Spectral bounds for the k-independence number of a graph

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Abstract

In this paper, we obtain two spectral upper bounds for the k-independence number of a graph which is is the maximum size of a set of vertices at pairwise distance greater than k. We construct graphs that attain equality for our first bound and show that our second bound compares favorably to previous bounds on the k-independence number.

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1. Introduction

The independence number of a graph G, denoted by $\alpha(G)$, is the size of the largest independent set of vertices in G. A natural generalization of the independence number is the *k-independence number* of G, denoted by $\alpha_k(G)$ with $k \geq 0$, which is the maximum number of vertices that are mutually at distance greater than k. Note that $\alpha_0(G)$ equals the number of vertices of G and $\alpha_1(G)$ is the independence number of G.

The k-independence number is an interesting graph theoretic parameter that is closely related to coding theory, where codes and anticodes are k-independent sets in Hamming graphs (see [24, Chapter 17]). In addition, the k-independence number of a graph has been studied in various other contexts (see [2, 8, 12, 13, 14, 21, 26] for some examples) and is related to other combinatorial parameters such as average distance [15], packing chromatic number [16], injective chromatic number [19], and strong chromatic index [25]. It is known that determining α_k is NP-Hard in general [22].

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In this article, we prove two spectral upper bounds for α_k that generalize two well-known bounds for the independence number: Cvetković's inertia bound [4] and the Hoffman ratio bound (see [3, Theorem 3.5.2] for example). Our motivation behind this work is obtaining non-trivial and tight generalizations of these classical results in spectral graph theory that depend on the parameters of the original graph and not of its higher powers. Note that α_k is the independence number of G^k, the k-th power of G. The graph G^k has the same vertex set as G and two distinct vertices are adjacent in G^k if their distance in G is k or less. In general, even the simplest spectral or combinatorial parameters of G^k cannot be deduced easily from the similar parameters of G (see [6, 7, 20]). The bounds in our main results (Theorem 3.2 and Theorem 4.2) depend on the eigenvalues and eigenvectors of the adjacency matrix of G and do not require the spectrum of G^k. We prove our main results in Section 3 and Section 4. We construct infinite examples showing that the bound in Theorem 3.2 is tight, but we have not been able to determine whether or not equality can happen in Theorem 4.2. We conclude our paper with a detailed comparison of our bounds to previous work of Fiol [10, 11] and some directions for future work.

2. Preliminaries

Throughout this paper $G = (V, E)$ will denote a graph (undirected, simple and loopless) on vertex set V with n vertices, edge set E and adjacency matrix A with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. The following result was proved by Haemers in his Ph.D. Thesis (see [18] for example).

Lemma 2.1 (Eigenvalue Interlacing, [18])**.** *Let A be a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. For some integer $m < n$, let S be a real $n \times m$ matrix such that $S^\top S = I$ (its columns are orthonormal), and consider the $m \times m$ matrix $B = S^\top AS$, with eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$. Then, the eigenvalues of B interlace the eigenvalues of A, that is, $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$, for $1 \leq i \leq m$.*

If we take $S = [\, I \;\; O\,]$, then B is just a principal submatrix of A and we have:

Corollary 2.2. *If B is a principal submatrix of a symmetric matrix A, then the eigenvalues of B interlace the eigenvalues of A.*

3. Generalized inertia bound

Cvetković [4] (see also [3, p.39] or [17, p.205]) obtained the following upper bound for the independence number.

Theorem 3.1 (Cvetković's inertia bound)**.** *If G is a graph, then*

$$\alpha(G) \leq \min\{|i : \lambda_i \geq 0|, |i : \lambda_i \leq 0|\}. \tag{1}$$

Let $w_k(G) = \min_i(A^k)_{ii}$ be the minimum number of closed walks of length k where the minimum is taken over all the vertices of G. Similarly, let $W_k(G) = \max_i(A^k)_{ii}$ be the maximum number of closed walks of length k where the maximum is taken over all the vertices of G. Our first main theorem generalizes Cvetković's inertia bound which can be recovered when $k = 1$.

Theorem 3.2. *Let G be a graph on n vertices. Then,*

$$\alpha_k(G) \leq |\{i : \lambda_i^k \geq w_k(G)\}| \quad \textit{and} \quad \alpha_k(G) \leq |\{i : \lambda_i^k \leq W_k(G)\}|. \tag{2}$$

Proof. Because G has a k-independent set U of size α_k, the matrix A^k has a principal submatrix (with rows and columns corresponding to the vertices of U) whose off-diagonal entries are 0 and whose diagonal entries equal the number of closed walks of length k starting at vertices of U. Corollary 2.2 leads to the desired conclusion. □

We now describe why the above theorem can be considered a spectral result in nature. Our bounds are functions of the eigenvalues of A and of certain counts of closed walks in G. We will now explain briefly how one may count closed walks in G using only the eigenvalues and eigenvectors of A (cf [5] Section 1.8 or [13]). Let $x_1, \cdots, x_n$ be an orthonormal basis of eigenvectors for A and let $e_1, \cdots, e_n$ be standard basis vectors. Then the number of closed walks of length j from a vertex v is given by

$$e_v^T A^j e_v = \left(\sum_{i=1}^n \langle e_v, x_i\rangle x_i\right)^T A^j \left(\sum_{i=1}^n \langle e_v, x_i\rangle x_i\right) = \sum_{i=1}^n \langle e_v, x_i\rangle^2 \lambda_i^j.$$

Therefore, one may apply our bounds with knowledge only of the eigenvalues and eigenvectors for A. In fact, we note that one does not need to compute the eigenvectors of A to count walks in G. It is enough to compute the idempotents which are given in terms of a polynomial in A and the eigenvalues of A [9].

3.1. Construction attaining equality

In this section, we describe a set of graphs for which Theorem 3.2 is tight. For $k, m \geq 1$ we will construct a graph G with $\alpha_{2k+2}(G) = \alpha_{2k+3}(G) = m$.

Le H be the graph obtained from the complete graph K_n by removing one edge. The eigenvalues of H are $\frac{n-3\pm\sqrt{(n+1)^2-8}}{2}, 0$ (each with multiplicity 1), and -1 with multiplicity $n-3$. This implies $|\lambda_i(H)| < 2$ for $i > 1$.

Let $H_1, ..., H_m$ be vertex disjoint copies of H with $u_i, v_i \in V(H_i)$ and $u_i \not\sim v_i$ for $1 \leq i \leq m$. Let x be a new vertex. For each $1 \leq i \leq m$, create a path of length k with x as one endpoint and u_i as the other. Let G be the resulting graph which has $nm + (k-2)m + 1$ vertices with $m\left(\binom{n}{2} - 1\right) + mk$ edges.

Because the distance between any distinct v_is is $2k + 4$, we get that

$$\alpha_{2k+2}(G) \geq \alpha_{2k+3}(G) \geq m. \tag{3}$$

We will use Theorem 3.2 to show that equality occurs in (3) for n large enough.

Starting from any vertex of G, one can find a closed walk of length $2k+2$ or $2k+3$ that contains an edge of some H_i. Therefore, $w_{2k+2}(G) \geq n-2$ and $w_{2k+3}(G) \geq n-2$. Choose n so that $n-2 > (\sqrt{m}+4)^{2k+3}$. If we can show that

$$|\lambda_i(G)| \leq \sqrt{m}+4 \tag{4}$$

for all $i > m$, then Theorem 3.2 will imply that $\alpha_{2k+3}(G) \leq \alpha_{2k+2}(G) \leq m$ and we are done. To show (4), note that the edge-set of G is the union of m edge disjoint copies of H, the star $K_{1,m}$, and m vertex disjoint copies of P_{k-1}. Since the star $K_{1,m}$ has spectral radius $\sqrt{m}$ and a disjoint union of paths has spectral radius less than 2, applying the Courant-Weyl inequalities again, along with the triangle inequality, proves (4) and shows the tightness of our examples.

4. Generalized Hoffman bound

The following bound on the independence number is an unpublished result of Hoffman known as the Hoffman's ratio bound (see [3, p.39] or [17, p.204]).

Theorem 4.1 (Hoffman ratio bound)**.** *If G is regular then*

$$\alpha(G) \leq n\frac{-\lambda_n}{\lambda_1 - \lambda_n},$$

and if a coclique C meets this bound then every vertex not in C is adjacent to precisely $-\lambda_n$ vertices of C.

Let G be a d-regular graph on n vertices having an adjacency matrix A with eigenvalues $d = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq -d$. Let $\lambda = \max\{|\lambda_2|, |\lambda_n|\}$. We use Alon's notation and say that G is an (n, d, λ)-graph (see also [23, p.19]). Let $\tilde{W}_k = \max_i \sum_{j=1}^{k} (A^j)_{ii}$ be the maximum over all vertices of the number of closed walks of length at most k. Our second theorem is an extension of the Hoffman bound to k-independent sets.

Theorem 4.2. *Let G be an (n, d, λ)-graph and k a natural number. Then*

$$\alpha_k(G) \leq n\frac{\tilde{W}_k + \sum_{j=1}^{k} \lambda^j}{\sum_{j=1}^{k} d^j + \sum_{j=1}^{k} \lambda^j}. \tag{5}$$

The proof of Theorem 4.2 will be given as a corollary of a type of Expander-Mixing Lemma (cf [1]). For k a natural number, denote

$$\lambda^{(k)} = \lambda + \lambda^2 + \cdots + \lambda^k,$$

and

$$d^{(k)} = d + d^2 + \cdots + d^k.$$

Theorem 4.3 (k-Expander Mixing Lemma)**.** *Let G be an (n,d,λ)-graph. For $S,T \subseteq G$ let $W_k(S,T)$ be the number of walks of length at most k with one endpoint in S and one endpoint in T. Then for any $S,T \subseteq V$, we have*

$$\left|W_k(S,T) - \frac{d^{(k)}|S||T|}{n}\right| \leq \lambda^{(k)}\sqrt{|S||T|\left(1-\frac{|S|}{n}\right)\left(1-\frac{|T|}{n}\right)} < \lambda^{(k)}\sqrt{|S||T|}.$$

Proof. Let $S,T \subset V(G)$ and let $\mathbf{1}_S$ and $\mathbf{1}_T$ be the characteristic vectors for S and T respectively. Then

$$W_k(S,T) = \mathbf{1}_S^t\left(\sum_{j=1}^{k} A^j\right)\mathbf{1}_T.$$

Let $x_1,...,x_n$ be an orthonormal basis of eigenvectors for A. Then $\mathbf{1}_S = \sum_{i=1}^n \alpha_i x_i$ and $\mathbf{1}_T = \sum_{i=1}^n \beta_i x_i$, where $\alpha_i = \langle \mathbf{1}_S, x_i\rangle$ and $\beta_i = \langle \mathbf{1}_T, x_i\rangle$. Note that $\sum \alpha_i^2 = \langle \mathbf{1}_S, \mathbf{1}_S\rangle = |S|$ and similarly, $\sum \beta_i^2 = |T|$. Because G is d-regular, we get that $x_1 = \frac{1}{\sqrt{n}}\mathbf{1}$ and so $\alpha_1 = \frac{|S|}{n}$ and $\beta_1 = \frac{|T|}{n}$. Now, since $i \neq j$ implies $\langle x_i, x_j\rangle = 0$, we have

$$\begin{aligned}
W_k(S,T) &= \left(\sum_{i=1}^n \alpha_i x_i\right)^t\left(\sum_{j=1}^k A^j\right)\left(\sum_{i=1}^n \beta_i x_i\right)\\
&= \sum_{i,j}(\alpha_i x_i)((\beta_j(\lambda_j + \lambda_j^2 + \cdots + \lambda_j^k)x_j)\\
&= \sum_{i=1}^n(\lambda_i + \lambda_i^2 + \cdots + \lambda_i^k)\alpha_i\beta_i\\
&= \frac{d^{(k)}}{n}|S||T| + \sum_{i=2}^n(\lambda_i + \lambda_i^2 + \cdots + \lambda_i^k)\alpha_i\beta_i
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
\left|W_k(S,T) - \frac{d^{(k)}}{n}|S||T|\right| &= \left|\sum_{i=2}^n(\lambda_i + \lambda_i^2 + \cdots + \lambda_i^k)\alpha_i\beta_i\right|\\
&\leq \lambda^{(k)}\sum_{i=2}^n|\alpha_i\beta_i|\\
&\leq \lambda^{(k)}\left(\sum_{i=2}^n\alpha_i^2\right)^{1/2}\left(\sum_{i=2}^n\beta_i^2\right)^{1/2},
\end{aligned}$$

where the last inequality is by Cauchy-Schwarz. Now since

$$\sum_{i=2}^n \alpha_i^2 = |S| - \frac{|S|^2}{n^2}$$

and

$$\sum_{i=2}^{n} \beta_i^2 = |T| - \frac{|T|^2}{n^2},$$

we have the result. $\square$

Now we are ready to prove the bound of Theorem 4.2.

Proof. [Proof of Theorem 4.2] Let S be a k-independent set in G with $|S| = \alpha_k(G)$, and let $W_k(S,S)$ be equal to the number of closed walks of length at most k starting in S. Theorem 4.3 gives

$$\frac{d^{(k)}|S|^2}{n} - W_k(S,S) \leq \lambda^{(k)}|S| \left(1 - \frac{|S|}{n}\right).$$

Recalling that $\tilde{W}_k = \max_i \sum_{j=1}^{k} (A^j)_{ii}$, we have $W_k(S,S) \leq |S|\tilde{W}_k$. This yields

$$\frac{d^{(k)}|S|}{n} - \tilde{W}_k \leq \lambda^{(k)} \left(1 - \frac{|S|}{n}\right).$$

Solving for $|S|$ and substituting $|S| = \alpha_k$ gives

$$\alpha_k \leq n\frac{\tilde{W}_k + \lambda^{(k)}}{d^{(k)} + \lambda^{(k)}}.$$

$\square$

Note that the bound from Theorem 4.2 behaves nicely if $\tilde{W}_k$ and $\lambda^{(k)}$ are small with respect of $d^{(k)}$. It is easy to see that $\tilde{W}_k \leq \frac{d^k - 1}{d-1}$ (we expand d in each step but in the last step we do not have any freedom since we assume that we are counting closed walks). Since G is d-regular and we know that $\tilde{W}_k \leq d^{k-1}$, the above bound performs well for graphs with a good spectral gap.

5. Concluding Remarks

In this section, we note how our theorems compare with previous upper bounds on α_k. Our generalized Hoffman bound for α_k is best compared with Firby and Haviland [15], who proved that if G is a connected graph of order $n \geq 2$ then

$$\alpha_k(G) \leq \frac{2(n-\epsilon)}{k+2-\epsilon} \tag{6}$$

where $\epsilon \equiv k \pmod 2$. If d is large compared to k and $\lambda = o(d)$, then Theorem 4.2 is much better than (6) (this may be expected, as we have used much more information than is necessary for (6)). We note that almost all d-regular graphs have $\lambda = o(d)$ as $d \to \infty$.

In [11], Fiol (improving work from [12]) obtained the bound

$$\alpha_k(G) \leq \frac{2n}{P_k(\lambda_1)}, \tag{7}$$

when G is a regular graph (later generalized to nonregular graphs in [10]), and P_k is the k-alternating polynomial of G. The polynomial P_k is defined by the solution of a linear programming problem which depends on the spectrum of the graph G. It is nontrivial to compute P_k, and there is not a closed form for it making it difficult to compare to our theorems in general. However, the reader may check the Appendix to see that (7), Theorem 4.2, and Theorem 3.2 are pairwise incomparable.

If p is a polynomial of degree at most k, and U is a k-independent set in G, then $p(A)$ has a principal submatrix defined by U that is diagonal, with diagonal entries defined by a linear combination of various closed walk. Theorems 3.2 and 4.2 are obtained by taking $p(A) = A^k$, but hold also for in general for other polynomials of degree at most k. It is not clear to us how to choose a polynomial p to optimize the upper bound on α_k for general graphs as such polynomial will likely depend on the graph. Finally, we were able to construct graphs attaining equality in Theorem 3.2 but not in Theorem 4.2. We leave open whether the bound in Theorem 4.2 is attained for some graphs or can be improved in general.

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Appendix

The following tables compare Fiol's bound on α_k, namely equation (7), with Theorem 3.2 and Theorem 4.2. We tested all of the named graphs in Sage that do not take any arguments, subject to the constraint that they are regular, connected, and have diameter greater than k. Table entries that say "time" denote that the computation took longer than 60 seconds on a standard laptop. The parameter α_k is computationally hard to determine, and it is not clear how long it would take to calculate the table entries that timed out. A standard laptop was not able to compute α_2 of the Balaban 11-cage in 1 hour. Part of the value of our theorems is that they give an efficient way to compute bounds for a parameter for which it may be infeasible to compute an exact value.

Appendix.1. $k = 2$

Graph name	Eq. (7)	Thm. 3.2	Thm. 4.2	α_k
Balaban 10-cage	73	43	32	17
Frucht graph	9	6	6	3
Meredith Graph	115	41	20	10
Moebius-Kantor Graph	8	10	10	4
Bidiakis cube	7	6	5	2
Gosset Graph	2	7	8	2
Balaban 11-cage	123	68	41	time
Gray graph	56	33	38	11
Nauru Graph	16	15	10	6
Blanusa First Snark Graph	16	10	8	4
Pappus Graph	9	11	14	3
Blanusa Second Snark Graph	16	10	8	4
Brinkmann graph	6	10	9	3
Harborth Graph	86	30	24	10
Perkel Graph	12	19	18	5
Harries Graph	73	43	32	17
Bucky Ball	86	35	23	12
Harries-Wong graph	73	43	32	17

Robertson Graph	4	9	6	3
Heawood graph	5	8	2	2
Cell 600	92	53	18	8
Cell 120	1018	351	302	time
Hoffman Graph	6	9	10	2
Sylvester Graph	8	14	10	6
Coxeter Graph	16	15	13	7
Holt graph	10	12	14	3
Szekeres Snark Graph	70	29	25	9
Desargues Graph	13	12	10	4
Horton Graph	177	60	50	24
Dejter Graph	91	64	44	16
Tietze Graph	6	6	5	3
Double star snark	34	17	12	6
Truncated Icosidodecahedron	211	75	60	26
Durer graph	9	6	5	2
Klein 3-regular Graph	54	32	22	12
Truncated Tetrahedron	6	6	5	3
Dyck graph	26	20	14	8
Klein 7-regular Graph	3	6	17	3
Tutte 12-Cage	132	78	44	time
Ellingham-Horton 54-graph	92	33	32	11
Tutte-Coxeter graph	20	18	10	6
Ellingham-Horton 78-graph	148	48	38	18
Ljubljana graph	132	70	44	26
Tutte Graph	76	28	21	10
F26A Graph	18	16	12	6
Watkins Snark Graph	74	30	25	9
Flower Snark	13	11	7	5
Markstroem Graph	29	14	11	6
Wells graph	6	12	22	2
Folkman Graph	11	12	10	3
Foster Graph	94	56	44	21
McGee graph	15	13	10	5
Franklin graph	6	7	6	2
Hexahedron	2	5	2	2
Dodecahedron	15	10	9	4
Icosahedron	2	3	7	2

Appendix.2. $k = 3$

Graph name	Eq. (7)	Thm. 3.2	Thm. 4.2	α_k

Balaban 10-cage	41	37	36	9
Frucht graph	4	5	6	2
Meredith Graph	85	35	45	7
Moebius-Kantor Graph	2	8	8	2
Balaban 11-cage	72	56	59	16
Gray graph	27	29	35	9
Nauru Graph	6	12	14	4
Blanusa First Snark Graph	8	8	8	2
Pappus Graph	3	9	11	3
Blanusa Second Snark Graph	9	7	8	2
Harborth Graph	70	27	20	6
Harries Graph	41	37	35	10
Bucky Ball	62	29	30	7
Harries-Wong graph	41	37	35	9
Cell 600	42	45	14	3
Cell 120	847	299	287	time
Hoffman Graph	2	8	11	2
Coxeter Graph	6	11	13	4
Szekeres Snark Graph	50	24	24	6
Desargues Graph	5	10	10	2
Horton Graph	162	51	50	14
Dejter Graph	42	57	56	8
Double star snark	19	13	15	4
Truncated Icosidodecahedron	180	64	60	18
Durer graph	4	4	7	2
Klein 3-regular Graph	28	24	29	7
Dyck graph	12	17	16	4
Tutte 12-Cage	72	67	77	21
Ellingham-Horton 54-graph	78	29	29	8
Tutte-Coxeter graph	7	16	20	5
Ellingham-Horton 78-graph	140	42	40	11
Ljubljana graph	80	60	63	17
Tutte Graph	62	23	21	6
F26A Graph	8	14	13	3
Watkins Snark Graph	54	24	24	6
Flower Snark	5	9	10	2
Markstroem Graph	19	11	10	3
Wells graph	2	7	13	2
Folkman Graph	4	10	15	2
Foster Graph	52	48	50	15
McGee graph	4	10	12	2
Dodecahedron	5	7	11	2

Appendix.3. $k = 4$

Graph name	Eq. (7)	Thm. 3.2	Thm. 4.2	α_k
Balaban 10-cage	21	40	32	5
Meredith Graph	63	39	20	5
Balaban 11-cage	37	60	39	9
Gray graph	17	31	14	3
Harborth Graph	55	27	13	4
Harries Graph	21	40	32	5
Bucky Ball	41	30	20	6
Harries-Wong graph	21	40	32	5
Cell 600	16	39	14	2
Cell 120	675	309	250	time
Szekeres Snark Graph	33	25	17	5
Desargues Graph	2	11	10	2
Horton Graph	144	55	26	8
Dejter Graph	20	59	16	2
Truncated Icosidodecahedron	151	70	40	11
Klein 3-regular Graph	14	25	22	4
Dyck graph	5	18	14	2
Tutte 12-Cage	38	72	44	9
Ellingham-Horton 54-graph	63	31	12	4
Ellingham-Horton 78-graph	129	44	24	6
Ljubljana graph	46	64	44	8
Tutte Graph	48	25	20	4
F26A Graph	3	14	12	2
Watkins Snark Graph	37	25	19	5
Markstroem Graph	11	11	6	3
Foster Graph	25	51	44	5
Dodecahedron	2	7	9	2