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A General Spectral Bound for Distant Vertex Subsets

M. A. FIOL†

Departament de Matemàtica Aplicada i Telemàtica, Universitat Politècnica de Catalunya, Jordi Girona 1-3, Mòdul C3, Campus Nord, 08034 Barcelona, Spain
(e-mail: fiol@mat.upc.es)

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A general spectral bound for the sizes of some vertex subsets, which are mutually at a given minimum distance in a graph, is derived. This unifies and improves some previous results. Some applications to the study of certain metric parameters of the graph are then discussed.

1. Preliminaries

Let $\Gamma = (V, E)$ be a (finite and simple) connected graph on $n := |V|$ vertices. The distance between two vertices $u, v \in V$ is denoted by $\mathrm{dist}(u, v)$; and the distance between two vertex subsets $U_1, U_2 \subset V$ is defined as

$$\mathrm{dist}(U_1, U_2) := \min_{u \in U_1, v \in U_2} \{\mathrm{dist}(u, v)\}.$$

The notation $\bar{U}$ is used to denote the complement of the set U in V. Let $\boldsymbol{A} = \boldsymbol{A}(\Gamma)$ be the adjacency matrix of Γ, with elements $a_{uv} = 1$ if $u \sim v$, that is, $uv \in E$, and $a_{uv} = 0$ otherwise. Its eigenvalues are denoted by $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, including multiplicities. Since Γ is supposed to be connected and nontrivial ($n > 1$), the Perron–Frobenius theorem ensures that λ_1 is simple, positive (in fact, it coincides with the *spectral radius* $r(\boldsymbol{A})$), and with positive eigenvector $\boldsymbol{v}$. Moreover, $\lambda_n < 0$. Here we suppose that $\boldsymbol{v}$ is normalized in such a way that its minimum entry is 1. In particular, when Γ is regular, such an eigenvector is just the all-1 vector, here represented by $\boldsymbol{j}$. When we are interested in the set of distinct eigenvalues, we denote it by

$$\mathrm{ev}\,\Gamma \equiv \mathrm{ev}\,\boldsymbol{A} := \{\theta_0 > \theta_1 > \cdots > \theta_d\}$$

(note that $\theta_0 = \lambda_1$ and $\theta_d = \lambda_n$). From the positive eigenvector $\boldsymbol{v}$, we consider the map

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$\boldsymbol{\rho} : 2^V \to \mathbb{R}^n$ defined by $\boldsymbol{\rho}U := \sum_{u\in U} v_u \boldsymbol{e}_u$ for any $U \neq \emptyset$, where $\boldsymbol{e}_u$ represents the uth canonical (column) vector, and $\boldsymbol{\rho}\emptyset := \mathbf{0}$. Note that, with $\boldsymbol{\rho}u := \boldsymbol{\rho}\{u\}$, we have $\|\boldsymbol{\rho}u\| = v_u$, so that we can see $\boldsymbol{\rho}$ as a function that assigns weights to the vertices of Γ, and 'regularize' the graph since $\frac{1}{v_u}\sum_{v\sim u} v_v = \theta_0$ for any vertex u. Accordingly, for any vertex subset $U \subset V$, we will refer to the square norm $w := \|\boldsymbol{\rho}U\|^2$ as the *weight* of U. This approach has been used in recent work to extend some algebraic results from regular graphs to general graphs. See, for example, [8, 10, 11].

As above, let Γ be a graph with $\operatorname{ev}\Gamma = \{\theta_0 > \theta_1 > \cdots > \theta_d\}$. The alternating polynomials, introduced in [10], can be thought of as the discrete version of the Chebyshev polynomials. For any integer $0 \leqslant k \leqslant d-1$, the *$k$-alternating polynomial* P_k, is the (unique) polynomial of degree k satisfying

$$P_k(\theta_0) = \max_{p\in\mathbb{R}_k[x]}\{p(\theta_0) : \|p\|_\infty \leqslant 1\}, \tag{1.1}$$

where $\|p\|_\infty := \max_{1\leqslant i\leqslant d} |p(\theta_i)|$. Thus, we obviously have $P_0 = 1$. Otherwise, for $k \geqslant 1$, it was proved in [10] that the k-alternating polynomial is characterized by taking $k+1$ alternating values ± 1 at $\operatorname{ev}\Gamma \setminus \{\theta_0\}$, with $P_k(\theta_1) = 1$ and $P_k(\theta_d) = (-1)^k$. Moreover,

$$1 < P_1(\theta_0) < P_2(\theta_0) < \cdots < P_{d-1}(\theta_0). \tag{1.2}$$

In particular, for the values $k = 1$ and $k = d-1$, the above characterization gives $P_1 = 2\frac{x-\theta_1}{\theta_1-\theta_d} + 1$, and the $(d-1)$-alternating polynomial is defined by $P_{d-1}(\theta_i) = (-1)^{i+1}$, $1 \leqslant i \leqslant d$. Thus, using Lagrange interpolation in the second case, we get

$$P_1(\theta_0) = 2\frac{\theta_0-\theta_1}{\theta_1-\theta_d} + 1, \qquad P_{d-1}(\theta_0) = \sum_{i=1}^{d} \frac{\pi_0}{\pi_i} \tag{1.3}$$

where the π_is are the moment-like parameters defined by

$$\pi_i := \prod_{j=0, j\neq i}^{d} |\theta_i - \theta_j|, \qquad 0 \leqslant i \leqslant d.$$

In general, it was shown in [10] that the k-alternating polynomial P_k can be found by solving a simple linear programming problem. Some particular cases of these polynomials were used by van Dam and Haemers [5, 4] in the same context. In fact, they constitute a standard tool in the theory of uniform approximations of continuous functions.

The *Kronecker product* of two matrices $\boldsymbol{A} = (a_{ij})$ and $\boldsymbol{B}$, denoted by $\boldsymbol{A} \otimes \boldsymbol{B}$, is obtained by replacing each entry a_{ij} with the matrix $a_{ij}\boldsymbol{B}$, for all i and j. If $\boldsymbol{u}$ and $\boldsymbol{v}$ are eigenvectors of $\boldsymbol{A}$ and $\boldsymbol{B}$, with corresponding eigenvalues λ and μ, respectively, then $\boldsymbol{u} \otimes \boldsymbol{v}$ (seeing $\boldsymbol{u}$ and $\boldsymbol{v}$ as matrices) is an eigenvector of $\boldsymbol{A} \otimes \boldsymbol{B}$, with eigenvalue $\lambda\mu$.

We finally recall that the spectral radii of two (nonnegative) matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ such that $\boldsymbol{A} \geqslant \boldsymbol{B}$ (which means that $\boldsymbol{A} - \boldsymbol{B}$ is componentwise nonnegative) coincide with their respective maximum eigenvalues and satisfy $r(\boldsymbol{A}) \geqslant r(\boldsymbol{B})$.

A brief sketch of the contents of the paper follows. Our main result is in Section 2, where we derive a new bound for the weights (or sizes) of some vertex subsets, which are mutually at a given minimum distance in a graph, in terms of its distinct eigenvalues. This result unifies and improves a number of similar bounds recently given in the literature by

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different authors; see [3, 4, 5, 7, 8, 9, 14]. Some applications of such a result are discussed in Section 3.

2. A general bound for distant subsets

In this section we derive our main result. As stated above, this can be thought of as a spectral bound for the weights of some vertex subsets that are at a given minimum distance from each other.

Theorem 2.1. *Let Γ be a graph on n vertices, with eigenvalues $\operatorname{ev}\Gamma = \{\theta_0 > \theta_1 > \cdots > \theta_d\}$. For a given graph G with vertices $1, 2, \ldots, N$, and eigenvalues $\operatorname{ev} G = \{\eta_0 > \eta_1 > \cdots > \eta_e\}$, assume that there exist some vertex subsets $U_1, U_2, \ldots, U_N$ of Γ such that $\operatorname{dist}(U_i, U_j) > k$ for some integer $k \geqslant 1$ and any vertices i, j adjacent in G. Let p be a polynomial of degree k such that $p(\theta_0) > 0$. Then, for any given positive reals $\alpha_1, \alpha_2, \ldots, \alpha_N$, we have*

$$\frac{p(\theta_0)}{|\min \eta p(\theta)|} \leqslant \Psi := \frac{\sum_{i=1}^{N} \alpha_i^2 \|\boldsymbol{\rho} U_i\|^2 \|\boldsymbol{\rho} \bar{U}_i\|^2}{\sum_{i\sim j} 2\alpha_i \alpha_j \|\boldsymbol{\rho} U_i\|^2 \|\boldsymbol{\rho} U_j\|^2}, \tag{2.1}$$

where $\min \eta p(\theta) := \min\{\eta p(\theta) : \eta \in \operatorname{ev} G, \theta \in \operatorname{ev}\Gamma \setminus \{\theta_0\}\}$.

Proof. Let us consider an orthonormal basis of the vector space $\ell^2(V(G)) \cong \mathbb{R}^N$ consisting of eigenvectors of $\boldsymbol{A}(G)$, say $\boldsymbol{\phi}_r := (\phi_{1r}, \ldots, \phi_{Nr})^\top$, with corresponding eigenvalues μ_r, $1 \leqslant r \leqslant N$. Then, if $\boldsymbol{\Phi} := (\phi_{ir})$ denotes the matrix with such vectors as its columns, we have $\boldsymbol{\Phi}^{-1} = \boldsymbol{\Phi}^\top$ and $\boldsymbol{A}(G) = \boldsymbol{\Phi}\boldsymbol{M}\boldsymbol{\Phi}^\top$, where $\boldsymbol{M} := \operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_N)$. Hence,

$$(\boldsymbol{A}(G))_{ij} = \sum_{r,s=1}^{N} \phi_{ir} (\boldsymbol{M})_{rs} \phi_{js} = \sum_{r=1}^{N} \phi_{ir} \phi_{jr} \mu_r. \tag{2.2}$$

Now, let us consider the vector space spanned by the eigenvectors of the Kronecker product $\boldsymbol{K} := \boldsymbol{A}(G) \otimes p(\boldsymbol{A}(\Gamma))$, which is isomorphic to $\mathbb{R}^n \times \cdots \times \mathbb{R}^n$ (N factors). In such a space we take the '$\boldsymbol{\alpha}$-weight characteristic vector' of the set $(1, U_1) \cup \cdots \cup (N, U_N)$, namely $\boldsymbol{f} := (\alpha_1 \boldsymbol{\rho} U_1 | \alpha_2 \boldsymbol{\rho} U_2 | \cdots | \alpha_N \boldsymbol{\rho} U_N)$, or 'concatenation' of the vectors $\alpha_1 \boldsymbol{\rho} U_1, \ldots, \alpha_N \boldsymbol{\rho} U_N$, with $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots \alpha_N) \in \mathbb{R}_+^N$; and consider its spectral decomposition:

$$\begin{aligned}
\boldsymbol{f} &= \sum_{r=1}^{N} \frac{\langle \boldsymbol{f}, \boldsymbol{\phi}_r \otimes \boldsymbol{v} \rangle}{\|\boldsymbol{\phi}_r \otimes \boldsymbol{v}\|^2} \boldsymbol{\phi}_r \otimes \boldsymbol{v} + \boldsymbol{z} = \sum_{r=1}^{N} \sum_{i=1}^{N} \frac{\alpha_i \phi_{ir} \langle \boldsymbol{\rho} U_i, \boldsymbol{v} \rangle}{\|\boldsymbol{v}\|^2} \boldsymbol{\phi}_r \otimes \boldsymbol{v} + \boldsymbol{z} \\
&= \frac{1}{\|\boldsymbol{v}\|^2} \sum_{i=1}^{N} \alpha_i \|\boldsymbol{\rho} U_i\|^2 \sum_{r=1}^{N} \phi_{ir} \boldsymbol{\phi}_r \otimes \boldsymbol{v} + \boldsymbol{z} \\
&= \sum_{i=1}^{N} \frac{\alpha_i \|\boldsymbol{\rho} U_i\|^2}{\|\boldsymbol{v}\|^2} \boldsymbol{e}_i \otimes \boldsymbol{v} + \boldsymbol{z},
\end{aligned}$$

where $\boldsymbol{z} \in \langle \boldsymbol{\phi}_1 \otimes \boldsymbol{v}, \ldots, \boldsymbol{\phi}_N \otimes \boldsymbol{v} \rangle^\perp = \langle \boldsymbol{e}_1 \otimes \boldsymbol{v}, \ldots, \boldsymbol{e}_N \otimes \boldsymbol{v} \rangle^\perp \cong \boldsymbol{v}^\perp \times \cdots \times \boldsymbol{v}^\perp$ and, since $\boldsymbol{\Phi}\boldsymbol{\Phi}^\top = \boldsymbol{I}$,

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we have used that $\sum_{r=1}^{N} \phi_{ir}\phi_{jr} = \delta_{ij}$. Hence, by taking norms, we get

$$\begin{aligned}\|\boldsymbol{z}\|^2 &= \|\boldsymbol{f}\|^2 - \sum_{i=1}^{N} \frac{\alpha_i^2 \|\boldsymbol{\rho} U_i\|^4}{\|\boldsymbol{v}\|^4} \|\boldsymbol{e}_i \otimes \boldsymbol{v}\|^2 \\ &= \sum_{i=1}^{N} \alpha_i^2 \|\boldsymbol{\rho} U_i\|^2 - \frac{1}{\|\boldsymbol{v}\|^2} \sum_{i=1}^{N} \alpha_i^2 \|\boldsymbol{\rho} U_i\|^4 \\ &= \frac{1}{\|\boldsymbol{v}\|^2} \sum_{i=1}^{N} \alpha_i^2 \|\boldsymbol{\rho} U_i\|^2 \|\boldsymbol{\rho} \bar{U}_i\|^2,\end{aligned}$$

since $\|\boldsymbol{v}\|^2 - \|\boldsymbol{\rho} U_i\|^2 = \|\boldsymbol{\rho} \bar{U}_i\|^2$.

On the other hand, since there is no path of length $k = \operatorname{dgr} p$ between (the vertices of) the subsets U_i and U_j, provided that $i \sim j$ in G, we have

$$\begin{aligned}0 &= \langle \boldsymbol{K}\boldsymbol{f}, \boldsymbol{f} \rangle \\ &= \left\langle \sum_{r=1}^{N} \sum_{i=1}^{N} \alpha_i \phi_{ir} \frac{\|\boldsymbol{\rho} U_i\|^2}{\|\boldsymbol{v}\|^2} \boldsymbol{K}(\boldsymbol{\phi}_r \otimes \boldsymbol{v}) + \boldsymbol{K}\boldsymbol{z}, \sum_{r=1}^{N} \sum_{i=1}^{N} \alpha_i \phi_{ir} \frac{\|\boldsymbol{\rho} U_i\|^2}{\|\boldsymbol{v}\|^2} \boldsymbol{\phi}_r \otimes \boldsymbol{v} + \boldsymbol{z} \right\rangle \\ &= \frac{1}{\|\boldsymbol{v}\|^2} \sum_{r=1}^{N} \left(\sum_{i=1}^{N} \alpha_i \phi_{ir} \|\boldsymbol{\rho} U_i\|^2 \right)^2 \mu_r p(\theta_0) + \langle [\boldsymbol{A}(G) \otimes p(\boldsymbol{A}(\Gamma))]\boldsymbol{z}, \boldsymbol{z} \rangle \\ &\geqslant \frac{p(\theta_0)}{\|\boldsymbol{v}\|^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \|\boldsymbol{\rho} U_i\|^2 \|\boldsymbol{\rho} U_j\|^2 \sum_{r=1}^{N} \phi_{ir}\phi_{jr}\mu_r + [\min \eta p(\theta)] \|\boldsymbol{z}\|^2 \\ &= \frac{p(\theta_0)}{\|\boldsymbol{v}\|^2} \sum_{i \sim j} 2\alpha_i \alpha_j \|\boldsymbol{\rho} U_i\|^2 \|\boldsymbol{\rho} U_j\|^2 + [\min \eta p(\theta)] \frac{1}{\|\boldsymbol{v}\|^2} \sum_{i=1}^{N} \alpha_i^2 \|\boldsymbol{\rho} U_i\|^2 \|\boldsymbol{\rho} \bar{U}_i\|^2\end{aligned}$$

because of (2.2). Note that, since $p(\theta_0) > 0$ and $\alpha_i > 0$ for any $1 \leqslant i \leqslant N$, for the above inequality to hold, we must have $\min \eta p(\theta) < 0$. Consequently, the claimed inequality (2.1) follows. □

To optimize the above result we now have a double task.

(a) First, we must choose the constants $\alpha_1, \ldots, \alpha_N$ in order to minimize the upper bound on the right-hand side of inequality (2.1), which can be seen as a multivariable function $\Psi(\alpha_1, \ldots, \alpha_N)$;

(b) Second, we must find the polynomial p which maximizes the quotient on the left-hand side of the same inequality.

Let us proceed with the study of each problem in turn.

(a) With the new variables $\beta_i := \alpha_i \|\boldsymbol{\rho} U_i\| \|\boldsymbol{\rho} \bar{U}_i\|$, the function Ψ to be minimized becomes

$$\boldsymbol{\Psi}(\beta_1, \ldots, \beta_N) = \frac{\sum_{i=1}^{N} \beta_i^2}{\sum_{i \sim j} 2\beta_i \frac{\|\boldsymbol{\rho} U_i\|}{\|\boldsymbol{\rho} \bar{U}_i\|} \beta_j \frac{\|\boldsymbol{\rho} U_j\|}{\|\boldsymbol{\rho} \bar{U}_j\|}} = \frac{\langle \boldsymbol{\beta}, \boldsymbol{\beta} \rangle}{\langle \boldsymbol{\beta}, \boldsymbol{B}\boldsymbol{\beta} \rangle},$$

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where $\boldsymbol{B}$ is a kind of weighted adjacency matrix of G, defined as

$$(\boldsymbol{B})_{ij} = \frac{\|\boldsymbol{\rho}U_i\|\|\boldsymbol{\rho}U_j\|}{\|\boldsymbol{\rho}\bar{U}_i\|\|\boldsymbol{\rho}\bar{U}_j\|} \quad \text{if } i \sim j \qquad \text{and} \qquad (\boldsymbol{B})_{ij} = 0 \quad \text{otherwise.}$$

But, from Rayleigh's principle, we know that $\langle \boldsymbol{\beta}, \boldsymbol{B}\boldsymbol{\beta}\rangle / \langle \boldsymbol{\beta}, \boldsymbol{\beta}\rangle$ takes its maximum at the spectral radius $r(\boldsymbol{B})$ of such a matrix. Consequently, we conclude that $\Psi_{\min} = r(\boldsymbol{B})^{-1}$.

(b) From the left-hand expression of (2.1) notice that the polynomial p can be chosen up to a multiplicative constant. Then, assuming that such a constant is fixed in such a way that $\min \eta p(\theta) \geqslant -1$, we are looking for the polynomial p which attains maximum value at θ_0, that is,

$$p(\theta_0) = \max_{q \in \mathbb{R}_k[x]} \big\{ q(\theta_0) : \min \eta q(\theta) \geqslant -1 \big\}. \tag{2.3}$$

But

$$\min \eta q(\theta) = \min \Big\{ \eta_0 \min_{1 \leqslant i \leqslant d} \{q(\theta_i)\},\ \eta_e \max_{1 \leqslant i \leqslant d} \{q(\theta_i)\} \Big\} \geqslant -1$$

leads to

$$p(\theta_0) = \max_{q \in \mathbb{R}_k[x]} \big\{ q(\theta_0) : -1/\eta_0 \leqslant q(\theta_i) \leqslant -1/\eta_e;\ 1 \leqslant i \leqslant d \big\}.$$

Alternatively, writing the above q in terms of a polynomial P with norm

$$\|P\|_\infty = \max_{1 \leqslant i \leqslant d} |p(\theta_i)| \leqslant 1,$$

namely

$$q := \frac{\eta_0 - \eta_e}{-2\eta_0\eta_e} P + \frac{\eta_0 + \eta_e}{-2\eta_0\eta_e},$$

we obtain the condition

$$p(\theta_0) = \max_{q \in \mathbb{R}_k[x]} \big\{ q(\theta_0) : \|P\|_\infty \leqslant 1 \big\}.$$

Hence, since $q(\theta_0)$ attains its maximum whenever $P(\theta_0)$ does, the above condition leads to taking, as the best choice for P, the k-alternating polynomial P_k defined in Section 1.

Thus, from the above discussion, the 'optimal version' of Theorem 2.1 turns out to be as follows.

Theorem 2.2. *Let Γ and G be graphs as above. Let P_k be the k-alternating polynomial of Γ. Assume that there exist some vertex subsets $U_1, U_2, \ldots, U_N$ of Γ such that* $\operatorname{dist}(U_i, U_j) > k$ for any $i \sim j$ in G. Let $\boldsymbol{B}$ be the weighted adjacency matrix of G, with spectral radius $r(\boldsymbol{B})$. Then,

$$P_k(\theta_0) \leqslant \frac{-2\eta_0\eta_e}{(\eta_0 - \eta_e) r(\boldsymbol{B})} - \frac{\eta_0 + \eta_e}{\eta_0 - \eta_e} \tag{2.4}$$

or

$$r(\boldsymbol{B}) \leqslant \frac{-2\eta_0\eta_e}{(\eta_0 - \eta_e) P_k(\theta_0) + (\eta_0 + \eta_e)}. \tag{2.5}$$

□

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Since we are free to choose the constants $\alpha_1, \alpha_2, \ldots$ we can also obtain suboptimal inequalities. For instance, assuming that $\boldsymbol{B}$ has nearly constant row sums, a good strategy would be to impose that $\beta_1 = \cdots = \beta_N$, which corresponds to

$$\alpha_1 \|\boldsymbol{\rho} U_1\| \|\boldsymbol{\rho} \bar{U}_1\| = \cdots = \alpha_N \|\boldsymbol{\rho} U_N\| \|\boldsymbol{\rho} \bar{U}_N\|.$$

(This is optimal, for example, when $G = K_2$.) Moreover, since Ψ is also invariant under multiplication of all its variables α_i by a constant, we can take $\alpha_1 = (\|\boldsymbol{\rho} U_1\| \|\boldsymbol{\rho} \bar{U}_1\|)^{-1}$, whence we get $\alpha_i = (\|\boldsymbol{\rho} U_i\| \|\boldsymbol{\rho} \bar{U}_i\|)^{-1}$ for any $1 \leqslant i \leqslant N$, and then

$$\Psi = \frac{N}{2} \left(\sum_{i \sim j} \frac{\|\boldsymbol{\rho} U_i\| \|\boldsymbol{\rho} U_j\|}{\|\boldsymbol{\rho} \bar{U}_i\| \|\boldsymbol{\rho} \bar{U}_j\|} \right)^{-1}.$$

With such a value, Theorem 2.1 becomes

$$P_k(\theta_0) \leqslant \frac{-\eta_0 \eta_e}{\eta_0 - \eta_e} N \left(\sum_{i \sim j} \frac{\|\boldsymbol{\rho} U_i\| \|\boldsymbol{\rho} U_j\|}{\|\boldsymbol{\rho} \bar{U}_i\| \|\boldsymbol{\rho} \bar{U}_j\|} \right)^{-1} - \frac{\eta_0 + \eta_e}{\eta_0 - \eta_e} \tag{2.6}$$

or

$$\sum_{i \sim j} \frac{\|\boldsymbol{\rho} U_i\| \|\boldsymbol{\rho} U_j\|}{\|\boldsymbol{\rho} \bar{U}_i\| \|\boldsymbol{\rho} \bar{U}_j\|} \leqslant \frac{-N \eta_0 \eta_e}{(\eta_0 - \eta_e) P_k(\theta_0) + (\eta_0 + \eta_e)}. \tag{2.7}$$

If Γ is regular, the above results are given in terms of the cardinalities of the vertex subsets. Indeed, in this case, we know that $\boldsymbol{v} = \boldsymbol{j}$ and hence $\|\boldsymbol{\rho} U_i\| = \sqrt{|U_i|}$, $\|\boldsymbol{\rho} \bar{U}_i\| = \sqrt{n - |U_i|}$ for any vertex subset U_i. Thus, for instance, (2.6) becomes

$$P_k(\theta_0) \leqslant \frac{-\eta_0 \eta_e}{\eta_0 - \eta_e} N \left(\sum_{i \sim j} \sqrt{\frac{|U_i||U_j|}{(n - |U_i|)(n - |U_j|)}} \right)^{-1} - \frac{\eta_0 + \eta_e}{\eta_0 - \eta_e}. \tag{2.8}$$

When we study nonregular graphs, but still want to consider the cardinalities of the vertex subsets, rather than their weights, we can use the Laplacian matrix. The *Laplacian matrix* of a graph is defined as $\boldsymbol{L} \equiv \boldsymbol{L}(\Gamma) := \boldsymbol{D} - \boldsymbol{A}(\Gamma)$, where $\boldsymbol{D} = \mathrm{diag}(\delta_1, \delta_2, \ldots, \delta_n)$ and δ_i denotes the degree of the ith vertex (see, for example, [15]). It turns out that $\boldsymbol{L}$ has eigenvalues $\mathrm{ev}\, \boldsymbol{L} = \{\theta_0 = 0 < \theta_1 < \cdots < \theta_d\}$ (they are usually enumerated in increasing order) and the eigenvalue 0 has eigenvector $\boldsymbol{j}$. As when using the adjacency matrix, the Laplacian matrix satisfies $(p(\boldsymbol{L}))_{uv} = 0$ for any vertices u, v at distance greater than k and any polynomial p of degree k. Thus, working now with the Kronecker product $\boldsymbol{K} := \boldsymbol{A}(G) \otimes p(\boldsymbol{L}(\Gamma))$, we get the analogue of Theorem 2.1.

Theorem 2.3. *Let Γ be a graph on n vertices, with Laplacian eigenvalues $\mathrm{ev}\, \boldsymbol{L} = \{0 < \theta_1 < \cdots < \theta_d\}$. For a given graph G with vertices $1, 2, \ldots, N$, and eigenvalues $\mathrm{ev}\, G = \{\eta_0 > \eta_1 > \cdots > \eta_e\}$, assume that there exist some vertex subsets $U_1, U_2, \ldots, U_N$ such that $\mathrm{dist}(U_i, U_j) > k$ for some integer $k \geqslant 1$ and any i, j adjacent in G. Let p be a polynomial of degree k such*

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that $p(0) > 0$. *Then, for any given positive reals* $\alpha_1, \alpha_2, \ldots, \alpha_N$, *we have*

$$\frac{p(0)}{|\min \eta p(\theta)|} \leqslant \Psi := \frac{\sum_{i=1}^{N} \alpha_i^2 |U_i|(n - |U_i|)}{\sum_{i \sim j} 2\alpha_i \alpha_j |U_i||U_j|} \tag{2.9}$$

where $\min \eta p(\theta) := \min\{\eta p(\theta) : \eta \in \operatorname{ev} G, \theta \in \operatorname{ev} \boldsymbol{L} \backslash \{0\}\}$. □

As before, the best choice for p is given by (2.3), where the k-alternating polynomial P_k must now be understood as the polynomial with $\max_{1 \leqslant i \leqslant d} \|P_k(\theta_i)\|_\infty \leqslant 1$ that attains maximum value at $\theta_0 = 0$, that is, on the left of the other eigenvalues.

Similar results can be obtained by using other matrices, such as the *Laplace operator* $\mathcal{L} := \boldsymbol{D}^{-1/2} \boldsymbol{L} \boldsymbol{D}^{-1/2}$ employed by Chung, Delorme and Solé in [3]. (In fact, this can be seen as a kind of normalized Laplacian matrix.) In this case, we have $\operatorname{ev} \mathcal{L} = \{\theta_0 = 0 < \theta_1 < \cdots < \theta_d \leqslant 2\}$ and the eigenvalue 0 has eigenvector $\boldsymbol{D}^{1/2} \boldsymbol{j}$. So the 'weight' of a vertex subset U_i turns out now to be $\operatorname{vol} U_i := \sum_{u \in U_i} \delta_i$.

3. Some applications

The above results generalize and unify a number of theorems previously offered in the literature to study some parameters of a graph from its spectrum. Most such theorems come from the following simplified version of Theorem 2.2.

Theorem 3.1. *Let* Γ *and* G *be graphs as above. Let* P_k *be the* k*-alternating polynomial of* Γ. *Assume that there exist some vertex subsets* $U_1, U_2, \ldots, U_N$ *of* Γ *such that* $\operatorname{dist}(U_i, U_j) > k$ *for any* $i \sim j$ *in* G; *and weights* $\|\boldsymbol{\rho} U_i\|^2 \geqslant w$ *for any* $1 \leqslant i \leqslant N$ *and* $w \in \mathbb{R}^+$. *Then,*

$$1 - \frac{\eta_0}{\eta_e} \leqslant \frac{2\|\boldsymbol{v}\|^2}{w(P_k(\theta_0) + 1)}. \tag{3.1}$$

Proof. From the hypothesis on the weights, we have that $\boldsymbol{B} \geqslant \frac{w}{\|\boldsymbol{v}\|^2 - w} \boldsymbol{A}(G)$, and hence

$$r(\boldsymbol{B}) \geqslant \frac{w}{\|\boldsymbol{v}\|^2 - w} r(\boldsymbol{A}(G)) = \frac{w}{\|\boldsymbol{v}\|^2 - w} \eta_0.$$

Then, the result is a consequence of (25). □

A particular case of this result, when each subset U_i consists of a single vertex with constant weight w, was derived in [8], together with some applications, such as a bound for the multiplicity of a certain eigenvalue of a distance-regular graph.

Perhaps the most interesting case of the above results is when all vertex subsets are mutually at distance greater than k. In this case, we say that the subsets are k-*independent*, a concept that generalizes the standard notion of independence (see [6, 7, 9]). Of course, such a situation corresponds to taking G as the complete graph on N vertices, K_N, with eigenvalues $\eta_0 = N - 1$ and $\eta_e = -1$. In particular, (2.7) and (3.1), respectively, become

$$\sum_{1 \leqslant i < j \leqslant N} \frac{\|\boldsymbol{\rho} U_i\| \|\boldsymbol{\rho} U_j\|}{\|\boldsymbol{\rho} \bar{U}_i\| \|\boldsymbol{\rho} \bar{U}_j\|} \leqslant \frac{N(N-1)}{N P_k(\theta_0) + N - 2} \tag{3.2}$$

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and

$$N \leqslant \frac{2\|\boldsymbol{v}\|^2}{w(P_k(\theta_0)+1)}. \tag{3.3}$$

Now we will give some examples of applications of these results. We begin by deriving an upper bound for an independence-like number concerning vertex subsets, whose definition follows. For any integer $k \geqslant 0$ and any weight $w \in \mathbb{R}$, $w \geqslant 1$, the (w,k)-*independence number* α_k^w, is the maximum number of k-independent subsets $U \subset V$ with weight $\|\boldsymbol{\rho} U\|^2 \geqslant w$. As in the standard notion of independence, it is assumed that every subset U is k-independent from itself, so that $\alpha_k^w \geqslant 1$. Then (3.3) gives the following result, which could have some relevance in coding theory.

Theorem 3.2. *Let G be a graph with eigenvalues $\operatorname{ev} G = \{\theta_0 > \theta_1 > \cdots > \theta_d\}$, positive eigenvector $\boldsymbol{v}$, and k-alternating polynomials P_k, $0 \leqslant k \leqslant d-1$. Then, given a real number $w \geqslant 1$, the (w,k)-independence number satisfies the bound*

$$\alpha_k^w \leqslant \frac{2\|\boldsymbol{v}\|^2}{w(P_k(\theta_0)+1)}. \tag{3.4}$$

□

Alternatively, we can also prove the above inequality by using (3.2). Indeed, if we consider $N = \alpha_k^w$ k-independent sets $U_1, \ldots, U_N$ with $\|\boldsymbol{\rho} U_i\|^2 \geqslant w$ for any $1 \leqslant i \leqslant N$, each of the $N(N-1)/2$ sum terms in (3.2) are bounded below by $w/(\|\boldsymbol{v}\|^2 - w)$, so giving

$$\frac{w}{\|\boldsymbol{v}\|^2 - w} \leqslant \frac{2}{NP_k(\theta_0) + N - 2}$$

and, solving for N, the result follows.

If we take $w := \min_{1 \leqslant i \leqslant N} \|\boldsymbol{\rho} U_i\|^2$, the above reasoning ensures that, among any N k-independent sets, it must be some set with weight

$$w \leqslant \frac{2\|\boldsymbol{v}\|^2}{N(P_k(\theta_0)+1)}.$$

The particular case of Theorem 3.2 where all subsets have equal weight w was proved in [8]. Such a case is, in turn, a generalization of a bound for the *k-independence number* α_k, that is, the maximum number of vertices that are mutually at distance greater than k, given in [7] for a regular graph:

$$\alpha_k \leqslant \frac{2n}{P_k(\theta_0)+1}.$$

In that paper, this bound was used to give an eigenvalue characterization of antipodal distance-regular graphs (among regular connected graphs).

A similar result can now be given for a general graph. Indeed, since every vertex u has weight $v_u^2 \geqslant 1$, we have $\alpha_k^1 \geqslant \alpha_k$. Moreover, as vertices in distinct k-independent sets are also k-independent, we also have $\alpha_k \geqslant \alpha_k^1$. Hence, $\alpha_k = \alpha_k^1$ and Theorem 3.2 has the following corollary.

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Corollary 3.3. *Let G be a graph as above. Then, its k-independence number satisfies the bound*

$$\alpha_k \leqslant \frac{2\|\boldsymbol{v}\|^2}{P_k(\theta_0)+1}. \tag{3.5}$$

□

A parameter closely related to the (w, k)-independence number is the (w, N)-*diameter*. This is a measure of how far apart N vertex subsets with minimum weight w can be from each other. More precisely, given an integer $N \geqslant 2$ and $w \in \mathbb{R}$, $w \geqslant 1$, the (w, N)-*diameter* is defined by

$$D_N^w := \max_{U_1,\ldots,U_N \subset V} \left\{ \min_{1 \leqslant i < j \leqslant N} \operatorname{dist}(U_i, U_j) : \|\boldsymbol{\rho} U_i\|^2 \geqslant w, 1 \leqslant i \leqslant N \right\}. \tag{3.6}$$

From this definition, we have that if $w_2 \geqslant w_1$, then $D_N^{w_2} \leqslant D_N^{w_1}$. In particular, the $(1, N)$-diameter D_N^1 measures the largest pairwise minimum distance of a set of N vertices. Hence, D_N^1 coincides with the N-diameter D_N considered by Chung, Delorme and Solé [3], as a generalization of the standard diameter D, which would be D_2 (for some previous results about the diameter, see [1, 2, 5, 9, 10, 13, 16].) More generally, if G is regular, the (w, N)-diameter is the same as the parameter $D_{N\times w}$, considered by Garriga and the author in [9] to measure the largest pairwise minimum distance of a family of N subsets with w vertices.

Theorem 3.4. *Let Γ be a graph as above. Then,*

$$P_k(\theta_0) > \frac{2\|\boldsymbol{v}\|^2}{wN} - 1 \Rightarrow D_N^w \leqslant k. \tag{3.7}$$

Proof. From the hypothesis and Theorem 3.2 we get $\alpha_k^w < N$, whence the result follows. □

The above results still hold if we replace P_k by the Chebyshev polynomial T_k 'shifted' from $[-1, 1]$ to $[\theta_d, \theta_1]$, that is,

$$T_k^*(x) := T_k\left(\frac{2x-\theta_1-\theta_d}{\theta_1-\theta_d}\right)$$

(since $\|T_k^*\|_\infty = \|P_k\|_\infty = 1$ and $P_k(\theta_0) \geqslant T_k^*(\theta_0)$). Then, since $T_k(x) = \cosh(k \cosh^{-1} x)$, (3.7) yields

$$D_N^w \leqslant \left\lfloor \frac{\cosh^{-1}\left(\frac{2\|\boldsymbol{v}\|^2}{wN} - 1\right)}{\cosh^{-1}\left(\frac{2\theta_0-\theta_1-\theta_d}{\theta_1-\theta_d}\right)} \right\rfloor + 1. \tag{3.8}$$

The case of regular graphs was proved in [8] by using eigenvalue interlacing. For the same case, Kahale [14] showed that, if $\vartheta_1 (= \theta_0), \vartheta_2, \ldots, \vartheta_n$ represent the eigenvalues of the graph with $|\vartheta_1| > |\vartheta_2| \geqslant \cdots \geqslant |\vartheta_n|$, then

$$D_N^w \leqslant \left\lfloor \frac{\cosh^{-1}\left(\frac{n}{w} - 1\right)}{\cosh^{-1}(\vartheta_1/|\vartheta_N|)} \right\rfloor + 1. \tag{3.9}$$

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In fact, some slightly stronger results can be obtained from Theorem 2.1 in its version in (2.6) and (3.2):

$$P_k(\theta_0) > (N-1)\left(\sum_{1\leqslant i<j\leqslant N}\frac{\|\boldsymbol{\rho}U_i\|\,\|\boldsymbol{\rho}U_j\|}{\|\boldsymbol{\rho}\bar{U}_i\|\,\|\boldsymbol{\rho}\bar{U}_j\|}\right)^{-1} - \frac{N-2}{N} \Rightarrow \min_{i\neq j}\{\mathrm{dist}(U_i,U_j)\}\leqslant k.$$

Thus, if we define $\omega := \min_{i\neq j}\{\|\boldsymbol{\rho}U_i\|\,\|\boldsymbol{\rho}U_j\|\}$, the inverse of the sum is bounded above by

$$\binom{N}{2}^{-1}\left(\frac{\|\boldsymbol{v}\|^2}{\omega}-1\right),$$

and hence

$$P_k(\theta_0) > \frac{2\|\boldsymbol{v}\|^2}{N\omega} - 1 \Rightarrow \min_{i\neq j}\{\mathrm{dist}(U_i,U_j)\}\leqslant k.$$

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