

A Heuristic for the Maximum Independent Set Problem Based on Optimization of a Quadratic Over a Sphere

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Abstract

For a given graph the maximum independent set problem is to find a maximum subset of vertices no two of which are adjacent. We propose a heuristic for the maximum independent set problem which utilizes classical results for the problem of optimization of a quadratic function over a sphere. The efficiency of the approach is confirmed by results of numerical experiments on DIMACS benchmarks.

1 Introduction

Let $G = (V, E)$ be a simple undirected graph with vertex set $V = \{1, \dots, n\}$ and set of edges E . The *complement graph* of G is the graph $\bar{G} = (V, \bar{E})$, where \bar{E} is the complement of E . For a subset $W \subseteq V$ let $G(W)$ denote the subgraph induced by W on G . $N(i)$ will denote the set of neighbors of vertex i and $d_i = |N(i)|$ is the degree of vertex i . We denote by $\Delta \equiv \Delta(G)$ the maximum degree of G .

A subset $I \subseteq V$ is called an *independent set* (*stable set*, *vertex packing*) if the edge set of the subgraph induced by I is empty. 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 *independence number* $\alpha(G)$ (also called the *stability number*) is the cardinality of a maximum independent set in G .

Along with the maximum independent set problem, we consider the *maximum clique* problem. 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 . It is easy to see that I is a maximum independent set of G if and only if I is a maximum clique of \bar{G} .

The maximum independent set and the maximum clique problems are NP-hard [11], so it is unlikely that a polynomial-time algorithm for computing the independence number of a graph can be devised.

Practical applications of these optimization problems are abundant. They appear in information retrieval, signal transmission analysis, classification theory, economics, scheduling, experimental design, and computer vision. See [2–6, 9, 20, 21] for details.

The paper is organized as follows. In Section 2 we review some continuous formulations of the maximum independent set problem. In Section 3 we discuss some well-known results concerning the problem of optimization of a quadratic function over a sphere. The heuristic that uses a quadratic polynomial formulation to find maximal independent sets is presented in Section 4. Computational efficiency of the proposed algorithm is discussed in Section 5.

2 Continuous formulations of the problem

The maximum independent set problem has many equivalent formulations as an integer programming problem and as a continuous nonconvex optimization problem [6, 20]. In this section we will give a brief review of some existing continuous approaches.

In 1965 Motzkin and Straus [19] formulated the maximum clique problem as a standard quadratic programming problem. The original proof of the Motzkin–Straus theorem was by induction. See [1] for another proof. Let A_G be the adjacency matrix of G and let e be the n -dimensional vector with all components equal to 1.

Theorem 1 (Motzkin–Straus) *The optimal value of the following quadratic*

program

$$\max f(x) = \frac{1}{2}x^T A_G x, \quad (1)$$

subject to

$$e^T x = 1, \quad (1a)$$

$$x \geq 0. \quad (1b)$$

is given by

$$\frac{1}{2} \left(1 - \frac{1}{\omega(G)} \right),$$

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

This result is extended in [13], by providing a characterization of maximal cliques in terms of local solutions. Moreover, optimality conditions of the Motzkin-Straus program have been studied and properties of a newly introduced parameterization of the corresponding quadratic program have been investigated.

In [12] Gibbons et al. proposed another, more tractable continuous formulation of the maximum independent set problem.

Theorem 2 (Gibbons et al.) *Consider the following optimization problem:*

$$V(k) = \min \frac{1}{2}x^T A_G x + \left(\sum_{i=1}^n x_i - 1 \right)^2 \quad (2)$$

subject to

$$\sum_{i=1}^n x_i^2 \leq \frac{1}{k}, \quad (2a)$$

$$x \geq 0. \quad (2b)$$

If \bar{x} is a solution to (2) then $V(k) = 0$ iff there exists an independent set I in G such that $|I| \geq k$.

Based on this theorem the authors proposed a heuristic for the maximum clique problem, which uses the global minimum of the problem (2)-(2a) to extract a maximal independent set from the graph. The approach that we propose in this paper is based on the same formulation as in Theorem 2.

Moreover, we also adopt the idea of using the problem of optimization of the same quadratic over a sphere to find a large independent set, but in our approach we use information about all stationary points of the problem (2)-(2a). We will use the computational results from [12] to estimate the efficiency of our approach in Section 5.

The following formulations were proposed in [15,16], where they were proved using probabilistic methods. See [1] for deterministic proofs. In the first case the objective is a degree $(\Delta + 1)$ polynomial, and the second is a quadratic formulation. The feasible region is the n -dimensional unit hypercube in both cases.

Theorem 3 *The independence number $\alpha(G)$ of G can be characterized as the following optimization problems:*

$$\alpha(G) = \max_{0 \leq x_i \leq 1, i=1, \dots, n} \sum_{i=1}^n (1 - x_i) \prod_{(i,j) \in E} x_j, \quad (3)$$

$$\alpha(G) = \max_{0 \leq x_i \leq 1, i=1, \dots, n} \left(\sum_{i=1}^n x_i - \sum_{(i,j) \in E} x_i x_j \right). \quad (4)$$

The reader is referred to [1] for description of several heuristics based on the results mentioned in the last theorem.

3 Optimization of a quadratic function over a sphere

Although optimization of a quadratic function subject to linear constraints is NP-hard, quadratic programming subject to an ellipsoid constraint is polynomially solvable. In fact, Ye in [22] proved that it can be solved in $O(\log(\log(1/\epsilon)))$ iterations, where ϵ is the error tolerance. Due to its application in trust region methods of nonlinear optimization, the problem of optimization of a quadratic function over a sphere is a well studied one [10, 14,17,18]. In this section we will discuss some results related to this problem.

Consider the following problem:

$$\min f(x) = 2c^T x + x^T Qx, \quad (5)$$

subject to

$$\|x\|_2 = r, \quad (5a)$$

where $x \in \mathbb{R}^n$ is the vector of variables, Q is a symmetric $n \times n$ matrix, $c \in \mathbb{R}^n$ is an arbitrary fixed vector, $r > 0$ is some number, and $\|\cdot\|_2$ is the second norm in \mathbb{R}^n , i.e. for any $x \in \mathbb{R}^n$: $\|x\|_2 = \left(\sum_{i=1}^n x_i^2\right)^{\frac{1}{2}}$.

We are interested in all stationary points of the problem (5), which can be found from the Lagrangian $\mathcal{L}(x, \lambda)$ of $f(x)$. We have

$$\mathcal{L}(x, \lambda) = f(x) - \lambda(\|x\|_2^2 - r^2), \quad (6)$$

where λ is the Lagrange multiplier of the constraint of (5), and the stationarity conditions:

$$\frac{\partial \mathcal{L}(x, \lambda)}{\partial x_i} = 0, i = 1, \dots, n; \quad (7)$$

$$\frac{\partial \mathcal{L}(x, \lambda)}{\partial \lambda} = 0. \quad (8)$$

The set of conditions (7) is equivalent to the system

$$(Q - \lambda I)x = -c, \quad (9)$$

where I stands for the $n \times n$ identity matrix. The condition (8) is simply the constraint (5a). Therefore, x is a stationary point of problem (5)-(5a) if and only if there exists a real number $\lambda = \lambda(x')$ such that

$$(Q - \lambda I)x = -c; \quad (10)$$

$$\sum_{i=1}^n x_i^2 = r^2. \quad (11)$$

The set Λ of all real λ for which there exists an x such that (10) and (11) are satisfied, is called the spectrum of the problem (5) - (5a).

Applying the eigenvalue decomposition for the matrix Q we have

$$Q = R \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) R^T,$$

where $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ are the eigenvalues of the matrix Q sorted in nondecreasing order, R is the matrix having a corresponding orthonormal set of eigenvectors as its columns. Transforming the vectors x and c to the basis R of the eigenvectors of Q , we obtain

$$\bar{x} = R^T x, \quad \bar{c} = R^T c.$$

Then (9) can be rewritten as

$$(\lambda_i - \lambda)\bar{x}_i = -\bar{c}_i, \quad i = 1, \dots, n. \quad (12)$$

Assuming that $\lambda \neq \lambda_i$, we have

$$\bar{x}_i = -\frac{\bar{c}_i}{\lambda_i - \lambda}. \quad (13)$$

Rewriting expression (11) in the basis associated with the rows of matrix R and substituting (13) into it, we obtain the so-called secular equation

$$\sum_{i=1}^n \frac{\bar{c}_i^2}{(\lambda_i - \lambda)^2} - r^2 = 0. \quad (14)$$

The left-hand side of the last expression is a univariate function consisting of $n + 1$ pieces each of which is continuous and convex. This implies that it can have at most two roots at any interval $(\lambda_i, \lambda_{i+1})$, $i = 0, \dots, n$ corresponding to the i -th piece, where by λ_0 and λ_{n+1} we mean $-\infty$ and $+\infty$ respectively. Moreover, the spectrum Λ includes the set Λ^0 of all solutions to the secular equation (14) and $\Lambda \setminus \Lambda^0 = \{\lambda_i : \bar{c}_i = 0\}$ (so, $\Lambda = \Lambda^0$ if $\{\lambda_i : \bar{c}_i = 0\} = \emptyset$).

In [10] it was shown that the global minimum of (5) corresponds to the smallest element of the spectrum $\lambda^* = \min \Lambda$. It implies that if $\bar{c}_i \neq 0$ then $\lambda^* = \min \Lambda^0$.

We mention one more result, which relates the maximum independent set problem to the problem of optimization of a quadratic over a sphere. Recently in [8] it has been shown that in the problem of optimizing a quadratic over a sphere of radius r a global solution $x^*(r)$ can be chosen, which depends continuously upon r . The last fact gives us a new point of view on the maximum independent set problem. Namely, it can be formulated as a problem of optimization of a quadratic function over a sphere with unknown radius:

Lemma 1 *There exists $r \in \left[\frac{1}{2}, \frac{\sqrt{n}}{2}\right]$ such that*

$$\alpha(G) = \max f_\alpha(x) = \sum_{i=1}^n x_i - \sum_{(i,j) \in E} x_i x_j \quad (15)$$

$$\text{subject to } \|x - \frac{1}{2}e\|_2 = r,$$

To show the validity of the lemma, consider formulation (4) and take two spheres S_1 (of radius $\frac{1}{2}$) and S_2 (of radius $\frac{\sqrt{n}}{2}$) inscribed in and circumscribed over the unit hypercube respectively. We have

$$\max_{x \in S_1} f_\alpha(x) \leq \alpha(G) = \max_{x \in [0,1]^n} f_\alpha(x) \leq \max_{x \in S_2} f_\alpha(x)$$

and by the Intermediate Value Theorem the lemma is correct.

4 Heuristic for the maximum independent set problem

In this section, we present the heuristic for the maximum independent set problem which employ the formulation mentioned in Theorem 2, and utilizes the methods similar to those in the so-called QUALEX heuristic [7]. In [7] the feasible region of the formulation (4) is changed from the unit hypercube to the sphere with the center $x^0 = 0$ and a certain radius r , depending on the input graph, resulting in the following problem:

$$\max f_\alpha(x) = \sum_{i=1}^n x_i - \sum_{(i,j) \in E} x_i x_j \quad (16)$$

subject to

$$\|x - x^0\|_2^2 = r^2. \quad (16a)$$

In short, QUALEX can be regarded as a sophisticated greedy heuristic, which first finds a local solution using a straightforward greedy approach, and then attempts to find a better solution using information provided by the stationary points of the above problem.

We apply similar techniques for the problem which is obtained from (2)-(2b) by changing the inequality to the equality in (2a) and relaxing nonnegativity constraints (2b):

$$\min \frac{1}{2} x^T A_G x + \left(\sum_{i=1}^n x_i - 1 \right)^2 \quad (17)$$

subject to

$$\sum_{i=1}^n x_i^2 = \frac{1}{k}. \quad (17a)$$

As the value of k we use the cardinality of a maximal independent set found by a simple greedy heuristic (numerical experiments suggest that varying k does not make results much better, but, naturally, requires more computational time). For each stationary point x of the problem (17)-(17a) we apply a greedy heuristic to find a maximal independent set I_x , which uses order of the vertices in the graph corresponding to the nonincreasing order of the components of x . The largest found I_x is reported as the output maximal independent set.

Below we present an outline of our algorithm.

Algorithm 1 [QSH]:

INPUT: Graph G with adjacency matrix A_G ; $\alpha = 0$

OUTPUT: A maximal independent set I^* and its cardinality α

0. Apply the following greedy heuristic:
 - (a) $G_0 = G$;
 - (b) In G_0 recursively remove the neighborhood of a vertex with the minimum degree in the current graph until an empty graph with vertex set I is obtained;
 - (c) **If** $|I| > \alpha$ **then begin** $I^* = I$, $\alpha = |I|$; **end**
 - (d) **If** $G_0 \setminus I \neq \emptyset$ **then begin** $G_0 = G_0 \setminus I$; **go to** step (b); **end**.
1. **For** $k = \alpha$ **begin**
 - For** each interval $(\lambda_i, \lambda_{i+1})$ **begin**
 - (a) Apply the techniques discussed in Section 3 for the problem (17)-(17a) to find the set of all stationary points S corresponding to $(\lambda_i, \lambda_{i+1})$;
 - (b) For each $x \in S$ find I_x by the following procedure:
 - i. Order the components of x in nonincreasing order
 $x_{i_1} \geq x_{i_2} \geq \dots \geq x_{i_n}$;
 - ii. $I_x = \emptyset$;
 - iii. **For** $j = 1$ **to** n **begin**
If $N(i_j) \cap I_x = \emptyset$ then $I_x = I_x \cup \{i_j\}$
end
 - (c) $x^* = \operatorname{argmax}\{|I_x| : x \in S\}$, $I = I_{x^*}$;

(d) If $|I| > \alpha$ then $I^* = I$ and $\alpha = |I|$;

end
end

The results of numerical experiments with the algorithm are reported in the next part of the paper.

5 Computational experiments

This section presents results of computational experiments for the proposed heuristic. The algorithm has been tested on the complement graphs of some of the DIMACS clique instances which can be downloaded from the URL <http://dimacs.rutgers.edu/Challenges/>. The performance of the algorithm (denoted by QSH) on the benchmarks is summarized in Tables 1 and 2. The columns “Name,” “ n ,” “Density,” and “ $\omega(G)$ ” represent the name of the graph, the number of its vertices, its density, and its clique number, respectively. This information is available from the DIMACS web site. Recall that we are working with complements of the considered graphs, and the densities are specified for the original (maximum clique) instances. The column “Sol. Found” contains the size of the clique found by each algorithm. Columns “CBH” and “QSH” in Table 1 represent the continuous based heuristic [12] and the heuristic proposed in this paper, correspondingly. Finally, the column “Time” reports computational times for QSH in seconds obtained using the C function `time`. The results for CBH were taken from [12]. A modification of the C++ QUALEX code available on-line from [7] was used to obtain the results for QSH. The code was compiled and executed on an IBM computer with 2 PowerPC processors, 333 Mhz each.

In Table 3 we compare the performance of CBH and QSH on different types of graphs. In each row of this table the first column contains a name of the family of graphs, where each family consists of a group of graphs with the same letter names (in Tables 1 and 2 such families are separated by horizontal lines). In the next three columns “+” represents the number of instances from each family for which CBH found a better solution than QSH; “-” represents the number of instances for which QSH found a better solution than CBH; finally, “=” stands for the number of instances for which cardinalities of the independent sets found by the two algorithms were equal.

Table 1: Results on benchmark instances.

Name	n	Density	$\omega(G)$	Sol. Found		Time (sec.)
				CBH	QSH	
MANN_a9	45	0.927	16	16	16	0
MANN_a27	378	0.990	126	121	125	8
brock200_1	200	0.745	21	20	21	1
brock200_2	200	0.496	12	12	12	1
brock200_3	200	0.605	15	14	15	1
brock200_4	200	0.658	17	16	17	2
brock400_1	400	0.748	27	23	27	21
brock400_2	400	0.749	29	24	29	21
brock400_3	400	0.748	31	23	31	20
brock400_4	400	0.749	33	24	33	21
brock800_1	800	0.649	23	20	17	245
brock800_2	800	0.651	24	19	24	243
brock800_3	800	0.649	25	20	25	228
brock800_4	800	0.650	26	19	26	233
c-fat200-1	200	0.077	12	12	12	1
c-fat200-2	200	0.163	24	24	24	1
c-fat200-5	200	0.426	58	58	58	1
c-fat500-1	500	0.036	14	14	14	33
c-fat500-10	500	0.374	≥ 126	126	126	20
c-fat500-2	200	0.073	26	26	26	31
c-fat500-5	500	0.186	64	64	64	23
hamming6-2	64	0.905	32	32	32	0
hamming6-4	64	0.349	4	4	4	0
hamming8-2	256	0.969	128	128	128	2
hamming8-4	256	0.639	16	16	16	1
johnson8-2-4	28	0.556	4	4	4	0
johnson8-4-4	70	0.768	14	14	14	0
johnson16-2-4	120	0.765	8	8	8	0
johnson32-2-4	496	0.879	16	16	16	24

As one can see QSH performed better on four families (MANN_a, brock, keller, san) and did worse on two (p_hat and sanr). Analyzing the dif-

Table 2: Results on benchmark instances (continued).

Name	n	Density	$\omega(G)$	Sol. Found CBH	QSH	Time (sec.)
keller4	171	0.649	11	10	11	1
keller5	776	0.751	27	21	24	149
p_hat300-1	300	0.244	8	8	7	6
p_hat300-2	300	0.489	25	25	24	6
p_hat300-3	300	0.744	36	36	33	6
p_hat500-1	500	0.253	9	9	9	48
p_hat500-2	500	0.505	36	35	33	49
p_hat500-3	500	0.752	≥ 49	49	46	48
p_hat700-1	700	0.249	11	11	8	143
p_hat700-2	700	0.498	44	44	42	143
p_hat700-3	700	0.748	≥ 62	60	59	143
san200_0.7_1	200	0.700	30	15	30	1
san200_0.7_2	200	0.700	18	12	18	1
san200_0.9_1	200	0.900	70	46	70	1
san200_0.9_2	200	0.900	60	36	60	1
san200_0.9_3	200	0.900	44	30	35	1
san400_0.5_1	400	0.500	13	8	9	20
san400_0.7_1	400	0.700	40	20	40	21
san400_0.7_2	400	0.700	30	15	30	19
san400_0.7_3	400	0.700	22	14	16	21
san400_0.9_1	400	0.900	100	50	100	23
sanr200_0.7	200	0.700	18	18	15	1
sanr200_0.9	200	0.900	≥ 42	41	37	1
sanr400_0.5	400	0.500	13	12	11	20
sanr400_0.7_1	400	0.700	≥ 21	20	18	19

ference in quality of the results, one can notice a huge gap between the solutions obtained for **san** group. The results of numerical experiments suggest that QSH is superior to CBH and many other heuristics presented in the literature.

Table 3: Comparison of the results on benchmark instances.

Graphs family name	CBH vs QSH		
	+	=	-
MANN_a	0	1	1
brock	1	1	10
c-fat	0	7	0
hamming	0	4	0
johnson	0	4	0
keller	0	0	2
p_hat	8	1	0
san	0	0	10
sanr	4	0	0
TOTAL	13	18	23

6 Conclusions and future research

In this paper we present a heuristic for the maximum independent set problem. The proposed approach utilizes techniques used in optimization of a quadratic over a sphere. We show the validity of this approach by demonstrating the results of numerical experiments. As it was discussed before, the idea of using the optimization of a quadratic over a sphere for the maximum independent set problem is not new. However, we want to stress that the information provided by the stationary points other than points of global optimality may help us to find better independent sets in the corresponding graph.

In Lemma 1 we formulated the maximum independent set problem as a problem of optimization of a quadratic over a sphere with unknown radius. In future research, when using similar techniques for combinatorial optimization problems, one should try to address the following issues:

- How to optimally choose the parameters of the quadratic objective and of the sphere used as the feasible set?
- What is the optimal way to extract the combinatorial object sought for, from the information provided by stationary (or optimal) points of the considered quadratic problem?

To answer these questions both theoretical and empirical studies are needed.

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