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# Spectral upper bounds for the order of a $k$ -regular induced subgraph

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**Abstract.** Let  $G$  be a simple graph with least eigenvalue  $\lambda$ , and let  $S$  be a set of vertices in  $G$  which induce a subgraph with mean degree  $k$ . We use a quadratic programming technique in conjunction with the main angles of  $G$  to establish an upper bound of the form  $|S| \leq \inf\{(k+t)q_G(t) : t > -\lambda\}$ , where  $q_G$  is a rational function determined by the spectra of  $G$  and its complement. In the case  $k = 0$  we obtain improved bounds for the independence number of various benchmark graphs.

Keywords: graph, main eigenvalue, independence number, clique number

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# 1 Introduction

Let  $G$  be a simple graph of order  $n$  with  $(0, 1)$ -adjacency matrix  $A$  and characteristic polynomial  $P_G(x) = \det(xI - A)$ . The  $i$ -th largest eigenvalue of  $A$  is denoted by  $\lambda_i(G)$ , and we write  $\lambda_i = \lambda_i(G)$ ,  $\bar{\lambda}_i = \lambda_i(\bar{G})$ , where  $\bar{G}$  denotes the complement of  $G$ .

Let  $S$  be a set of vertices in  $G$  which induce a subgraph with mean degree  $k$ . We use a quadratic programming technique [2, 3] in conjunction with the main angles of  $G$  [8, Section 4.5] to prove that

$$|S| \leq \inf\{h_k^G(t) : t > -\lambda_n(G)\}, \quad (1)$$

where

$$h_k^G(t) = (k + t) \left\{ 1 - \frac{P_{\bar{G}}(t-1)}{(-1)^n P_G(-t)} \right\}.$$

Thus if we write  $H_G(t)$  for the walk-generating function of  $G$  (see [4] or [14]) then

$$h_k^G(t) = \left(1 + \frac{k}{t}\right) H_G\left(-\frac{1}{t}\right).$$

We give computational results which demonstrate that the bound (1) is superior to previous bounds. We make use of the functions  $f_{k,t}^A : \mathbb{R}^n \rightarrow \mathbb{R}$  defined for  $t > 0$  by

$$f_{k,t}^A(\mathbf{x}) = 2\mathbf{j}^\top \mathbf{x} - \frac{1}{k+t} \mathbf{x}^\top (A + tI) \mathbf{x},$$

where  $\mathbf{j}$  denotes the all-1 vector in  $\mathbb{R}^n$ . These functions were constructed in [3] to determine upper bounds for the order of a  $k$ -regular induced subgraph in terms of eigenvalues. The problem of finding the largest order of such a subgraph is NP-complete [2, Section 2], whereas spectral upper bounds can be computed in polynomial time. We too state our results in terms of  $k$ -regular induced subgraphs, but they apply equally to induced graphs with mean degree  $k$  (for example, induced unicyclic graphs, with mean degree 2). When  $k = 0$  we obtain an upper bound for the independence number  $\alpha(G)$ ; a spectral lower bound for  $\alpha(G)$ , in terms of  $n$ ,  $\bar{\lambda}_n$  and the mean degree of  $G$ , is derived in [13].

We shall first summarize the basic argument in [3]. Recall that the eigenvalue  $\lambda$  of  $G$  is a *main* eigenvalue if the eigenspace  $\mathcal{E}_A(\lambda)$  is not orthogonal to  $\mathbf{j}$ . In particular,  $\lambda_1$  is a main eigenvalue because the Perron-Frobenius theory ensures that  $A$  has a corresponding eigenvector whose entries are all non-negative.

If  $t \geq -\lambda_n$  then  $f_{k,t}^A$  is concave, that is,

$$f_{k,t}^A(\theta \mathbf{x} + (1 - \theta) \mathbf{y}) \geq \theta f_{k,t}^A(\mathbf{x}) + (1 - \theta) f_{k,t}^A(\mathbf{y})$$

whenever  $0 \leq \theta \leq 1$ . (To see this, express  $\mathbf{x}, \mathbf{y}$  as sums of eigenvectors of  $A$ ; alternatively, note that the Hessian matrix of  $f_{k,t}^A(t)$  is  $\frac{-2}{k+t}(A + tI)$ , which is negative semi-definite when  $t \geq -\lambda_n$ .) Accordingly,  $f_{k,t}^A$  has a global maximum at  $\mathbf{x}^*$  if and only if  $\nabla f_{k,t}^A(\mathbf{x}^*) = \mathbf{0}$ , that is,

$$\mathbf{j} - \frac{1}{k+t}(A + tI)\mathbf{x}^* = \mathbf{0}.$$

Then  $f_{k,t}^A(\mathbf{x}^*) = \mathbf{j}^\top \mathbf{x}^*$ . If  $\mathbf{x}_S$  is the characteristic vector of  $S$  then  $\mathbf{x}_S^\top A \mathbf{x}_S = k|S|$  and so  $|S| = f_{k,t}^A(\mathbf{x}_S) \leq f_{k,t}^A(\mathbf{x}^*)$ . Note that  $f_{k,t}^A(\mathbf{x}_S) = f_{k,t}^A(\mathbf{x}^*)$  if and only if  $(A + tI)\mathbf{x}_S = (k + t)\mathbf{j}$ , equivalently  $S$  is a  $(k, k + t)$ -regular set (that is,  $S$  induces a  $k$ -regular subgraph, while each vertex outside  $S$  is adjacent to  $k + t$  vertices inside  $S$ ).

Let  $J$  denote an all-1 matrix. If  $G \neq \overline{K}_n$  and  $\bar{\lambda}$  is a main eigenvalue of  $\overline{G}$  such that  $\bar{\lambda} \geq -\lambda_n - 1$ , then we may take  $t = \bar{\lambda} + 1$  and

$$\mathbf{x}^* = \frac{k + t}{\mathbf{j}^\top \mathbf{u}} \mathbf{u},$$

where  $\mathbf{u}$  is an eigenvector of  $J - I - A$  corresponding to  $\bar{\lambda}$  such that  $\mathbf{j}^\top \mathbf{u} \neq 0$ . (Note that then  $(A + tI)\mathbf{u} = J\mathbf{u} = \mathbf{j} \mathbf{j}^\top \mathbf{u}$ .) The Courant - Weyl inequalities imply that

$$\lambda_2(\overline{G}) + \lambda_n(G) \leq \lambda_2(K_n) = -1 = \lambda_n(K_n) \leq \lambda_1(\overline{G}) + \lambda_n(G).$$

Thus we may always take  $\bar{\lambda} = \bar{\lambda}_1$ , and the remaining possibility is  $\bar{\lambda} = -\lambda_n - 1$  when  $-\lambda_n - 1$  is a main eigenvalue of  $\overline{G}$ . Since  $f_{k,t}^A(\mathbf{x}^*) = \bar{\lambda} + k + 1$ , we obtain:

**Theorem 1.1** (cf. [3, Section 3]). *Let  $G$  be a graph of order  $n$ , and let  $S$  be a set of vertices which induces a  $k$ -regular subgraph of  $G$  ( $0 \leq k \leq n - 1$ ). Then*

$$|S| \leq \bar{\lambda}_1 + k + 1. \quad (2)$$

*If  $-\lambda_n - 1$  is a main eigenvalue of  $\overline{G}$  then*

$$|S| \leq -\lambda_n + k \quad (3)$$

Two remarks are in order:

(i) When  $k = 0$  we obtain from (2) the well-known upper bound  $\bar{\lambda}_1 + 1$  for the independence number  $\alpha(G)$ . This bound is attained when, for example,  $G$  is a complete graph or a complete bipartite graph.

(ii) If  $-\lambda_n - 1$  is a main eigenvalue of  $\overline{G}$  then  $\lambda_n$  is a non-main eigenvalue of  $G$ , and  $-\lambda_n - 1$  is a multiple eigenvalue of  $\overline{G}$ . This is a particular case of the following observation, essentially Theorem 2.12 of [5], for which we give a direct proof.

**Proposition 1.2.** *If  $\lambda$  is an eigenvalue of  $G$  such that  $-\lambda - 1$  is a main eigenvalue of  $\overline{G}$ , then  $\lambda$  is a non-main eigenvalue of  $G$ ; moreover, if  $\lambda$  has multiplicity  $d$  as an eigenvalue of  $G$  then  $-\lambda - 1$  has multiplicity  $d + 1$  as an eigenvalue of  $\overline{G}$ .*

**Proof.** Let  $(J - I - A)\mathbf{y} = (-\lambda - 1)\mathbf{y}$ , where  $\mathbf{j}^\top \mathbf{y} \neq 0$ . Let  $\mathbf{x} \in \mathcal{E}_A(\lambda)$ . Then  $(J - A)\mathbf{y} = -\lambda\mathbf{y}$  and  $\mathbf{x}^\top A = \lambda\mathbf{x}^\top$ . Hence  $\mathbf{x}^\top (J - A)\mathbf{y} = -\lambda\mathbf{x}^\top \mathbf{y}$  and  $\mathbf{x}^\top A\mathbf{y} = \lambda\mathbf{x}^\top \mathbf{y}$ . Adding, we have  $\mathbf{x}^\top J\mathbf{y} = 0$ , that is,  $\mathbf{x}^\top \mathbf{j} \mathbf{j}^\top \mathbf{y} = 0$ . Hence  $\mathbf{x}^\top \mathbf{j} = 0$  for all  $\mathbf{x} \in \mathcal{E}_A(\lambda)$ ; in other words,  $\lambda$  is a non-main eigenvalue of  $G$ . Now  $\mathcal{E}_{J-I-A}(-\lambda - 1) \cap \mathbf{j}^\perp = \mathcal{E}_A(\lambda)$ , and the second assertion follows.  $\square$

## 2 Further bounds

Here we introduce improved bounds by involving the main angles of  $G$ . We write  $\mu_1, \dots, \mu_s$  for the main eigenvalues of  $G$  in decreasing order. Then  $\mathbf{j}$  is expressible as

$$\mathbf{j} = \mathbf{u}_1 + \dots + \mathbf{u}_s \quad (\mathbf{u}_i \in \mathcal{E}_A(\mu_i)).$$

Thus  $\mu_1 = \lambda_1$ , and the non-zero main angles of  $G$  are  $\beta_1, \dots, \beta_s$  where  $\sqrt{n}\beta_i = \|\mathbf{u}_i\|$  ( $i = 1, \dots, s$ ).

**Theorem 2.1.** *Let  $G$  be a graph of order  $n$ , and let  $S$  be a set of vertices which induces a  $k$ -regular subgraph of  $G$  ( $0 \leq k \leq n-1$ ). If  $t > -\lambda_n$  then*

$$|S| \leq n \sum_{i=1}^s \frac{t+k}{t+\mu_i} \beta_i^2; \quad (4)$$

equivalently,

$$|S| \leq h_k^G(t), \quad (5)$$

where

$$h_k^G(t) = (k+t) \left\{ 1 - \frac{P_G(t-1)}{(-1)^n P_G(-t)} \right\}. \quad (6)$$

**Proof.** If  $t > -\lambda_1$  then the function  $f_{k,t}^A$  is concave and attains its maximum at

$$\mathbf{x}^* = \sum_{i=1}^s \frac{k+t}{\mu_i+t} \mathbf{u}_i.$$

Hence

$$|S| = f_{k,t}^A(\mathbf{x}_S) \leq \mathbf{j}^\top \mathbf{x}^* = n \sum_{i=1}^s \frac{t+k}{t+\mu_i} \beta_i^2.$$

The equivalent bound (5) is obtained by setting  $x = t-1$  in the formula [7, p.90]

$$P_G(x) = (-1)^n P_G(-x-1) \left\{ 1 - \sum_{i=1}^s \frac{n\beta_i^2}{x+1+\mu_i} \right\}. \quad (7)$$

□

When  $\lambda_n$  is a main eigenvalue of  $G$ , the graph of  $y = h_k^G(t)$  has  $t = -\lambda_n$  as an asymptote, and so we state our main result as follows. Here the second assertion follows from our remarks in Section 1.

**Corollary 2.2.** *If  $S$  induces a  $k$ -regular subgraph of  $G$  then*

$$|S| \leq \inf \{ h_k^G(t) : t > -\lambda_n(G) \}.$$

We have  $|S| = h_k^G(t_0)$  if and only if  $S$  is a  $(k, k+t_0)$ -regular set.

When  $\lambda_n$  is a non-main eigenvalue of  $G$ , we have  $G \neq \overline{K}_n$  and we may take  $t = -\lambda_n$  to obtain the following reformulation of [3, Theorem 3.4]:

**Theorem 2.3.** *Let  $G$  be a graph of order  $n$ , and let  $S$  be a set of vertices which induces a  $k$ -regular subgraph of  $G$  ( $0 \leq k \leq n-1$ ). If  $\lambda_n$  is a non-main eigenvalue of  $G$  then*

$$|S| \leq n \sum_{i=1}^s \frac{-\lambda_n + k}{-\lambda_n + \mu_i} \beta_i^2. \quad (8)$$

In Equation (5) we should cancel factors common to  $P_{\overline{G}}(t-1)$  and  $P_G(-t)$ . To this end, let  $M_G(x) = (x - \mu_1) \cdots (x - \mu_s)$ , and  $M_{\overline{G}}(x) = (x - \overline{\mu}_1) \cdots (x - \overline{\mu}_s)$ , where  $\overline{\mu}_1, \dots, \overline{\mu}_s$  are the main eigenvalues of  $\overline{G}$  (cf. [14]). By Proposition 1.2 applied to  $G$  and  $\overline{G}$ , or by Equation (8) of [14], we have

$$\frac{P_{\overline{G}}(t-1)}{(-1)^n P_G(-t)} = \frac{M_{\overline{G}}(t-1)}{(-1)^s M_G(-t)}; \quad (9)$$

moreover,  $M_{\overline{G}}(t-1)$  and  $M_G(-t)$  have no common factors. Thus  $h_k^G(t) = k + t$  if and only if  $t - 1$  is a main eigenvalue of  $\overline{G}$ . In particular, we may take  $t = 1 + \overline{\lambda}_1$  to obtain the bound (1). In the case that  $-1 - \lambda_n$  is a main eigenvalue of  $\overline{G}$ , we take  $t = -\lambda_n$  in (4) and (6) to deduce:

**Proposition 2.4.** *When  $-\lambda_n - 1$  is a main eigenvalue of  $\overline{G}$ , the upper bounds (3) and (8) coincide.*

To discuss the improvements on (2) afforded by Corollary 2.2, we write  $h_k(t)$  for  $h_k^G(t)$ . If either

$$-\lambda_n < \overline{\lambda}_1 + 1 \text{ and } h'_k(1 + \overline{\lambda}_1) \neq 0$$

or

$$-\lambda_n = \overline{\lambda}_1 + 1 \text{ and } h'_k(1 + \overline{\lambda}_1) < 0,$$

then an improvement on (1) is assured in a neighbourhood of  $1 + \overline{\lambda}_1$ . We have

$$h'_k(1 + \overline{\lambda}_1) = 1 - (k + 1 + \overline{\lambda}_1)(-1)^s \left\{ \frac{M'_{\overline{G}}(\overline{\lambda}_1)}{M_G(-1 - \overline{\lambda}_1)} \right\},$$

but it is more revealing to inspect two small examples.

**Example 2.5.** Let  $G = 3K_1 \dot{\cup} K_2 \dot{\cup} K_3$ . Then  $P_G(x) = (x-2)(x-1)x^3(x+1)^3$ . Using the computer package GRAPH, we find that  $P_{\overline{G}}(x) = (x^3 - 2x^2 - 21x - 24)x^3(x+1)^2$ ; moreover,  $0 (= -\lambda_8 - 1)$  is not a main eigenvalue of  $\overline{G}$ . We have  $\overline{\lambda}_1 \approx 6.0930$ , and so the bound (1) yields  $|S| \leq 7$  when  $k = 0$ . Here  $\mu_s = 0 = k$  and  $y = h_0(t)$  does not have  $t = 0$  as an asymptote. We have

$$h_0(t) = \frac{2(2t+3)(2t+1)}{(t+1)(t+2)},$$

a function which increases monotonically on  $[-\lambda_8, \infty)$ . Whenever  $h_k(t)$  has this property, and  $\mu_s > \lambda_n$ , the best bound arises when  $t = -\lambda_n$ , giving a formula that coincides with (8). In this example, we obtain  $|S| \leq 5$  (a sharp upper bound since  $\alpha(G) = 5$ ).  $\square$

**Example 2.6.** Let  $G$  be the graph on 6 vertices numbered 50 in the table [6], where characteristic polynomials are listed and main angles are identified; the complement of  $G$  is numbered 100 in [6]. We have  $s = 4$ ,  $\mu_4 = \lambda_6 \approx -2.508$  and  $\overline{\lambda}_1 \approx 2.228$ . We take  $k = 0$  again, and then the upper bound (1) for  $|S|$  is 3.228. In this case  $y = h_0(t)$  has  $t = -\lambda_6$  as an asymptote. Explicitly,

$$h_0(t) = \frac{2t(3t^3 - 9t^2 + t + 7)}{t^4 - 9t^2 + 4t + 7}.$$

This function has a unique local minimum on  $(-\lambda_6, \infty)$ . Using Mathematica, we find that this minimum is 3.132 at  $t = 2.834$  (to three places of decimals).

This new upper bound is smaller, but of course both bounds yield  $|S| \leq 3$  (a sharp inequality since  $\alpha(G) = 3$ ).  $\square$

These examples are provided to illustrate differences in the behaviour of  $h_k$ . To demonstrate the superiority of the bound in Corollary 2.2, we should consider larger graphs, and this we do in the the next section. Here we first discuss properties of  $h_k$  in the general case.

**Proposition 2.7** *The function  $h_k(t)$  has at most one local minimum in  $(-\mu_s, \infty)$ .*

**Proof.** The result is immediate if  $s = 1$  (that is, if  $G$  is regular), since then  $h_k(t)$  is monotonic. Accordingly we suppose that  $s > 1$ . We have

$$h_k(t) = n - \sum_{i=1}^s \frac{n(\mu_i - k)\beta_i^2}{t + \mu_i}. \quad (10)$$

Suppose first that  $k$  is not a main eigenvalue of  $G$ , so that the graph  $\mathcal{G}$  of  $y = h_k(t)$  has asymptotes  $t = -\mu_i$  ( $i = 1, \dots, s$ ). Note also that  $h_k(t) \rightarrow n$  as  $t \rightarrow \infty$  and as  $t \rightarrow -\infty$ .

If  $\mu_s < k$  then the line  $y = d$  cuts  $\mathcal{G}$  in (at least)  $s - 1$  points of  $(-\infty, -\mu_s)$  when  $d > n$ , and (at least)  $s - 2$  points of  $(-\infty, -\mu_s)$  when  $d < n$ . If  $\mu_s > k$  then the line  $y = d$  cuts  $\mathcal{G}$  in (at least)  $s$  points of  $(-\infty, -\mu_s)$  when  $d > n$ , and (at least)  $s - 1$  points of  $(-\infty, -\mu_s)$  when  $d < n$ .

Now suppose that  $h_k(t)$  has a local minimum at  $t_0 \in (-\mu_s, \infty)$ . Then  $h'_k(t) \geq 0$  for all  $t \geq t_0$ , for otherwise  $h_k(t)$  has a local maximum at some point  $t_1 \in (t_0, \infty)$ . If  $h_k(t_1) > n$  then for some  $d > n$ , the line  $y = d$  cuts  $\mathcal{G}$  in (at least) 3 points in  $(-\mu_s, \infty)$ . If  $h_k(t_1) \leq n$  then for some  $d < n$ , the line  $y = d$  cuts  $\mathcal{G}$  in (at least) 4 points in  $(-\mu_s, \infty)$ . In any case, the function  $h_k(t) - d$  has more than  $s$  zeros in  $\mathbb{R}$ . This is a contradiction because  $h_k(t) - d$  ( $d \neq n$ ) has the form  $p(t)/q(t)$ , where  $p(t), q(t)$  are polynomials of degree  $s$ .

If  $k$  is a main eigenvalue of  $G$ , then the same arguments apply to a graph with  $s - 1$  vertical asymptotes.

It follows that  $h_k(t)$  has no more than one local minimum in  $(-\mu_s, \infty)$ .  $\square$

**Corollary 2.8** *For a non-regular graph  $G$ , we have:*

- (i) *if  $\mu_s < 0$  then  $h_0^G(t)$  has a unique local minimum in  $(-\mu_s, \infty)$ ,*
- (ii) *if  $\mu_s = 0$  then  $h_0^G(t)$  is increasing on  $(-\mu_{s-1}, \infty)$ ,*
- (iii) *if  $\mu_s > 0$  then  $h_0^G(t)$  is increasing on  $(-\mu_s, \infty)$ .*

**Proof.** We have  $h_0(1 + \bar{\lambda}_1) = 1 + \bar{\lambda}_1 < n$  and  $1 + \bar{\lambda}_1 \in (-\mu_s, \infty)$ . Thus if  $\mu_s < 0$  then  $h_0(t)$  has a local minimum on  $(-\mu_s, \infty)$ , and this minimum is unique by Proposition 2.7. If  $\mu_s = 0$  then from (10) we see that  $h'_0(t) > 0$  for all  $t \in (-\mu_{s-1}, \infty)$ , and if  $\mu_s > 0$  then  $h'_0(t) > 0$  for all  $t \in (-\mu_s, \infty)$ .  $\square$

We conclude this section by deriving sharp upper bounds in two special cases. First, if  $G$  is  $r$ -regular, we may apply Theorem 2.3 to obtain

$$|S| \leq \frac{n(k - \lambda_n)}{r - \lambda_n}.$$

This bound, known as the Hoffman bound when  $k = 0$ , coincides with that obtained from interlacing (cf. [10, Lemma 9.6.2]). It is attained in some of

the regular graphs  $\overline{G}$  discussed in Section 3. Other generalizations of the Hoffman bound may be found in [1, Theorem 7] and [9, Corollary 3.2].

Secondly, consider a connected harmonic graph  $G$ , that is, a connected graph  $G$  for which  $A\mathbf{d} = \mu_1\mathbf{d}$ , where  $\mathbf{d}$  is the vector whose entries are the vertex degrees. We show that if  $G$  has  $e$  edges then

$$\alpha(G) \leq n - \frac{e}{\mu_1}. \quad (11)$$

The main eigenvalues of  $G$  are  $\mu_1$  and 0 [14, Proposition 3.3], and so

$$\alpha(G) \leq h_0(-\lambda_n) = n \left\{ 1 - \frac{\mu_1}{\mu_1 - \lambda_n} \beta_1^2 \right\} \leq n(1 - \frac{1}{2}\beta_1^2).$$

To determine  $\beta_1$  when  $G$  is connected, note that

$$\mathbf{u}_1 = \frac{1}{\|\mathbf{d}\|^2} (\mathbf{d}^\top \mathbf{j}) \mathbf{d}, \quad \text{whence } n\beta_1^2 = \frac{4e^2}{\|\mathbf{d}\|^2}.$$

Since  $\mathbf{d} - \mu_1\mathbf{j} \in \mathcal{E}_A(0) \subseteq \mathcal{E}_A(\mu_1)^\perp = \mathbf{d}^\perp$ , we have  $\|\mathbf{d}\|^2 = 2e\mu_1$ , and so  $n(1 - \frac{1}{2}\beta_1^2) = n - \frac{e}{\mu_1}$ , proving (11). We note that this bound is attained in all Grünwald trees [11, 14]: for such a tree  $T$  we have  $\lambda_n = -\mu_1$ ,  $e = n - 1 = \mu_1(\mu_1^2 - \mu_1 + 1)$  and  $\alpha(T) = (\mu_1 - 1)(\mu_1^2 - \mu_1 + 1) + 1$ .

### 3 Computational results

Here we apply our results to  $\overline{G}$  with  $k = 0$  to obtain bounds on the clique number  $\omega(G) = \alpha(\overline{G})$ . We compare old and new bounds for  $\omega(G)$  for graphs  $G$  from the Second DIMACS Implementation Challenge [12]: these are benchmark graphs used for testing algorithms that determine or estimate  $\omega(G)$ . The old bounds in the table are given by  $1 + \lambda_1(G)$ , while the new bounds  $h_0^{\overline{G}}(t^*)$  are calculated in accordance with Corollary 2.8: if  $\overline{\mu}_s \geq 0$  (in particular, if  $\overline{G}$  is regular) then  $t^* = -\overline{\lambda}_n$ ; otherwise  $h_0^{\overline{G}}(t^*)$  is the unique local minimum on  $(-\overline{\lambda}_n, \infty)$ . In practice,  $t^*$  is determined to within a computational error, and so

$$h_0^{\overline{G}}(t^*) \approx \inf\{h_0^{\overline{G}}(t) : t > -\lambda_n(\overline{G})\}.$$

Most of the graphs in the table have  $\lambda_n(\overline{G})$  as a main eigenvalue, with  $h_0'(1 + \lambda_1(G)) > 0$ , where  $h_0 = h_0^{\overline{G}}$ . Then  $\overline{\mu}_s < 0$  and we estimate  $t^*$  using successive bisections of intervals, starting with  $[-\lambda_n(\overline{G}) + 10^{-6}, \lambda_1(G) + 1]$ , where the value of  $h_0$  at the mid point is less than the value at each end point. For an interval  $[a, b]$  with mid-point  $c$ , let  $x, y$  be the mid points of  $[a, c], [c, b]$  respectively. If  $h_0(x)$  and  $h_0(y)$  are both greater than  $h_0(c)$  then we replace  $[a, b]$  with  $[x, y]$ . Otherwise,  $[a, b]$  is replaced with  $[a, c]$  if  $h_0(x) \leq h_0(c)$ , or with  $[c, b]$  if  $h_0(x) > h_0(c)$ . The process is repeated until we reach an interval where the values of  $h_0$  at the mid point and end points coincide to within four decimal places.

In the graph c-fat200-1.clq,  $-\lambda_n(\overline{G}) - 1$  is a main eigenvalue of  $G$  and  $h_0'(-\lambda_n(\overline{G})) > 0$ ; thus the best upper bound is that in (3), attained when  $t^* = h_0(t^*) = -\lambda_n(\overline{G}) = 17.2675$ .



$G$	$n$	$\omega(G)$	$\lambda_1(G) + 1$	$t^*$	$h_0^{\bar{G}}(t^*)$	Notes
brock200-1.clq	200	21	149.5707	12.4952	43.3005	(a)
brock200-2.clq	200	12	100.1963	14.0483	26.4234	(a)
brock200-3.clq	200	15	121.8181	13.9645	32.0650	(a)
brock200-4.clq	200	17	132.2037	13.5104	35.3994	(a)
brock400-1.clq	400	27	299.8496	17.2781	62.8351	(a)
brock400-2.clq	400	29	300.1480	17.4017	62.8164	(a)
brock400-3.clq	400	31	299.6317	17.6204	63.9385	(a)
brock400-4.clq	400	33	300.0543	17.5317	63.3207	(a)
c-fat200-1.clq	200	12	17.8135	17.2675	17.2675	
c-fat200-2.clq	200	24	33.6036	32.7001	32.9611	(a)
c-fat200-5.clq	200	58	85.7778	64.7787	72.9051	
hamming6-2.clq	64	32	58		32	(b)
hamming6-4.clq	64	4	23		13.5385	(b)
hamming8-2.clq	256	128	248		128	(b)
hamming8-4.clq	256	16	164		72	(b)
johnson8-2-4.clq	28	4	16		4	(b)
johnson8-4-4.clq	70	14	54		14	(b)
johnson16-2-4.clq	120	8	92		8	(b)
johnson32-2-4.clq	496	16	436		16	(b)
MANN-a9.clq	45	16	41.8039	2.3885	19.7076	
MANN-a27.clq	378	126	374.3035	6.7405	278.9118	
p-hat300-1.clq	300	8	80.7579	16.6554	26.3647	(a)
p-hat300-2.clq	300	25	158.9345	30.3485	78.1328	(a)
p-hat300-3.clq	300	36	225.8307	19.3401	88.3742	(a)
keller4.clq	171	11	111.8552	17.7206	41.1585	
san200-0.7-1.clq	200	30	140.5107	51.6650	94.7681	(a)
san200-0.7-2.clq	200	18	143.5080	68.3020	117.1690	(a)
san200-0.9-1.clq	200	70	180.3256	22.8092	118.7377	(a)
san200-0.9-2.clq	200	60	180.1964	17.4725	98.3736	(a)
san200-0.9-3.clq	200	44	180.1697	14.1434	86.5558	(a)
san400-0.5-1.clq	400	13	202.9588	151.2577	179.3039	(a)
san400-0.7-1.clq	400	40	280.4968	102.2726	184.7757	(a)
san400-0.7-2.clq	400	30	280.5105	98.4703	182.4865	(a)
san400-0.7-3.clq	400	22	280.8343	93.7929	183.7393	(a)

Notes: (a)  $-\lambda_n(\bar{G})$  is a main eigenvalue, (b)  $G$  is regular.

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