_i = \begin{cases} 1, & \text{if } i = k; \\ x^o_i, & \text{if } i \in V \setminus \{k\}. \end{cases}$$

Since x^o is a local maximizer, $f(x'') \leq f(x^o)$, where

$$f(x^o) = \sum_{i \in I^o} \frac{1}{1 + |N(i) \cap I^o|}.$$

If $N(k) \cap I^o = \emptyset$, then

$$f(x'') = \sum_{i \in I^o \cup \{k\}} \frac{1}{1 + |N(i) \cap (I^o \cup \{k\})|} = f(x^o) + 1 > f(x^o),$$

which is a contradiction. Hence, for every $k \notin I^o$, $N(k) \cap I^o \neq \emptyset$, so I^o is a dominating set. □

THEOREM 5. *If I^o is a maximal independent set and $x^o \equiv I^o$, then x^o is a local maximizer of* (2) *in the binary neighborhood.*

Proof. Since I^o is an independent set, $f(x^o) = |I^o|$. Any vector in the binary neighborhood of x^o can be obtained by either changing x^o_k from 1 to 0 for some $k \in I^o$ or changing x^o_k from 0 to 1 for some $k \notin I^o$. We analyze these two cases separately.

First, let $k \in I^o$, then $x^o_k = 1$. Construct x' in the binary neighborhood of x^o as follows,

$$x'_i = \begin{cases} 0, & \text{if } i = k; \\ x^o_i, & \text{if } i \in V \setminus \{k\}. \end{cases}$$

Then

$$f(x') = |I^o| - 1 < f(x^o).$$

Now let $k \in V \setminus I^o$, then $x^o_k = 0$. Construct x'' as follows,

$$x''_i = \begin{cases} 1, & \text{if } i = k; \\ x^o_i, & \text{if } i \in V \setminus \{k\}. \end{cases}$$

Then

$$\begin{aligned} f(x'') &= \frac{x''_k}{1+\sum_{j\in N(k)} x''_j} + \sum_{i\in I^o\cap N(k)} \frac{x''_i}{1+\sum_{j\in N(i)} x''_j} + \sum_{i\in I^o\setminus N(k)} \frac{x''_i}{1+\sum_{j\in N(i)} x''_j} \\ &= \frac{1}{1+|N(k)\cap I^o|} + \frac{|N(k)\cap I^o|}{2} + |I^o| - |N(k)\cap I^o| \\ &= |I^o| - \left(\frac{p^2+p-2}{2(1+p)}\right), \end{aligned}$$

where $p=|N(k)\cap I^o|\geq 1$ is integer and hence $\frac{p^2+p-2}{2(1+p)}\geq 0$. Thus, $f(x'')\leq f(x^o)$ and for any x in the binary neighborhood of x^o, $f(x)\leq f(x^o)$. □

REMARK. Note that x^o does not have to be a strict local maximum. For instance when $p=1$, there is a vertex outside the set that has exactly one neighbor inside and hence including that induces an IUC with the same number of components as in I^o (*i.e.*, $|I^o|-1$ cliques of size 1 and a clique of size 2). So, the objective function value does not change and the local maximizer is not strict.

5. Modified Formulation

We now modify the above formulation to obtain one with more desirable properties. In particular, we are interested in a one-to-one correspondence between local maximizers of the formulation and maximal independent sets of the graph.

Given graph $G=(V,E)$ with the adjacency matrix A_G, consider the following function:

$$\begin{aligned} g(x) &= \sum_{i\in V} \frac{x_i}{1+\sum_{j\in N(i)} x_j} - \frac{1}{2}x^T A_G x \\ &= \sum_{i\in V} x_i \left(\frac{1}{1+\sum_{j\in N(i)} x_j} - \frac{1}{2}\sum_{j\in N(i)} x_j\right). \end{aligned}$$

Then, $\forall\ x\in[0,1]^n$,

$$g(x)\leq f(x)\leq \max_{x\in[0,1]^n} f(x) = \alpha(G),$$

and for x^* corresponding to a maximum independent set, $g(x^*) = \alpha(G)$. Hence we have

$$\alpha(G) = \max_{x\in[0,1]^n} \left\{ \sum_{i\in V} x_i \left(\frac{1}{1 + \sum\limits_{j\in N(i)} x_j} - \frac{1}{2} \sum_{j\in N(i)} x_j \right) \right\}. \tag{6}$$

As in (Balasundaram and Butenko, 2005), for a given k, we can rewrite $g(x)$ as

$$g(x) = x_k A_k(x) + B_k(x) + C_k(x),$$

where

$$A_k(x) = \frac{1}{1 + \sum\limits_{j\in N(k)} x_j} - \sum_{j\in N(k)} x_j,$$

$$B_k(x) = \sum_{i\in N(k)} \frac{x_i}{x_k + 1 + \sum\limits_{j\in N(i)\setminus\{k\}} x_j},$$

$$C_k(x) = \sum_{i\in S} x_i \left(\frac{1}{1 + \sum\limits_{j\in N(i)} x_j} - \frac{1}{2} \sum_{j\in N(i)} x_j \right).$$

Here $S = V \setminus (\{k\} \cup N(k))$. Using this representation and arguments similar to ones used in (Balasundaram and Butenko, 2005), it is easy to show that $g(x)$ is convex with respect to each variable and every local (and global) maximizer is a binary vector.

We now look at the local maxima of (6). Note that every local maximum is a binary vector and is a regular point.

THEOREM 6. *x^o is a point of local maximum of* (6) *if and only if I^o is a maximal independent set, where $x^o \equiv I^o$.*

Proof. Let x^o be a local maximum of (6). Then the KKT conditions imply the existence of λ^o, μ^o such that

$$\begin{aligned} \forall\ k \in V:\ \left.\frac{\partial g}{\partial x_k}\right|_{x=x^o} &= \lambda_k^o - \mu_k^o; \\ \lambda_k^o(x_k^o - 1) &= 0; \\ \mu_k^o(-x_k^o) &= 0; \\ \lambda_k^o &\geq 0; \\ \mu_k^o &\geq 0; \end{aligned}$$

where

$$\left.\frac{\partial g}{\partial x_k}\right|_{x=x^o} = \frac{1}{1+\sum_{j\in N(k)} x_j^o} - \sum_{j\in N(k)} x_j - \sum_{i\in N(k)} \frac{x_i^o}{(x_k^o+1+\sum_{j\in N(i)\setminus\{k\}} x_j^o)^2}.$$

Let $x^o \equiv I^o$, then $\forall\ k\in I^o$, $x_k^o = 1$ and from KKT-FONC we have,

$$\mu_k^o = 0;$$
$$\lambda_k^o = \frac{1}{1+|N(k)\cap I^o|} - |N(k)\cap I^o| - \sum_{i\in N(k)\cap I^o} \frac{1}{(1+|N(i)\cap I^o|)^2} \geq 0.$$

Since k is an arbitrary vertex from I^o, in order to show that I^o is an independent set it suffices to prove that $N(k)\cap I^o = \emptyset$. Assume that this is not the case, *i.e.*, $|N(k)\cap I^o| \geq 1$. Then $\lambda_k^o \leq 1/2 - 1 < 0$, which contradicts the nonnegativity of λ_k^o. Hence, $|N(k)\cap I^o| = 0$ for any $k\in I^o$ and I^o is an independent set. Now suppose this independent set is not maximal. Then there exists $x_k^o = 0$, $k\in V\setminus I^o$ such that $N(k)\cap I^o = \emptyset$. Construct x', such that

$$x'_j = \begin{cases} \epsilon > 0, & \text{if } j = i; \\ x_j^o, & \text{if } j\in V\setminus\{i\}. \end{cases}$$

Then we have, $f(x') = f(x^o) + \epsilon$, which contradicts the fact that x^o is a local maximum. Hence, I^o must be a *maximal* independent set.

To prove the other direction, suppose I^o is a maximal independent set and $x^o \equiv I^o$. In order to show that x^o is a local maximum, we show that it satisfies the KKT-FONC and use Lemma 1. The unique solution to the KKT system is

$$\lambda_k^o = \begin{cases} 1, & \text{if } k\in I^o; \\ 0, & \text{if } k\in V\setminus I^o; \end{cases}$$
$$\mu_k^o = \begin{cases} 0, & \text{if } k\in I^o; \\ 2|N(k)\cap I^o| - \frac{1}{1+|N(k)\cap I^o|}, & \text{if } k\in V\setminus I^o. \end{cases}$$

Note that $\mu_k^o > 0$ as $|N(k)\cap I^o| \geq 1$ for any $k\in V\setminus I^o$ since I^o is a maximal independent set.

Here again, all conditions of Lemma 1 are satisfied for problem (6) with $x^* = x^o$, so x^o is a local maximizer of (6). □

COROLLARY 2. *x^* is a global maximum of* (6) *if and only if V^* is a maximum independent set of G, where $x^* \equiv V^*$.*

We now proceed to show that similar properties hold in case of the binary neighborhood for formulation (6).

THEOREM 7. *x^o is a local maximum of* (6) *in the binary neighborhood if and only if I^o is a maximal independent set, where $x^o \equiv I^o$.*

Proof. Let I^o be a maximal independent set with $x^o \equiv I^o$, then $g(x^o) = |I^o|$. Let x' be a binary neighbor obtained from x^o by changing a component that was 1 to 0. Then $g(x') = |I^o| - 1 < g(x^o)$ as x' would still correspond to an independent set.

Now, let x'' denote a binary neighbor obtained by changing the component, say k, in x^o from 0 to 1. Let I'' be the corresponding set of vertices. Then

$$\begin{aligned} g(x'') &= \sum_{i \in I''} \frac{1}{1+|N(i)\cap I''|} - |N(k)\cap I^o| \\ &= \frac{1}{1+|N(k)\cap I''|} + \sum_{i\in I^o\setminus N(k)} \frac{1}{1+|N(i)\cap I''|} \\ &\quad + \sum_{i\in I^o\cap N(k)} \frac{1}{1+|N(i)\cap I''|} - |N(k)\cap I^o| \\ &= \frac{1}{1+|N(k)\cap I^o|} + \sum_{i\in I^o\setminus N(k)} \frac{1}{1+|N(i)\cap I^o|} \\ &\quad + \sum_{i\in I^o\cap N(k)} \frac{1}{2+|N(i)\cap I^o|} - |N(k)\cap I^o| \\ &= \frac{1}{1+|N(k)\cap I^o|} + |I^o\setminus N(k)| + \frac{1}{2}|N(k)\cap I^o| - |N(k)\cap I^o| \\ &= \frac{1}{1+|N(k)\cap I^o|} + |I^o| - |N(k)\cap I^o| - \frac{1}{2}|N(k)\cap I^o| \\ &= |I^o| - \frac{3}{2}|N(k)\cap I^o| + \frac{1}{1+|N(k)\cap I^o|} \\ &= |I^o| - \frac{3p^2+3p-2}{2(1+p)}, \end{aligned}$$

where $p = |N(k)\cap I^o| \geq 1$ as I^o is maximal. Note that $\frac{3p^2+3p-2}{2(1+p)} > 0$ if $p \geq 1$ and integer, so we have $g(x'') < g(x^o)$, which establishes one direction.

To show the other direction, suppose that x^o is a local maximum in the binary neighborhood and $x^o \equiv I^o$.

$$g(x^o) = \sum_{i\in I^o} \frac{1}{1+|N(i)\cap I^o|} - |E\cap(I^o\times I^o)|.$$

Suppose that I^o is not an independent set. Then $\exists\ u, v \in I^o$ such that $(u, v) \in E$. Construct x' in the binary neighborhood of x^o as follows,

$$x_i' = \begin{cases} x_i^o, & \text{if } i \neq u; \\ 0, & \text{if } i = u; \end{cases} \quad i \in V.$$

Let I' be the corresponding vertex set, $I' = I^o \setminus \{u\}$. Then we have,

$$g(x') = \sum_{i \in I'} \frac{1}{1 + |N(i) \cap I'|} - |E \cap (I' \times I')|.$$

Note that

$$|E \cap (I' \times I')| = |E \cap (I^o \times I^o)| - |N(u) \cap I^o|$$

and

$$\begin{aligned} &\sum_{i \in I'} \frac{1}{1 + |N(i) \cap I'|} \\ &\quad = \sum_{i \in I' \setminus N(u)} \frac{1}{1 + |N(i) \cap I'|} + \sum_{i \in I' \cap N(u)} \frac{1}{1 + |N(i) \cap I'|} \\ &\quad = \sum_{i \in I' \setminus N(u)} \frac{1}{1 + |N(i) \cap I^o|} + \sum_{i \in I' \cap N(u)} \frac{1}{1 + |N(i) \cap I^o| - 1}, \end{aligned}$$

so

$$\begin{aligned} g(x^o) - g(x') = &\frac{1}{1 + |N(u) \cap I^o|} + \sum_{i \in I' \cap N(u)} \left(\frac{1}{1 + |N(i) \cap I^o|} - \frac{1}{|N(i) \cap I^o|} \right) \\ &- |N(u) \cap I^o| < 0, \end{aligned}$$

since

$$\frac{1}{1 + |N(u) \cap I^o|} - |N(u) \cap I^o| < 0$$

as $v \in N(u) \cap I^o$. But x^o was assumed to be a local maximum and hence by contradiction I^o is an independent set.

Now suppose that I^o is not maximal. Then there exists at least one vertex a that can be added to I^o. That is, $I'' = I^o \cup \{a\}$ is an independent set with the corresponding binary vector x'' given by

$$x_i'' = \begin{cases} x_i^o, & \text{if } i \neq a; \\ 1, & \text{if } i = a; \end{cases}$$

and $g(x'') = |I''| = |I^o| + 1 > |I^o| = g(x^o)$. This contradiction with the local maximality of x^o in the binary neighborhood establishes that I^o is a maximal independent set and hence the required result. □

6. Numerical Experiments

Numerical experiments were conducted to compare the performance of the original formulation (2) and the modified formulation (6) as objective functions for a simple local search algorithm and a constrained optimization function available in the MATLAB® Optimization Toolbox. Complements of selected DIMACS clique benchmark graphs (DIMACS, 1995) were used as instances for testing.

The local search algorithm starts at a random binary vector and reaches a local maximum in the binary neighborhood by successively moving to the first improving neighbor found. Table 1 presents the results that were obtained, where average and the maximum objective function value obtained starting from ten random binary vectors are shown for formulations (2) and (6).

MATLAB® function `fmincon` uses a sequential quadratic programming approach for solving medium-scale constrained optimization problems. Details and relevant references can be found at (MathWorks, 2004). The

Table 1. Results for local search

Instance	Vertices	Edges	$\alpha(G)$	Original Formulation		Modified Formulation	
				Avg	Best	Avg	Best
c-fat200-1	200	18366	12	9.86	12.00	12.00	12.00
c-fat200-2	200	16665	24	18.12	24.00	23.60	24.00
c-fat200-5	200	11427	58	57.40	58.00	57.90	58.00
johnson16-2-4	120	1680	8	7.68	8.00	8.00	8.00
johnson8-2-4	28	210	4	3.62	4.00	4.00	4.00
johnson8-4-4	70	560	14	14.00	14.00	11.20	14.00
keller4	171	5100	11	10.00	11.00	8.20	10.00
hamming6-2	64	192	32	30.70	32.00	24.30	32.00
hamming6-4	64	1312	4	3.04	4.00	2.80	4.00
hamming8-2	256	1024	128	125.90	128.00	74.60	82.00
hamming8-4	256	11776	16	16.00	16.00	10.20	13.00
san200_0.7_2	200	5970	18	12.30	13.00	12.70	14.00
san200_0.9_1	200	1990	70	46.70	48.00	37.70	47.00
san200_0.9_2	200	1990	60	37.30	40.00	29.10	32.00
san200_0.9_3	200	1990	44	32.60	35.00	27.60	29.00
brock200_1	200	5066	21	17.30	19.00	14.00	16.00
brock200_2	200	10024	12	9.10	11.00	7.90	9.00
brock200_3	200	7852	15	12.00	13.00	10.20	12.00
brock200_4	200	6811	17	12.70	15.00	10.80	12.00
p_hat300-1	300	33917	8	7.20	8.00	5.60	6.00
p_hat300-2	300	22922	25	23.80	25.00	17.60	19.00
p_hat300-3	300	11460	36	30.70	32.00	23.90	28.00
mann_a27	378	702	126	117.20	118.00	117.80	119.00
mann_a9	45	72	16	15.10	16.00	14.30	15.00

Table 2. Results for MATLAB® – `fmincon`

Instance	Vertices	Edges	$\alpha(G)$	Original Formulation		Modified Formulation	
				Avg	Best	Avg	Best
c-fat200-1	200	18366	12	9.86	12.00	11.88	12.00
c-fat200-2	200	16665	24	21.78	24.00	22.40	24.00
c-fat200-5	200	11427	58	54.79	58.00	57.30	58.00
johnson16-2-4	120	1680	8	4.37	4.44	8.00	8.00
johnson8-2-4	28	210	4	2.54	3.00	4.00	4.00
johnson8-4-4	70	560	14	13.30	14.00	11.50	14.00
keller4	171	5100	11	7.29	9.00	7.00	7.00
hamming6-2	64	192	32	30.30	32.00	22.30	32.00
hamming6-4	64	1312	4	2.54	3.33	4.00	4.00
hamming8-2	256	1024	128	104.14	128.00	78.00	90.00
hamming8-4	256	11776	16	14.93	16.00	10.50	16.00
san200_0.7_2	200	5970	18	12.00	12.00	12.00	12.00
san200_0.9_1	200	1990	70	45.39	47.00	45.20	46.00
san200_0.9_2	200	1990	60	35.78	38.00	36.95	40.00
san200_0.9_3	200	1990	44	31.38	34.00	30.90	33.00
brock200_1	200	5066	21	17.20	19.00	16.50	18.00
brock200_2	200	10024	12	8.59	10.00	8.00	9.00
brock200_3	200	7852	15	11.40	13.00	10.20	12.00
brock200_4	200	6811	17	13.40	15.00	12.20	14.00
p_hat300-1	300	33917	8	7.20	8.00	6.30	7.00
p_hat300-2	300	22922	25	22.80	25.00	21.00	24.00
p_hat300-3	300	11460	36	32.02	33.00	29.90	32.00
mann_a27	378	702	126	116.99	117.00	117.10	118.00
mann_a9	45	72	16	15.10	16.00	15.00	16.00

results tabulated in Table 2 show the average and best objective function value attained in ten runs starting from random initial feasible points inside $[0, 1]^n$ with formulations (2) and (6) as objective functions.

A total of 24 DIMACS clique benchmark graphs with up to 378 vertices were complemented and used in testing. Note that the values could be rounded up to get lower bounds on $\alpha(G)$. In terms of the average objective function value achieved in 10 runs of the local search algorithm, formulation (2) produced better results than formulation (6) with 17 instances whereas formulation (6) was better in 7 cases. In terms of the best solution obtained in 10 runs, formulation (2) beats formulation (6) 14 to 2, with the rest being equal. Similarly with `fmincon`, in terms of average performance, the ratio was 15 to 8 in favor of formulation (2) with one instance producing identical results with both. In terms of best solution obtained, the ratio was 11 to 5 again in favor of formulation (2), with the rest being equal.

Note that given a graph $G = (V, E)$, every maximal independent set in G corresponds to a local maximum for both formulations. The original formulation can have additional "spurious" local maxima besides these. However, with both algorithms, test results indicate that formulation (2) produces better quality solutions more often than formulation (6). The main advantage we gain by using the modified formulation is that the locally optimal solution will correspond to a maximal independent set as the spurious local maxima that exist in the other formulation are eliminated here. Note that in the original formulation, although the objective attained is a lower bound on the independence number, the solution may not even correspond to an independent set.

7. Conclusion

We have shown that a local maximum of a continuous formulation for the independence number of a graph corresponds to a dominating set in the graph and every maximal independent set of the graph corresponds to a local maximum of this formulation. We modify the formulation in order to strengthen these characterizations and obtain a one to one correspondence between local maxima and maximal independent sets in this case. Based on computational test results, we find the original formulation to be more suitable for the purposes of computing bounds on independence number. We find the modified formulation to be appropriate whenever maximal independent sets are to be found.

Acknowledgement

We would like to thank the anonymous referee who suggested a simplification of the proof of Theorem 2.

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