A New Spectral Bound
on the Clique Number of Graphs

Samuel Rota Bulò and Marcello Pelillo

Dipartimento di Informatica - University of Venice - Italy
{srotabul,pelillo}@dsi.unive.it

Abstract. Many computer vision and patter recognition problems are intimately related to the maximum clique problem. Due to the intractability of this problem, besides the development of heuristics, a research direction consists in trying to find good bounds on the clique number of graphs. This paper introduces a new spectral upper bound on the clique number of graphs, which is obtained by exploiting an invariance of a continuous characterization of the clique number of graphs introduced by Motzkin and Straus. Experimental results on random graphs show the superiority of our bounds over the standard literature.

1 Introduction

Many problems in computer vision and pattern recognition can be formulated in terms of finding a completely connected subgraph (i.e. a *clique*) of a given graph, having largest cardinality. This is called the maximum clique problem (MCP). One popular approach to object recognition, for example, involves matching an input scene against a stored model, each being abstracted in terms of a relational structure [1,2,3,4], and this problem, in turn, can be conveniently transformed into the equivalent problem of finding a maximum clique of the corresponding *association graph*. This idea was pioneered by Ambler et. al. [5] and was later developed by Bolles and Cain [6] as part of their local-feature-focus method. Now, it has become a standard technique in computer vision, and has been employing in such diverse applications as stereo correspondence [7], point pattern matching [8], image sequence analysis [9]. Other interesting applications of the maximum clique problem arise in the context of cluster analysis, where graph-theoretical methods have long proven to be especially effective [10,11,12], and in the context of category learning and knowledge discovery [13,14]. Furthermore, clique finding is also linked with the learning of graphical structure by the Hammersley-Clifford theorem [15].

From a computational point of view, the maximum clique problem (MCP) belongs to the class of NP-Complete problems, whose intractability forces us to fall back on approximation methods. Unfortunately, even approximating the MCP is intractable [16]. Due to this pessimistic state of affairs, much attention has gone into developing efficient heuristics for the MCP, for which no formal guarantee of performance may be provided, but are nevertheless useful in practical

applications. We refer to Bomze et al. [17] for a survey concerning algorithms, applications, and complexity issues of this important problem.

Another interesting direction of research consists in trying to bound the clique number of a graph. In the literature we find both upper and lower bounds [18]. The former however are in general more interesting because any heuristics for the MCP can be used to generate lower bounds. In this paper we propose a new spectral upper bound by exploiting an invariance of a continuous characterization of the clique number of graphs introduced by Motzkin and Straus [19], and we present an algoritm for efficiently computing the bound. Experiments on random graphs demonstrate the effectiveness of our result. The bound proposed here can be used in the bounding phase of branch-and-bound style algorithms for finding maximal cliques, with applications in such problems as graph matching [1,20] and clustering [12] (see also [21] for the use of bounds in graph matching problems).

2   Bounds on the Clique Number of Graphs

Let $G = (V, E)$ be a (undirected) graph, where $V = \{1, \ldots, n\}$ is the vertex set and $E \subseteq \binom{V}{2}$ is the edge set, with $\binom{V}{k}$ denoting the set of all k-element subsets of V. A *clique* of G is a subset of mutually adjacent vertices in V. A clique is called *maximal* if it is not contained in any other clique. A clique is called *maximum* if it has maximum cardinality. The maximum size of a clique in G is called the *clique number* of G and is denoted by $\omega(G)$.

Several spectral bounds on the clique number of graphs have been inspired by a theorem due to Motzkin and Straus [19]. This result establishes a link between the problem of finding the clique number of a graph G and the problem of optimizing the Lagrangian of G over the simplex Δ, where the Lagrangian of a graph $G = (V, E)$ is the function $L_G : \mathbb{R}^n \rightarrow \mathbb{R}$ defined as

$$L_G(\mathbf{x}) = \sum_{\{i,j\} \in E} x_i x_j \, ,$$

and the *standard simplex* Δ is the set of nonnegative n-dimensional real vectors that sum up to 1, i.e., $\Delta = \{\mathbf{x} \in \mathbb{R}^n_+ : \sum_{i=1}^n x_i = 1\}$.

Theorem 1 (Motzkin-Straus). *Let G be a graph with clique number $\omega(G)$, and $\mathbf{x}^*$ a maximizer of L_G over Δ then*

$$L_G(\mathbf{x}^*) = \frac{1}{2} \left[1 - \frac{1}{\omega(G)} \right] \, .$$

Assuming S a maximum clique of G, Motzkin and Straus additionally proved that the *characteristic vector* $\mathbf{x}^S$ of S defined as

$$x_i^S = \begin{cases} \frac{1}{|S|} & i \in S \\ 0 & i \notin S \end{cases}$$

is a global maximizer of L_G over Δ.

Before reviewing some existing bounds on ω, we briefly introduce some concepts from spectral graph theory. The *spectral radius* $\rho(G)$ of a graph G is the largest eigenvalue of the adjacency matrix of G. An eigenvector of unit length having $\rho(G)$ as eigenvalue will be called *Perron eigenvector* of G. The Perron eigenvector is always nonnegative and it may not be unique unless the multiplicity of the largest eigenvalue is exactly 1. By definition, the spectral radius ρ and an associated Perron eigenvector $\mathbf{x}_P$ of a graph G satisfy the eigenvalue equation

$$A_G \mathbf{x}_P = \rho \mathbf{x}_P \,,$$

which can be equivalently expressed in terms of the graph Lagrangian L_G as follows

$$\nabla L_G(\mathbf{x}_P) = \rho \mathbf{x}_P \,,$$

where ∇ is the standard gradient operator. Since G is undirected and hence, A_G is symmetric, a useful variational characterization of ρ and $\mathbf{x}_P$ is given by the following constrained program,

$$\rho = \max_{\mathbf{x} \in S_2} \mathbf{x}^T A_G \mathbf{x} = 2 \max_{\mathbf{x} \in S_2} L_G(\mathbf{x}) \,, \tag{1}$$

where $S_k = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_k^k = 1\}$. Note that the eigenvectors of A_G are the critical points of this maximization problem. A further alternative characterization of the spectral radius and Perron eigenvector, that will be useful in the sequel, consists in maximizing the *Rayleigh quotient*, i.e.,

$$\rho = \max_{\mathbf{x} \in \mathbb{R}^n} \frac{\mathbf{x}^T A_G \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = 2 \max_{\mathbf{x} \in \mathbb{R}^n} \frac{L_G(\mathbf{x})}{\mathbf{x}^T \mathbf{x}} \,. \tag{2}$$

Note that every eigenvector associated to ρ is a maximizer in (2), whereas in (1) only a Perron eigenvector is a global maximizer.

We present now two upper bounds for ω that turned out to be the tightest ones in a paper of Budinich [18], where different bounds have been compared on random graphs. For a review of further spectral bounds we refer to [18,22].

The fist upper bound can be obtained by exploiting both the Motzkin-Straus theorem and (2).

Theorem 2. *Let G be an undirected graph with clique number $\omega(G)$ and spectral radius ρ. Then*

$$\omega(G) \leq \rho + 1 \,. \tag{B1}$$

Proof. Let $\mathbf{x}_\omega$ be the characteristic vector of a maximum clique of G, then $\mathbf{x}_\omega^T \mathbf{x}_\omega = 1/\omega(G)$ and by the Motzkin-Straus theorem $\mathbf{x}_\omega^T A_G \mathbf{x}_\omega = 1 - 1/\omega(G)$. By (2) we have that

$$\frac{\mathbf{x}_\omega^T A_G \mathbf{x}_\omega}{\mathbf{x}_\omega^T \mathbf{x}_\omega} = \frac{1 - \frac{1}{\omega(G)}}{\frac{1}{\omega(G)}} = \omega(G) - 1 \leq \rho \,,$$

from which the property derives.

This bound can also be derived as a straightforward implication of the result of Wilf [23]. The second bound is due to Amin and Hakimi [24]:

Theorem 3. *Let G be an undirected graph with adjacency matrix A_G and clique number $\omega(G)$. Moreover, let N_{-1} be the number of eigenvalues of A_G that are less or equal to -1. Then*

$$\omega(G) \leq N_{-1} + 1 \,. \tag{B2}$$

3   The η-Bound

We will introduce a new class of upper bounds generalizing (B1), where we exploit the fact that the maximizers of the Motzkin-Straus formulation are invariant with respect to shifts of the adjacency matrix of a graph G, whereas the maxima and the spectrum of the shifted matrix are not. Our intuition is that we can tighten (B1) by opportunely shifting the adjacency matrix of G.
   We define

$$\phi_G(t, \mathbf{x}) = \mathbf{x}^T \left[A_G + (t - 1)\mathbf{1}\mathbf{1}^\top \right] \mathbf{x} \,,$$

where $\mathbf{1}$ is an opportunely sized column vector of all 1's. Then by the Motzkin-Straus theorem we have

$$\max_{\mathbf{x} \in \Delta} \phi_G(t, \mathbf{x}) = \mathbf{x}^T \left[A_G + (t - 1)\mathbf{1}\mathbf{1}^\top \right] \mathbf{x} = t - \frac{1}{\omega(G)} \,.$$

We will denote with $\phi_G(t)$ the leading eigenvalue of $A_G + (t-1)\mathbf{1}\mathbf{1}^\top$, i.e.,

$$\phi_G(t) = \max_{\mathbf{x} \in S_2} \phi_G(t, \mathbf{x}) \,,$$

and with $\Phi_G(t)$ the set of eigenvectors associated to $\phi_G(t)$, i.e.,

$$\Phi_G(t) = \arg \max_{\mathbf{x} \in S_2} \phi_G(t, \mathbf{x}) \,.$$

Theorem 4 (t-bound). *Let G be a graph with adjacency matrix A_G and clique number $\omega(G)$. Then for any $t > 0$*

$$\omega(G) \leq \frac{\phi_G(t) + 1}{t}$$

Proof. Let $\mathbf{x}_\omega$ be the characteristic vector of a maximum clique of G. Then

$$\phi_G(t) \geq \phi_G\left(t, \frac{\mathbf{x}_\omega}{\|\mathbf{x}_\omega\|_2}\right) = \frac{\phi_G(t, \mathbf{x}_\omega)}{\mathbf{x}_\omega^T \mathbf{x}_\omega} = \frac{t - \frac{1}{\omega(G)}}{\frac{1}{\omega(G)}} = \omega(G)t - 1 \,, \tag{3}$$

from which the result follows.

Theorem 4 introduces a class of upper bounds that contains (B1) as the special case $t = 1$. Let us define the *t-bound* as

$$\eta_G(t) = \frac{\phi_G(t) + 1}{t}.$$

Of course the more interesting t-bound is the tightest one, which will be called *η-bound* and denoted by $\eta(G)$, i.e.,

$$\eta(G) = \inf_{t>0} \eta_G(t).$$

Note that $\eta(G)$ is well defined, because by Theorem 4 it is lower bounded by the clique number of G.

4   Computation of the η-Bound

This section is dedicated to showing that the computation of $\eta(G)$ is not difficult, although not obvious at first glance, and we will provide an efficient algorithm for its computation.

Proposition 1. *Let $s > t > 0$. For any $\mathbf{x}(s) \in \Phi_G(s)$ and $\mathbf{x}(t) \in \Phi_G(t)$ we have*

$$(s - t)\mathbf{x}(t)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(t) \leq \phi_G(s) - \phi_G(t) \leq (s - t)\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s).$$

Proof

$$\begin{aligned}
\phi_G(s) - \phi_G(t) &= \phi_G(s, \mathbf{x}(s)) - \phi_G(t) \\
&= \phi_G(t, \mathbf{x}(s)) + (s - t)\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s) - \phi_G(t) \\
&\leq \phi_G(t, \mathbf{x}(t)) + (s - t)\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s) - \phi_G(t) \\
&= \phi_G(t) + (s - t)\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s) - \phi_G(t) \\
&= (s - t)\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s)
\end{aligned}$$

$$\begin{aligned}
\phi_G(s) - \phi_G(t) &= \phi_G(s, \mathbf{x}(s)) - \phi_G(t) \\
&\geq \phi_G(s, \mathbf{x}(t)) - \phi_G(t) \\
&= \phi_G(t, \mathbf{x}(t)) + (s - t)\mathbf{x}(t)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(t) - \phi_G(t) \\
&= \phi_G(t) + (s - t)\mathbf{x}(t)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(t) - \phi_G(t) \\
&= (s - t)\mathbf{x}(t)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(t)
\end{aligned}$$

Proposition 2. *Let $s > t > 0$. For any $\mathbf{x}(s) \in \Phi_G(s)$ and $\mathbf{x}(t) \in \Phi_G(t)$ the following propositions hold*

1. *if $\phi_G(0, \mathbf{x}(s)) \geq -1$ then $\eta_G(s) \leq \eta_G(t)$,*
2. *if $\phi_G(0, \mathbf{x}(t)) \leq -1$ then $\eta_G(s) \geq \eta_G(t)$.*

Proof. If $\phi_G(0, \mathbf{x}(s)) \geq -1$ then

$$
\begin{aligned}
\eta_G(s) - \eta_G(t) &= \frac{\phi_G(s) + 1}{s} - \frac{\phi_G(t) + 1}{t} \\
&\leq \frac{\phi_G(t) + (s - t)\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s) + 1}{s} - \frac{\phi_G(t) + 1}{t} \quad \text{(by Prop. 1)} \\
&= \frac{(s - t)\left[-\phi_G(t) - 1 + t\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s)\right]}{ts} \\
&\leq \frac{(s - t)\left\{-\phi_G(t, \mathbf{x}(s)) - 1 + t\mathbf{x}(s)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(s)\right\}}{ts} \\
&= \frac{(s - t)\left[-\phi_G(0, \mathbf{x}(s)) - 1\right]}{ts} \leq 0 \, .
\end{aligned}
$$

While if $\phi_G(0, \mathbf{x}(t)) \leq -1$ then

$$
\begin{aligned}
\eta_G(s) - \eta_G(t) &= \frac{\phi_G(s) + 1}{s} - \frac{\phi_G(t) + 1}{t} \\
&\geq \frac{\phi_G(t) + (s - t)\mathbf{x}(t)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(t) + 1}{s} - \frac{\phi_G(t) + 1}{t} \quad \text{(by Prop. 1)} \\
&= \frac{(s - t)\left[-\phi_G(t) - 1 + t\mathbf{x}(t)^T \mathbf{1}\mathbf{1}^\top \mathbf{x}(t)\right]}{ts} \\
&= \frac{(s - t)\left[-\phi_G(0, \mathbf{x}(t)) - 1\right]}{ts} \geq 0 \, .
\end{aligned}
$$

Theorem 5. *Let $s > t > 0$. For any $\mathbf{x}(s) \in \Phi_G(s)$ and $\mathbf{x}(t) \in \Phi_G(t)$ if*

$$
\phi_G(0, \mathbf{x}(s)) \leq -1 \leq \phi_G(0, \mathbf{x}(t)) \, ,
$$

then there exists $t \leq q \leq s$ such that $\eta(G) = \eta_G(q)$.

Moreover, if for any $q > 0$ and $\mathbf{x}(q) \in \Phi_G(q)$ we have $\phi_G(0, \mathbf{x}(q)) = -1$ then $\eta(G) = \eta_G(q)$.

Proof. By Proposition 2 it follows that

- for any $r < t$ we have $\eta(G) \leq \eta_G(t) \leq \eta_G(r)$;
- for any $r > s$ we have $\eta(G) \leq \eta_G(s) \leq \eta_G(r)$,

from which the first part of the result follows.

For the second part note that for any $r < q$ we have $\eta(G) \leq \eta_G(q) \leq \eta_G(r)$, while for any $r > q$ we have $\eta(G) \leq \eta_G(q) \leq \eta_G(r)$. Hence, $\eta_G(q) = \eta(G)$.

Proposition 3. *Let $\mathbf{x}(1) \in \Phi_G(1)$ be a Perron eigenvector of A_G. For any $\mathbf{x}(0) \in \Phi_G(0)$ we have*

$$
\phi_G(0, \mathbf{x}(1)) \leq -1 \leq \phi_G(0, \mathbf{x}(0)) \, .
$$

Algorithm 1. Bisection search for computing $\eta(G)$

1: **function** η-BOUND(G,ϵ)
2:     $l = 0$
3:     $p = 0$
4:     $r = 1$
5:     Take any $\mathbf{x}(l) \in \Phi_G(l)$
6:     $\mathbf{x}(r) \leftarrow$ normalized Perron vector of A_G
7:     **while** $r - l > \epsilon$ **do**
8:         $p = (l + r)/2$ ▷ or any other selection mechanism
9:         Take any $\mathbf{x}(p) \in \Phi_G(p)$
10:        **if** $\phi_G(0, \mathbf{x}(p)) < -1$ **then**
11:            $r \leftarrow p$
12:            $\mathbf{x}(r) \leftarrow \mathbf{x}(p)$
13:        **else if** $\phi_G(0, \mathbf{x}(p)) > -1$ **then**
14:            $l \leftarrow p$
15:            $\mathbf{x}(l) \leftarrow \mathbf{x}(p)$
16:        **else**
17:            **return** $\eta_G(p)$
18:        **end if**
19:    **end while**
20:    **return** $\eta_G(p)$
21: **end function**

Proof. It follows from (3) that $\phi_G(0) = \phi_G(0, \mathbf{x}(0)) \geq -1$.

Because of the nonnegativity of the Perron vector, trivially $\mathbf{x}(1)^T A_G \mathbf{x}(1) \leq \mathbf{x}(1)^T (\mathbf{1}\mathbf{1}^\top - I)\mathbf{x}(1)$, from which it follows that

$$\phi_G(0, \mathbf{x}(1)) + 1 = $$
$$= \mathbf{x}(1)^T \left[A_G - \mathbf{1}\mathbf{1}^\top \right] \mathbf{x}(1) + 1 \leq \mathbf{x}(1)^T \left[(\mathbf{1}\mathbf{1}^\top - I) - \mathbf{1}\mathbf{1}^\top \right] \mathbf{x}(1) + 1 = 0.$$

Theorem 5 and Proposition 3 suggest an effective way of computing $\eta(G)$ by performing a section search (like the bisection search) in the interval (0,1]. Indeed, Theorem 5 allows us to bisect an interval having sign-discording values of $f(t) = \phi_G(0, \mathbf{x}(t)) + 1$ at the endpoints, and restrict the attention to the subinterval that preserves this property. Proposition 3, instead, entitles us to start the search procedure from the interval $[0, 1]$. Note that we can stop the search if we encounter an endpoint t, where $f(t) = 0$, as in this case $\eta_G(t)$ is our η-bound. Otherwise, the size of the interval is an indicator of the precision of the solution and we can stop as soon as this is small enough. Algorithm 1 reports an implementation that can be used for the computation of $\eta(G)$ with an arbitrary precision ϵ.

5   Experiments on Random Graphs

In this section, we evaluate the performance of our η-bound. We compare our bound against other spectral bounds, which were the best performing approaches

Table 1. Experiments on random graphs. The columns n, δ and ω are the order, density and average clique number of the random graphs, respectively. The results, expecting the last row, are expressed in terms of relative error.

Random graphs			Bound errors		
n	δ	ω	(B1)	(B2)	η
100	0.05	3.12	1.25	10.58	**0.79**
	0.10	3.96	1.99	9.26	**0.87**
	0.20	5.00	3.33	7.84	**1.07**
	0.30	6.13	4.17	6.52	**1.11**
	0.40	7.51	4.49	5.24	**1.08**
	0.50	9.11	4.58	4.19	**1.02**
	0.60	11.51	4.28	3.16	**0.91**
	0.70	14.55	3.85	2.33	**0.84**
	0.80	19.99	3.03	1.45	**0.64**
	0.90	30.69	1.94	0.61	**0.42**
	0.95	43.50	1.19	**0.16**	0.27
200	0.10	4.17	4.25	19.97	**1.45**
	0.50	11.00	8.19	7.71	**1.47**
	0.90	?	180.10	99.08	**68.45**

reviewed in the work of Budinich [18]. Specifically, we compare against bounds (B1) and (B2), which have been previously introduced.

Table 1 reports the results obtained on random graphs, where η is the column relative to our η-bound. The columns n, δ and ω are the order, density and average clique number of the random graphs, respectively. The results, except the last row, are expressed in terms of relative error, i.e. if $\overline{\omega}$ is the value of the bound then the relative error for the upper and lower bounds are $(\overline{\omega} - \omega)/\omega$ and $(\omega - \overline{\omega})/\omega$, respectively. In the last row, where the average clique number could not be computed, we reported the absolute value of the bounds. It is clear that, as expected, our η-bound improves (B1). Moreover, our bound outperforms also Amin's one on all instances excepting very dense graphs. Interestingly, it exhibits on average a remarkable improvement over the competitors by keeping an overall small relative error.

6   Conclusions

In this paper, we introduced a new spectral bounds on the clique number of graphs, called η-bound, which has been obtained by combining spectral graph theory with a result due to Motzkin and Straus. Specifically, we exploit an invariance of the Motzkin-Sraus formulation with respect to shifts of the adjacency matrix of graphs in order to tighten a well-known bound.

Finally, we tested our bounds on random graphs comparing them against state-of-the-art spectral approaches. The results outlined a marked improvement over the competitors.

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