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Note

Spectral Bounds for the Clique and Independence Numbers of Graphs

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TO THE MEMORY OF ERNST G. STRAUS

We obtain a sequence $k_1(G) \leqslant k_2(G) \leqslant \cdots \leqslant k_n(G)$ of lower bounds for the clique number (size of the largest clique) of a graph G of n vertices. The bounds involve the spectrum of the adjacency matrix of G. The bound $k_1(G)$ is explicit and improves earlier known theorems. The bound $k_2(G)$ is also explicit, and is shown to improve on the bound from Brooks' theorem even for regular graphs. The bounds $k_3,..., k_r$ are polynomial-time computable, where r is the number of positive eigenvalues of G.

We give lower bounds for the clique number $k(G)$ and for the (vertex) independence number $\alpha(G)$ of a graph G. They improve earlier results, and they involve the spectrum of the graph G. The derivation of these bounds rests on a theorem of T. Motzkin and Ernst Straus (Theorem 1).

In fact, we obtain a sequence of (increasingly hard to compute) bounds $k_1(G) \leqslant k_2(G) \leqslant \cdots \leqslant k_n(G) = k(G)$. The first two of these give explicit theorems. The first p^+ of them are polynomial-time-computable, where p^+ is the number of nonnegative eigenvalues of G.

If d is the maximum valence of vertices of G then Brooks' theorem gives the bound

$$\alpha(G) \geqslant n/d \qquad (n = |V(G)|) \tag{1}$$

unless G is complete or an odd circuit. This bound may be quite weak. If $G = K_{n,n}$, for example, then (1) yields only the estimate $\alpha(K_{n,n}) \geqslant 2$.

Any upper bound for the chromatic number $\chi(G)$ can be used, of course. Since [1] it is known that $\chi(G) \leqslant 1 + \lambda_1$, where λ_1 is the largest eigenvalue of G, we can replace (1) by $\alpha(G) \geqslant n/(1 + \lambda_1)$.

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To do much better than this we need tools that are specific to the clique number or independence number problem, rather than to be the chromatic number problem. The following elegant result is of this kind.

THEOREM 1 (Motzkin and Straus [2]). *For a given graph G the maximum value of*

$$\sum_{(i,j) \in E(G)} x_i x_j \tag{2}$$

taken over the simplex

$$\mathscr{S}: \quad x \geqslant 0; \qquad \sum_{i=1}^{n} x_i = 1 \tag{3}$$

is $\frac{1}{2}(1 - 1/k(G))$.

This theorem can provide a bridge to the spectral theory of graphs. Let A be the $n \times n$ vertex adjacency matrix of G. Then the Motzkin–Straus theorem asserts that

$$1 - \frac{1}{k(G)} = \max_{\mathscr{S}} (x, Ax). \tag{4}$$

After some obvious manipulation we find that, dually,

$$\frac{1}{\alpha(G)} = \min_{\mathscr{S}} (x, (I + A)x). \tag{5}$$

There are many ways to get useful inequalities from these extremal principles. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of (the vertex adjacency matrix of) G, and let $u_1, \ldots, u_n$ be the corresponding *normalized* eigenvectors. We can suppose that $u_1 > 0$. Then the vector $x = u_1/S$, where S is the sum of the entries of u_1, belongs to the simplex $\mathscr{S}$ of (3). Consequently

$$\begin{aligned} 1 - \frac{1}{k(G)} &\geqslant (x, Ax) \\ &= \lambda_1 / S^2 \end{aligned}$$

THEOREM 2. *For the clique number $k(G)$ of a graph G (and a fortiori for the chromatic number $\chi(G)$) we have*

$$k(G) \geqslant \frac{S^2}{S^2 - \lambda_1}, \tag{6}$$

where S is the sum of the entries of the normalized principal eigenvector of G.

To see the relationship of (6) to earlier bounds, note that $S \leqslant \sqrt{n}$ always, so (6) implies that

$$k(G) \geqslant \frac{n}{n-\lambda_1}. \tag{7}$$

Further, since $\chi(G) \geqslant k(G)$, (7) implies that $\chi(G) \geqslant n/(n-\lambda_1)$. The latter is a result of Cvetković [3], which in turn refined an earlier result of Geller and Schmeichel [4]. Hence (6) sharpens both of these.

For regular graphs one has to work a little more in order to improve on the bounds given by Brooks' theorem. Let G be d-regular and have n vertices. Then $u_1 = e/\sqrt{n}$ where $e = (1, 1,..., 1)$, and $\lambda_1 = d$. Consider the vector

$$x = \frac{1}{n} e + \theta u_2, \tag{8}$$

where θ is to be determined. Since $(e, u_2) = 0$, it follows that in order for x to belong to the simplex $\mathscr{S}$ of (3) we need only require that $x \geqslant 0$, i.e.,

$$\theta(u_2)_i \geqslant -\frac{1}{n} \qquad (i = 1, 2,..., n). \tag{9}$$

For such θ we have from (4),

$$1 - \frac{1}{k(G)} \geqslant \frac{d}{n} + \lambda_2 \theta^2. \tag{10}$$

By a theorem of J. H. Smith [5] (see also [6, Theorem 6.7]), a graph for which $\lambda_2 \leqslant 0$ consists of isolated points together with a complete multipartite graph. Suppose G is not of this form. Then $\lambda_2 > 0$, and we want to maximize θ^2 subject to (9). After a short computation, the result can be expressed as follows.

Let

$$M_+ = \min_{(u_2)_i > 0} \frac{1}{(u_2)_i}; \qquad M_- = \min_{(u_2)_i < 0} \frac{1}{|(u_2)_i|}. \tag{11}$$

THEOREM 3. *Let G be a d-regular graph of n vertices. Then*

$$k(G) \geqslant \frac{n}{\{n - d - (\lambda_2/n) \max (M_+^2, M_-^2)\}}. \tag{12}$$

The corresponding result for the independence number $\alpha(G)$ begins with

$$M_+ = \min_{(u_n)_i > 0} \frac{1}{(u_n)_i}; \qquad M_- = \min_{(u_n)_i < 0} \frac{1}{|(u_n)_i|} \tag{13}$$

and leads to

THEOREM 4. *Let G be a d-regular graph of n vertices. Then*

$$\alpha(G) \geqslant \frac{n}{\{d+1+((\lambda_n+1)/n)\max(M_+^2, M_-^2)\}}. \tag{14}$$

The inequality (12) for the clique number sheds light on the case of equality in the simpler estimate $k(G) \geqslant n/(n-d)$, namely if $k(G) = n/(n-d)$ then $\lambda_2 \leqslant 0$. After Smith's theorem, G must be a regular complete multipartite graph, together with 0 or more isolated vertices. Similarly if $\alpha(G) = n/(d+1)$ then (14) requires that $\lambda_n = -1$, and that happens ([6], Theorem 0.13) only when the connected components of G are complete graphs.

The bound (14) may considerably improve (1). If we use $K_{n,n}$ as an example again, we find that (14) gives $\alpha(K_{n,n}) \geqslant n$, which is of course best possible.

We consider briefly the computational problem that is posed by extending the method. Given a regular graph G of n vertices, fix r, $2 \leqslant r \leqslant n$, and consider the maximization of (x, Ax) over just those vectors of $\mathscr{S}$ that have the form

$$x = \frac{1}{n} e + \sum_{j=2}^{r} \theta_j u_j \tag{15}$$

by analogy with (8). Then we want

$$\max_x (x, Ax) = \frac{d}{n} + \max_\theta \sum_{j=2}^{r} \lambda_j \theta_j^2. \tag{16}$$

For x to belong to $\mathscr{S}$ we need

$$\sum_{j=2}^{r} \theta_j (u_j)_i \geqslant -\frac{1}{n} \qquad (i = 1, \ldots, n). \tag{17}$$

To find the best x we would want to find the maximum in (16) subject to (17). This is a standard quadratic programming problem, and we have here another proof of the NP-hardness of such problems (Sahni [7]). Indeed if we could solve (16), (17) in polynomial time when $r = n$ we would have calculated the clique number of G.

There is one small redeeming feature, however. Suppose G has p^+ nonnegative eigenvalues, and $n - p^+$ negative ones. Then in polynomial time we can solve (16), (17) if $r \leqslant p^+$, for then the objective function in (16) is *convex*. The polynomial time solvability of convex quadratic programming is proved in [8].

As two questions for future research we ask first for a nontrivial bound, that approaches 0 as $r \to n$, for the difference between the restricted maximum in (16), (17), and the full maximum in (2), (3). Second, (14) is a good bound in particular if G admits as an eigenvector a vector of all ± 1 entries. What kind of a graph can have such an eigenvector?

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