Isoperimetric Inequalities and Eigenvalues

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Abstract

An upper bound is given on the minimum distance between i subsets of same size of a regular graph in terms of the i-th largest eigenvalue in absolute value. This yields a bound on the diameter in terms of the i-th largest eigenvalue, for any integer i. Our bounds are shown to be asymptotically tight for explicit families of graphs having asymptotically optimal i-th largest eigenvalue. A recent result by Quenell relating the diameter, the second eigenvalue, and the girth of a regular graph is obtained as a byproduct.

Key words. eigenvalues, diameter, Chebychev polynomials, expanders

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1 Introduction

Many combinatorial properties of a graph are related to the spectrum of its adjacency matrix [2, 3, 4, 17]. The adjacency matrix A of an undirected graph is the $0-1$ matrix indexed by the vertices, and such that the entry (u, v) is equal to 1 if and only if (u, v) is an edge. Since the adjacency matrix of any graph H on n vertices is symmetric and real, its eigenvalues are real and will be denoted by $\lambda_0(H) \geq \lambda_1(H) \geq \cdots \geq \lambda_{n-1}(H)$. In this paper, we explore the relation between the spectrum of a graph and its isoperimetric properties. We focus our attention on the diameter, which is defined to be the maximum distance in H between any pair of vertices, and will be denoted by $D(H)$. The diameter plays an important role in network design, in parallel and distributed computing.

Let $\lambda = \lambda(H) = \max(\lambda_1, |\lambda_{n-1}|)$. It is known that if a graph is k-regular, then $\lambda_0 = k$ and $\lambda \leq k$, with equality if and only if the graph is disconnected or bipartite. Moreover, the graph is an expander if and only if [2] there exists a gap between k and λ_1. Thus, the existence of an upper bound on the diameter in terms of the eigenvalue gap is not surprising. Such a bound first appeared in [3], where it was shown that, when G is k-regular,

$$D(G) \leq 2\sqrt{\frac{2k}{(k-\lambda_1)}} \log_2 n. \tag{1}$$

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Chung [5] (see also [12]) established that

$$D(G) \leq \left\lfloor \frac{\log(n-1)}{\log(k/\lambda)} \right\rfloor + 1, \tag{2}$$

which beats Eq. 1 when λ is small. Eq. 2 was further improved in [6, 16], where it was shown that

$$D(G) \leq \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(k/\lambda)} \right\rfloor + 1. \tag{3}$$

In this paper, we establish isoperimetric bounds that are function of the subsequent eigenvalues and do not depend on the second eigenvalue. More precisely,

Theorem 1 *Let $G = (V, E)$ be an undirected k-regular graph and $\delta_0, \delta_1, \ldots, \delta_{n-1}$ the eigenvalues of its adjacency matrix, with $|\delta_0| \geq |\delta_1| \geq \ldots \geq |\delta_{n-1}|$. Let $d(X, Y)$ denote the distance between two subsets X and Y. If $|\delta_i| < k$ and $X_1, X_2, \ldots, X_{i+1}$ are $i+1$ subsets of V of same cardinality xn, then*

$$\min_{1 \leq j < h \leq i+1} d(X_j, X_h) \leq \left\lceil \frac{\cosh^{-1}(x^{-1}-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rceil + 1.$$

■

Eq. 2 is (up to an additive constant 1) a particular case of Theorem 1. We will use Theorem 1 to derive upper bounds on the diameter of G in terms of δ_i. In Section 3, we establish a lower bound on the size of $N^t(X)$, where X is a set of vertices and $N^t(X)$ is the set of nodes that can be reached from X by a path of length t, that is,

$$\underbrace{N(N(\ldots N(}_{t \text{ times}}X))\ldots).$$

The lower bound on $|N^t(X)|$ is a function of the size of X and of the second eigenvalue in absolute value λ of the graph. As a first corollary, we obtain an upper bound on the distance between two subsets of given size. As a second corollary, we get a simple proof of a recent result [15] relating the diameter, the girth, and λ. Section 3 combines ideas in [3, 12, 17]. In Section 4, we prove Theorem 1 and derive a relation between the diameter of a graph and its subsequent eigenvalues.

In Section 5, we study the tightness of the aforementioned bounds. For fixed n and k, the right-hand side of Eq. 3 is small when λ is small. It is known, however, that for any sequence $G_{n,k}$ of k-regular graphs on n vertices, $\liminf \lambda(G_{n,k}) \geq 2\sqrt{k-1}$ as n goes to infinity [2, 12, 14]. A Ramanujan graph is a k-regular graph where all eigenvalues not equal to $\pm k$ are at most $2\sqrt{k-1}$ in absolute value. Ramanujan graphs have been constructed explicitly in [12, 13]. It is known [12] (and in the non-bipartite case, follows from Eq. 3) that the diameter of a k-regular Ramanujan graph on n vertices is at most $(2+o(1))\log_{k-1} n$. On the other hand, it is easy to see that it is at least $(1+o(1))\log_{k-1} n$. To our knowledge, these are the best known asymptotic bounds on the diameter of the known explicit families of Ramanujan graphs [12, 13]. In Section 5, for many integers k, we construct explicitly a family of k-regular graphs with $\lambda = (2+o(1))\sqrt{k-1}$ and diameter $(2+o(1))\log_{k-1} n$. We generalize our construction to show that our bound on the diameter in terms of δ_i is asymptotically tight for explicit families of graphs having asymptotically optimal i-th largest eigenvalue.

Section 3 is based on [9]. A longer version of the paper appears in [10].

2 Notation and background

Let $G = (V, E)$ be an undirected k-regular graph on n vertices. Denote by $L^2(V)$ the set of real valued functions on V and $L_0^2(V) = \{f \in L^2(V);\ \sum_{v\in V} f(v) = 0\}$. As usual, we define the scalar product of two vectors f and g of $L^2(V)$ by

$$f \cdot g = \sum_{v\in V} f(v)g(v),$$

and the euclidean norm of a vector f by $||f|| = \sqrt{f \cdot f}$. The adjacency matrix A of G defines a linear operator in $L^2(V)$ that maps every vector $f \in L^2(V)$ to the vector Af defined by

$$(Af)(v) = \sum_{(v,w)\in E} f(w). \tag{4}$$

This operator is selfadjoint since $\forall f, g \in L^2(V)$, we have

$$(Af) \cdot g = f \cdot (Ag) = \sum_{(v,w)\in E} f(v)g(w). \tag{5}$$

For any subset W of V, we denote by χ_W the characteristic vector of W:

$$\chi_W(v) = \begin{cases} 1 & \text{if } v \in W \\ 0 & \text{otherwise.} \end{cases}$$

The support of a vector $f \in L^2(V)$ is defined to be the set of nodes v for which $f(v) \neq 0$. We sometimes order the eigenvalues of a graph H according to their absolute values and denote them by $\delta_i(H)$, so that $|\delta_0(H)| \geq |\delta_1(H)| \geq \cdots \geq |\delta_{n-1}(H)|$. Denote by $\lambda_i(B)$ the $(i+1)$-st largest eigenvalue of a matrix B with real eigenvalues. The l_1-norm $||h||_1$ of a vector h is defined to be $\sum_{v\in V} |h(v)|$.

The Chebychev polynomial of degree t is the unique polynomial P_t satisfying the equation

$$P_t(\cosh z) = \cosh(tz), \tag{6}$$

for any complex number z. Chebychev polynomials have been used in [12] in the study of expanders. The following facts easily follow from Eq. 6:

Fact 1 *For any complex number z, we have $P_t(-z) = (-1)^t P_t(z)$.* ■

Fact 2 *For any real number s between -1 and 1, we have $|P_t(s)| \leq 1$.* ■

3 Bounds on the distance between two subsets

The following theorem generalizes a result of Tanner [17]. We use a similar proof-technique.

Theorem 2 *Let $G = (V, E)$ be a k-regular graph on n vertices and λ its second largest eigenvalue in absolute value. For any subset X of V and any integer $t \geq 1$, we have*

$$|N^t(X)| \geq \frac{{P_t}^2(k/\lambda)|X|}{1 + ({P_t}^2(k/\lambda) - 1)|X|/n}. \tag{7}$$

If G is a non-bipartite Ramanujan graph of degree k, then

$$\frac{|N^t(X)|}{|X|} \geq \frac{((k-1)^t + 1)^2}{4(k-1)^t + ((k-1)^t - 1)^2|X|/n} \geq \frac{(k-1)^t}{4 + (k-1)^t|X|/n}.$$

In particular, if $|X|/n$ is at most $4(k-1)^{-t-1}$, then $|N^t(X)| \geq (k-2)(k-1)^{t-1}|X|/4$.

Proof Denote by f be the characteristic vector of X. Let $f = \bar{f} + f_0$, where $\bar{f}$ is a constant vector and $f_0 \in L_0^2(V)$. It follows from Fact 1 that P_t is of the form $P_t(s) = c_t s^t + c_{t-2} s^{t-2} + \cdots$, and so $P_t(\lambda^{-1}A)\ f = c_t \lambda^{-t} A^t f + c_{t-2}\lambda^{-(t-2)} A^{t-2} f + \cdots$. This implies that the support of the vector $g = P_t(\lambda^{-1}A)\ f$ is a subset of $N^t(X)$. This is because the support of the vector $A^l f$ is $N^l(X)$, and $N^t(X) \supseteq N^{t-2}(X) \supseteq \cdots$. We will obtain a lower bound on the size of $N^t(X)$ by comparing the norm of g to its sum of coordinates. Since $A\bar{f} = k\bar{f}$, we have

$$g = P_t(\lambda^{-1}A)\ \bar{f} + P_t(\lambda^{-1}A)\ f_0 = P_t(k/\lambda)\ \bar{f} + P_t(\lambda^{-1}A)\ f_0.$$

Eq. 4 shows that $L_0^2(V)$ is invariant under A, and so $P_t(\lambda^{-1}A)\ f_0 \in L_0^2(V)$. The eigenvalues of the restriction $A_{|L_0^2(V)}$ of A to $L_0^2(V)$ are λ_i, for $1 \leq i \leq n-1$. By the Pythagorean theorem, we have

$$||g||^2 = {P_t}^2(k/\lambda)||\bar{f}||^2 + ||P_t(\lambda^{-1}A)\ f_0||^2 \leq {P_t}^2(k/\lambda)||\bar{f}||^2 + ||f_0||^2.$$

The second inequality follows from the fact that the operator $P_t(\lambda^{-1}A_{|L_0^2(V)})$ is selfadjoint and its eigenvalues $P_t(\lambda_i/\lambda)$, $1 \leq i \leq n-1$, are at most 1 in absolute value (Fact 2.) It follows from the Cauchy-Schwartz inequality that

$$\begin{aligned} |\chi_{N^t(X)} \cdot g|^2 &\leq |N^t(X)|\ ({P_t}^2(k/\lambda)||\bar{f}||^2 + ||f_0||^2) \\ &= |N^t(X)|\ ({P_t}^2(k/\lambda)||\bar{f}||^2 + |X| - ||\bar{f}||^2). \end{aligned} \tag{8}$$

The sum of coordinates $\chi_{N^t(X)} \cdot g$ of g is equal to $P_t(k/\lambda)|X|$. This is because the sum of coordinates of Ah is equal to k times the sum of coordinates of h, as follows immediately from Eq. 4. By replacing the terms $\chi_{N^t(X)} \cdot g$ and $||\bar{f}||$ by their values in Eq. 8, we get

$$\frac{|X|}{|N^t(X)|} \leq \frac{|X|}{n} + \frac{1 - |X|/n}{{P_t}^2(k/\lambda)}, \tag{9}$$

which implies Eq. 7.

If G is a non-bipartite Ramanujan graph, we can replace λ by $2\sqrt{k-1}$ in Eq. 7. We have

$$\begin{aligned} P_t\left(\frac{k}{2\sqrt{k-1}}\right) &= P_t\left(\cosh\left(\frac{\ln(k-1)}{2}\right)\right) \\ &= \cosh\left(t\frac{\ln(k-1)}{2}\right) \\ &= \frac{(k-1)^{t/2} + (k-1)^{-t/2}}{2}. \end{aligned}$$

The rest of the theorem follows by an easy calculation. ■

Corollary 1 *If G is non-bipartite and X and Y are two subsets of V of cardinality xn and yn respectively,*

$$d(X,Y) \leq \left\lfloor \frac{\cosh^{-1}\sqrt{(x^{-1}-1)(y^{-1}-1)}}{\cosh^{-1}(k/\lambda)} \right\rfloor + 1.$$

Proof If t is an integer such that the right-hand side of Eq. 9 is less than $|X|/(n-|Y|)$, then $|N^t(X)| > n - |Y|$, and so the distance between X and Y is at most t. Let $\theta = \cosh^{-1}(k/\lambda)$, so that $P_t(k/\lambda) = \cosh(t\theta)$. We want t to be such that

$$x + \frac{1-x}{\cosh^2(t\theta)} < \frac{x}{1-y}.$$

Solving for t yields the desired bound on $d(X, Y)$. ■

By applying Corollary 1 to any pair of subsets consisting of single vertices, we obtain Eq. 3, which has already been established in [6, 16].

Corollary 2 ([15]) *If G is non-bipartite,*

$$D(G) \leq \left\lfloor \frac{\cosh^{-1}\left(\frac{n}{k(k-1)^{r-1}} - 1\right)}{\cosh^{-1}(k/\lambda)} \right\rfloor + 2r + 1,$$

where $r = \lfloor (c(G) - 1)/2 \rfloor$ is the injectivity radius *of G.*

Proof We remind the reader that $c(G)$ is the girth of G. Consider any pair of vertices u and v. The subsets $N^r(\{u\})$ and $N^r(\{v\})$ have size $k(k-1)^{r-1}$. By applying Corollary 1 to these subsets, we get

$$d(N^r(\{u\}, N^r(\{v\}) \leq \left\lfloor \frac{\cosh^{-1}\left(\frac{n}{k(k-1)^{r-1}} - 1\right)}{\cosh^{-1}(k/\lambda)} \right\rfloor + 1.$$

Corollary 2 follows immediately. ■

Corollary 2 has first been established by Quenell [15].

4 Relation with subsequent eigenvalues

We now show the following special case of Theorem 1.

Theorem 3 *If $G = (V, E)$ is a k-regular graph and $|\delta_i| < k$, then for any set S of $i + 1$ vertices of V,*

$$\min_{\{u,v\} \subset S, u \neq v} d(u, v) \leq \left\lceil \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rceil + 1.$$

Proof Let e_j be an eigenvector of A corresponding to the eigenvalue δ_j, and let $f \in L^2(V)$ be a nonzero function nul on $V - S$, and such that f belongs to the vector space E_i spanned by $e_i, e_{i+1}, \ldots, e_{n-1}$. The existence of f follows from the fact that $\dim L^2(S) = i+1$ and $\dim E_i = n - i$. Given an integer t, let $g = P_t(|\delta_i|^{-1}A)f$. The vector space E_i is invariant under A, and the eigenvalues of the restriction of A to E_i are δ_h, for $i \leq h \leq n-1$. By a similar reasoning to the proof of Theorem 2 the eigenvalues $P_t(\delta_h/|\delta_i|)$, for $i \leq h \leq n-1$, of the restriction of the operator $P_t(|\delta_i|^{-1}A)$ to E_i, are at most 1 in absolute value, and so $||g|| \leq ||f||$. Assume now that $\min_{\{u,v\} \subset S, u \neq v} d(u, v) > 2t$. Then the vectors $P_t(|\delta_i|^{-1}A)\chi_{\{u\}}$, for $u \in S$, have disjoint supports, and so

$$\begin{aligned} ||g||_1 &= ||\sum_{u \in S} f(u)\ P_t(|\delta_i|^{-1}A)\chi_{\{u\}}||_1 \qquad (10) \\ &= \sum_{u \in S} |f(u)|\ ||P_t(|\delta_i|^{-1}A)\chi_{\{u\}}||_1 \\ &\geq \sum_{u \in S} |f(u)| P_t(k/|\delta_i|) \\ &= P_t(k/|\delta_i|)||f||_1. \end{aligned}$$

The third equation follows from the fact that the sum of coordinates of the vector $P_t(|\delta_i|^{-1}A)\chi_{\{u\}}$ is $P_t(k/|\delta_i|)$.

On the other hand,

$$\begin{aligned} ||g||_1 &\leq \sqrt{n}||g|| \\ &\leq \sqrt{n}||f|| \\ &\leq \sqrt{n/2}||f||_1. \end{aligned} \tag{11}$$

The first inequality is a consequence of the Cauchy-Schwartz inequality. The last inequality is valid because $f \in L_0^2(V)$. Indeed,

$$\begin{aligned} ||f||^2 &= ||f^+||^2 + ||f^-||^2 \\ &\leq ||f^+||_1^2 + ||f^-||_1^2 \\ &= \frac{||f||_1^2}{2}, \end{aligned}$$

where $f^+ = \max(f, 0)$ and $f^- = \min(f, 0)$.

Combining Eqs. 10 and 11 shows that

$$P_t(k/|\delta_i|) \leq \sqrt{n/2}. \tag{12}$$

Eq. 12 does not hold for $t = \lfloor l \rfloor + 1$, where

$$l = \frac{\cosh^{-1}\sqrt{n/2}}{\cosh^{-1}(k/|\delta_i|)},$$

and so $\min_{\{u,v\}\subset S, u\neq v} d(u,v) \leq 2\lfloor l \rfloor + 2$.

This bound can be slighlty improved when l is an integer. Indeed, let $t = l$ and assume as before that $\min_{\{u,v\}\subset S, u\neq v} d(u,v) > 2l$. Since $P_l(k/|\delta_i|) = \sqrt{n/2}$, all terms of Eq. 11 are equal (otherwise, Eq. 12 would be a strict inequality for $t = l$.) This implies that the support of g is equal to V. It follows that every point in G is at distance at most l from some point in S, and so $\min_{\{u,v\}\subset S, u\neq v} d(u,v) \leq 2l + 1$. We conclude (whether l is an integer or not) that $\min_{\{u,v\}\subset S, u\neq v} d(u,v) \leq \lceil 2l \rceil + 1$. The lemma follows by noting that $2\cosh^{-1}\sqrt{n/2} = \cosh^{-1}(n-1)$. ■

Theorem 1 can be shown in a similar way to Theorem 3. The main difference is that we consider a function f in $L^2(\cup_{j=1}^{i+1} X_j)$ which is constant on each X_j.

Corollary 3 *If G is a k-regular connected graph and $|\delta_i| < k$, where i is an integer between 1 and $n-1$,*

$$D(G) \leq i\left\lceil \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(k/|\delta_i|)} \right\rceil + 2i - 1. \tag{13}$$

If r is the injectivity radius of G then

$$D(G) \leq i\left\lceil \frac{\cosh^{-1}(\frac{n}{k(k-1)^{r-1}} - 1)}{\cosh^{-1}(k/|\delta_i|)} \right\rceil + 2ir + 2i - 1.$$

Proof Let u and v be two vertices at maximal distance in G. Consider a shortest path between u and v. There exists a sequence of $i+1$ vertices $u_0 = u, u_1, \ldots, u_i = v$ on this path at distance at least $\lfloor D(G)/i \rfloor$ from each other. By applying Theorem 3 to the set $\{u_0, u_1, \ldots, u_i\}$, we get the first bound on $D(G) = d(u,v)$. The second bound can be established similarly by applying Theorem 1 to the subsets $N^r(\{u_j\})$. ■

5 Tightness of bounds

We show that, for any fixed i, Eq. 13 is asymptotically tight for certain families of k-regular graphs having asymptotically optimal $|\delta_i|$. We use techniques similar to [11]. We start with the case $i = 1$.

Theorem 4 *For any integer k such that $k-1$ is prime congruent to 1 modulo 4, there exists an infinite explicit family of k-regular graphs G_n on n vertices with $\lambda(G_n) = (2+o(1))\sqrt{k-1}$ and diameter $(2+o(1))\log_{k-1} n$.*

Proof Let H be a non-bipartite k-regular Ramanujan graph on n' vertices, of girth at least $(2/3+o(1))\log_{k-1} n'$. Such a graph has been explicitly constructed in [12]. Consider two identical trees T and T' of depth $l = \lfloor \log_{k-1} m - 2 \rfloor$, where $m = \lfloor n'/\log n' \rfloor$, and whose internal nodes have degree k. All leaves in T and T' have same depth, and H, T and T' are disjoint. Let F be a set of edges in H at distance at least $r = \Omega(\log_{k-1}(n'/m))$ from each other, and such that the number of edges in F is equal to the number of leaves in T (F can be found greedily.) Identify one endpoint of each edge in F to a leaf in T, and the other endpoint to a leaf in T', in such a way that all leaves of T and T' are identified to distinct vertices in H. By deleting the edges in F, we obtain a k-regular graph G on n vertices. The diameter of G is at least twice the depth of T, which is $(1+o(1))\log_{k-1} n$. We show that $\lambda(G) = (2+o(1))\sqrt{k-1}$. Eq. 3 then implies that the diameter of G is equal to $(2+o(1))\log_{k-1} n$. We only need to show the upper bound on $\lambda' = \lambda(G)$, since $\lambda' \geq (2+o(1))\sqrt{k-1}$ for any family of k-regular graphs as the number of vertices goes to infinity [2, 12, 14]. Let A be the adjacency matrix of H and A' the adjacency matrix of G. We assume that $\lambda' > 2\sqrt{k-1}$ (otherwise, we are done), and let $\lambda' = 2\sqrt{k-1}\cosh\theta'$, with $\theta' > 0$. We also assume that $\lambda' = \lambda_1(G)$. The case $\lambda' = -\lambda_{n-1}(G)$ can be treated similarly. Denote by $V(G)$, $V(H)$, $V(T)$ and $V(T')$ the vertex sets of G, H, T and T', respectively.

Let $g \in L^2(V(G))$ be an eigenvector of A' corresponding to λ', and let $f \in L^2(V(H))$ be the vector of $L^2(V(H))$ that coincides with g on $V(H)$. By Eq. 5, we have

$$\begin{aligned}
\lambda'||g||^2 &= g \cdot A'g \qquad (14)\\
&= f \cdot Af - \sum_{(u,v)\in F} g(u)g(v) + \sum_{(u,v)\in E(T)} g(u)g(v) + \sum_{(u,v)\in E(T')} g(u)g(v)\\
&\leq f \cdot Af + (2\sqrt{k-1}+1) \sum_{v\in V(T)\cup V(T')} g(v)^2.
\end{aligned}$$

The third equation follows from the fact that the largest eigenvalue of T is at most $2\sqrt{k-1}$. Since $g \in L_0^2(V(G))$,

$$\sum_{w\in V(H)} f(w) = -\sum_{w\in(V(T)\cup V(T'))-V(H)} g(w).$$

We need the following lemma, whose proof can be found in [11].

Lemma 1 *If $H = (V, E)$ is k-regular on n vertices, then for any $f \in L^2(V)$, we have*

$$f \cdot Af \leq \lambda_1(H)||f||^2 + \frac{k-\lambda_1(H)}{n}\Big(\sum_{v\in V} f(v)\Big)^2.$$

■

Using Lemma 1 and the Cauchy-Schwartz inequality, we get

$$f \cdot Af \quad \leq \quad \lambda_1(H)||f||^2 + \frac{k}{n}\left(\sum_{w\in(V(T)\cup V(T'))-V(H)} g(w)\right)^2$$

$$\begin{aligned} &\le 2\sqrt{k-1}\left(||g||^2 - \sum_{w\in(V(T)\cup V(T'))-V(H)} g(w)^2\right) + \frac{2km}{n}\sum_{w\in(V(T)\cup V(T'))-V(H)} g(w)^2 \\ &\le 2\sqrt{k-1}||g||^2, \end{aligned}$$

for sufficiently large n. Combining this with Eq. 14 yields

$$\lambda'||g||^2 \le 2\sqrt{k-1}\left(||g||^2 + 2\sum_{v\in V(T)\cup V(T')} g(v)^2\right). \tag{15}$$

Next, we show that $\sum_{v\in V(T)\cup V(T')} g(v)^2$ is small compared to $||g||^2$. We use the following lemma, whose proof is implicit in [11], and given in detail in [10, Sec. 5.3].

Lemma 2 *Let $G = (V, E)$ be a k-regular graph and g an eigenvector of G corresponding to the eigenvalue $2\sqrt{k-1}\cosh\theta$, with $\theta > 0$. If l and l' are two nonegative integers with $l < l'$, and u is a node of G such that the subgraph induced on the set of nodes at distance at most l' from u is a tree, then*

$$\sum_{v\in V:d(u,v)=l} g(v)^2 \le e^{-2(l'-l)\theta}||g||^2.$$

■

By applying Lemma 2 in the case where u is the root of T and $l' = l + r$, we see that

$$||g||^2 \ge e^{2r\theta'} \sum_{v\in V(T):d(u,v)=l} g(v)^2.$$

By applying the lemma to $l-1, l-2, \ldots, 0$, we obtain

$$||g||^2 \ge e^{2r\theta'}(1-e^{-2\theta'}) \sum_{v\in V(T)} g(v)^2.$$

Combining this with Eq. 15 yields

$$\cosh\theta' \le 1 + 4\frac{e^{-2r\theta'}}{1-e^{-2\theta'}}.$$

As a consequence, $\theta' \le 2(\log r)/r$, for large n, and so $\lambda' \le (2+o(1))\sqrt{k-1}$. ■

It is known (see, e.g. [8]) that $|\delta_i(G_n)| \ge (2+o(1))\sqrt{k-1}$ for any family of k-regular graphs, as the number of vertices goes to infinity. For graphs such that $|\delta_i(G_n)| = (2+o(1))\sqrt{k-1}$, Eq. 13 implies that $D(G) \le (2+o(1))i\log_{k-1} n$. The following theorem, obtained jointly with Noga Alon [1], shows that this bound is tight for some families of graphs. The proof uses the max-min characterization of the eigenvalues.

Fact 3 *If B is a selfadjoint operator in a vector space L and $\lambda_i(B)$ its $(i+1)$-st largest eigenvalue, then*

$$\lambda_i(B) = \max_H \min_{g\in H-\{0\}} \frac{g\cdot Bg}{||g||^2},$$

where H ranges over the vector subspaces of L of dimension $i+1$. ■

Theorem 5 *If $k-1$ is a prime congruent to 1 modulo 4 and i is a positive integer, there exists an infinite explicit family of k-regular graphs G_n on n vertices of diameter $(2+o(1))i\log_{k-1} n$ and such that $\delta_j(G_n) = k - O(1/n)$, for $0 \le j \le i-1$, and $|\delta_i(G_n)| = (2+o(1))\sqrt{k-1}$.*

Proof Consider a family (F_n) of k-regular graphs satisfying the conditions of Theorem 4, and whose girth goes to infinity as n goes to infinity. Such a family can be constructed explicitly, as shown in the proof proof of Theorem 4. We construct the graphs G_n (for n multiple of i and such that $F_{n/i}$ exists) as follows: consider i distinct copies of $F_{n/i}$, denoted by $F^j_{n/i}$, for $1 \leq j \leq i$. Let (u_j, v_j) be a pair of vertices in $F^j_{n/i}$ at maximal distance from each other, and let u'_j (resp. v'_j) be a vertex of $F^j_{n/i}$ adjacent to u_j (resp. v_j). We form the graph G_n by connecting v_j (resp. v'_j) to u_{j+1} (resp. u'_{j+1}), for $1 \leq j \leq i-1$, and deleting the edge between u_j and u'_j, for $2 \leq j \leq i$, and the edge between v_j and v'_j, for $1 \leq j \leq i-1$. Clearly, the diameter of G_n is $(2+o(1))i \log_{k-1} n$.

The eigenvalues of the union of the $F_{n/i}$ satisfy the conditions of Theorem 5. Indeed, the first i eigenvalues are equal to k, and the $(i+1)$-st largest eigenvalue in absolute value is, in absolute value, equal to $\lambda(F_{n/i}) = (2+o(1))\sqrt{k-1}$. This is because the eigenvalues of a graph are the union of the eigenvalues of its connected components. We now show that the $i+1$ largest eigenvalues of G_n are close to the $i+1$ largest eigenvalues of the union of the $F_{n/i}$.

Let A (resp. A') be the adjacency matrix of the union of the $F_{n/i}$ (resp. G_n.) Let V_j be the vertex set of $F^j_{n/i}$, and V the vertex set of G_n. It follows from Eq. 5 that for any $f \in L^2(V)$,

$$\begin{aligned} |A'f \cdot f - Af \cdot f| &= 2\Big|\sum_{j=1}^{i-1}(f(v_j)f(u_{j+1}) + f(v'_j)f(u'_{j+1}) - f(u_{j+1})f(u'_{j+1}) - f(v_j)f(v'_j))\Big| \quad (16) \\ &\leq 2\sum_{j=1}^{i}\left(f(u_j)^2 + f(u'_j)^2 + f(v_j)^2 + f(v'_j)^2\right). \end{aligned}$$

Denote by H the subspace of $L^2(V)$ of vectors wich are constant on each V_j. Eq. 16 shows that, for each $f \in H$, we have $A'f \cdot f \geq (k - 8i/n)||f||^2$. Since $\dim H = i$, it follows from Fact 3 that $\lambda_{i-1}(G)$ is lower bounded by $k - 8i/n$, and so are $|\delta_0|, |\delta_1|, \ldots, |\delta_{i-1}|$.

We now show that $|\delta_i(G_n)| = (2+o(1))\sqrt{k-1}$. We only need to show the upper bound, as the lower bound holds for any family of k-regular graphs [8]. Let r be the injectivity radius of G_n. It is at least the injectivity radius of $F_{n/i}$. If $|\delta_i| \leq 2\sqrt{k-1}$, we are done, so we will assume in the rest of the proof that $\delta_i > 2\sqrt{k-1}$ (the case where $\delta_i < -2\sqrt{k-1}$ can be treated similarly.) Let $\delta_i = 2\sqrt{k-1}\cosh\theta$, with $\theta > 0$, and e_h an eigenvector of A' corresponding to δ_h, for $0 \leq h \leq i$. Since $|\delta_h| \geq \delta_i$, for $0 \leq j \leq i$, it follows from Lemma 2 that $|e_h(u_j)| \leq e^{-r\theta}||e_h||$. Using the Cauchy-Schwartz inequality and the orthogonality of the vectors e_h, this implies that for any vector $f \in \mathrm{Vect}(e_0, e_1, \ldots, e_i)$,

$$|f(u_j)| \leq \sqrt{i+1}e^{-r\theta}||f||. \quad (17)$$

Indeed, if $f = \sum_{h=0}^{i} c_h e_h$, then

$$\begin{aligned} f(u_j)^2 &\leq (i+1)\sum_{h=0}^{i} {c_h}^2 e_h(u_j)^2 \\ &\leq (i+1)e^{-2r\theta}\sum_{h=0}^{i} {c_h}^2||e_h||^2 \\ &= (i+1)e^{-2r\theta}||f||^2. \end{aligned}$$

Eq. 17 remains valid if u_j is replaced by u'_j, v_j or v'_j. Since the vector space $\mathrm{Vect}(e_0, e_1, \ldots, e_i)$ is of dimension greater than H, it intersects $H^\perp - \{0\}$. Let g be an element of this intersection. Since the restriction of g to each V_j belongs to $L^2_0(V_j)$,

$$||Ag||^2 \leq \lambda(F_{n/i})^2||g||^2 \leq (4+o(1))(k-1)||g||^2.$$

Combining this with Eq. 17 applied to the vector $f = A'g$ yields

$$\begin{aligned} ||A'g||^2 &\leq ||Ag||^2 + \sum_{j=1}^{i} (A'g)(u_j)^2 + (A'g)(u'_j)^2 + (A'g)(v_j)^2 + (A'g)(v'_j)^2 \\ &\leq (4 + o(1))(k-1)||g||^2 + 4i(i+1)e^{-2r\theta}||A'g||^2. \end{aligned} \tag{18}$$

But since $g \in \mathrm{Vect}(e_0, e_1, \ldots, e_i)$, we have $||A'g||^2 \geq {\delta_i}^2 ||g||^2$. Combining this with Eq. 18 shows that

$$\cosh^2\theta \leq 1 + o(1) + 4i(i+1)e^{-2r\theta}\cosh^2\theta,$$

which implies that $\theta = o(1)$, since $r = \omega(1)$. We conclude that $|\delta_i| \leq (2 + o(1))\sqrt{k-1}$. ■

Concluding Remark

The results in Sections 3– 4 (including Theorem 1) can be easily extended to general graphs, using the techniques in [6]. This yields bounds in terms of the eigenvalues of the laplacian. Recently, other generalizations and extensions of our results, notably to continuous spaces, have been accomplished in [7].

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