The Alternating and Adjacency Polynomials, and their Relation with the Spectra and Diameters of Graphs *

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Abstract

Let Γ be a graph on n vertices, adjacency matrix $\boldsymbol{A}$, and distinct eigenvalues $\lambda > \lambda_1 > \lambda_2 > \cdots > \lambda_d$. For every $k = 0, 1, \ldots, d-1$, the *k-alternating polynomial* P_k is defined to be the polynomial of degree k and norm $\|P_k\|_\infty = \max_{1\leq l\leq d}\{|P_k(\lambda_l)|\} = 1$ that attains maximum value at λ. These polynomials, which may be thought of as the discrete version of the Chebychev ones, were recently used by the authors to bound the diameter $D(\Gamma)$ of Γ in terms of its eigenvalues. Namely, it was shown that $P_k(\lambda) > \|\boldsymbol{\nu}\|^2 - 1 \Rightarrow D(\Gamma) \leq k$, where $\boldsymbol{\nu}$ is the (positive) eigenvector associated to λ with minimum component 1. In this work we improve upon this result by assuming that some extra information about the structure of Γ is known. To this end, we introduce the so-called *τ-adjacency polynomial* Q_τ. For each $0 \leq \tau \leq d$, the polynomial Q_τ is defined to be the polynomial of degree τ and norm $\|Q_\tau\|_A = \max_{1\leq i\leq n}\{\|Q_\tau(\boldsymbol{A})\boldsymbol{e}_i\|\} = 1$ that attains maximum value at λ. Then it is shown that $P_k(\lambda) > \|\boldsymbol{\nu}\|^2/Q_\tau^2(\lambda) - 1 \Rightarrow D(\Gamma) \leq k + 2\tau$. Some applications of the above results, together with new bounds for generalized diameters, are also presented.

Keywords: Adjacency polynomials; Conditional diameters, Eigenvalues

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1 Introduction

In this paper $\Gamma = (V, E)$ denotes a (simple and finite) connected graph, with vertex set $V = V\Gamma$, $|V| = n$, and edge set $E = E\Gamma$. For any vertex $e_i \in V$, $\Gamma(e_i)$ denotes the set of vertices adjacent to e_i, and $\delta(e_i) = |\Gamma(e_i)|$ denotes its *degree*. Then, Γ is *(δ-)regular* if $\delta(e_i) = \delta$ for all $1 \le i \le n$. The *distance* between two vertices e_i and e_j will be denoted by $\partial(e_i, e_j)$. The *eccentricity* of a vertex e_i is $\varepsilon_i = \varepsilon(e_i) = \max_{e_j \in V} \partial(e_i, e_j)$, the *diameter* of Γ is $D = D(\Gamma) = \max_{e_i \in V} \varepsilon(e_i)$, and its *radius* is $r = r(\Gamma) = \min_{e_i \in V} \varepsilon(e_i)$.

Recently, much work has been done to give upper bounds on the diameter of a graph in terms of its spectrum. Let $\lambda_0 (= \delta) > \lambda_1 > \cdots > \lambda_d$ be the $d+1$ distinct eigenvalues of a δ-regular graph Γ, with order n and diameter D. Thus, Alon and Milman [1] and Mohar [28] gave results in terms of the two first eigenvalues λ_0 and λ_1. Then, several results using the first eigenvalue λ_0 and either the second largest eigenvalue in absolute value, $\lambda_* = \max\{\lambda_1, -\lambda_d\}$, or both λ_1 and λ_d have been given by Lubotzky, Phillips, and Sarnak [27], and Chung [4]:

$$D \le \left\lfloor \frac{\ln(n-1)}{\ln(\lambda_0/\lambda_*)} \right\rfloor + 1, \tag{1}$$

Sarnak [31], and Chung, Faber and Manteuffel [5]:

$$D \le \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}(\lambda_0/\lambda_*)} \right\rfloor + 1, \tag{2}$$

and Van Dam and Haemers [13]:

$$D < \frac{\ln 2(n-1)}{\ln \frac{\sqrt{\lambda_0-\lambda_d}+\sqrt{\lambda_0-\lambda_1}}{\sqrt{\lambda_0-\lambda_d}-\sqrt{\lambda_0-\lambda_1}}} + 1. \tag{3}$$

As expected, most of the previous results can be improved if we have further information about the structure of Γ. This is the case, for instance, when the graph is bipartite, as it was shown by Delorme and Solé [14] and the authors [18], or when it is vertex-transitive, see Delorme and Tillich [15]. Another example is that considered by Quenell [29], where it is assumed that the girth g of Γ is known. More precisely, this author managed to prove the following diameter estimates:

$$D \le \left\lfloor \frac{\cosh^{-1}\left(\frac{n}{\lambda_0(\lambda_0-1)^{\ell-1}} - 1\right)}{\cosh^{-1}(\lambda_0/\lambda_*)} \right\rfloor + 2\ell + 1, \tag{4}$$

where $\ell = \lfloor \frac{g-1}{2} \rfloor (\ge 1)$ is the so-called 'injectivity radius' [29] or 'parameter ℓ' [16] (in the latter paper this parameter was used in the context of connectivity problems.) This result improves, for 'large enough' graphs (more precisely, when $\lambda_* \ge 2\sqrt{\lambda_0 - 1}$), the result (2) of Sarnak [31], and Chung, Faber and Manteuffel [5].

The results (1), (2) and (3) admit the following unified presentation. Let P be a real polynomial and set $\|P\|_\infty = \max_{1\le i\le d}\{|P(\lambda_i)|\}$. Then,

$$P(\lambda_0) > \|P\|_\infty(n-1) \;\Rightarrow\; D(\Gamma) \le \operatorname{dgr} P, \tag{5}$$

whereas the result in (4) stems from the implication

$$P(\lambda_0) > \|P\|_\infty \left(\frac{n}{\lambda_0(\lambda_0-1)^{\ell-1}} - 1\right) \Rightarrow D(\Gamma) \le \operatorname{dgr} P + 2\ell. \tag{6}$$

With the formulation in (5), Chung [4] considered the case $P = x^k$, Delorme and Solé [14] generalized her results by taking $P = x^k + tx^{k-1}$, $t \in \mathbb{R}^+$, which has the advantage of being useful to the case of bipartite biregular graphs (that is, bipartite graphs such that vertices in the same vertex class have the same degree), and Sarnak [31], Chung, Faber and Manteuffel [5], and Van Dam and Haemers [13] used Chebychev polynomials shifted to the interval $[\lambda_d, \lambda_1]$. Such polynomials were also used by Quenell [29] to derive (4) from (6). Other results, using the Laplacian matrix, can be found in [5, 18, 19, 28, 11, 12, 30]. Besides, in [14, 5, 18] the case of regular digraphs was also considered.

However, the formulations in (5) and (6) suggest that, to optimize the results, we must face the discrete nature of the problem, and look for the polynomials that maximize the quotient $P(\lambda_0)/\|P\|_\infty$. Or, alternatively, we should try to maximize $P(\lambda_0)$ when the considered polynomials are normalized by $\|P\|_\infty = 1$. This has been done by Yebra and the authors in [18, 19], for not necessarily regular graphs, introducing the *alternating polynomials* P_k of degree k. We collect here some of its main properties, referring the reader to [18] for a more detailed study:

- There is a unique k-alternating polynomial P_k for $0 \le k \le d-1$;
- $P_0(\lambda_0) = 1 < P_1(\lambda_0) < \cdots < P_{d-1}(\lambda_0)$;
- P_k maximizes $P_k(x)$ for all $x > \lambda_1$ and, for $k \ne 0$, it is strictly increasing in $[\lambda_1, \infty)$;
- P_k takes $k+1$ alternating values ± 1 at $\{\lambda_1, \lambda_2, \ldots, \lambda_d\}$, starting with $P_k(\lambda_1) = 1$ and ending with $P_k(\lambda_d) = (-1)^k$;
- There are explicit formulae for $P_0(=1)$, P_1, P_2, and P_{d-1}, while the other polynomials can be computed by solving a linear programming problem (for instance, by the simplex method.)

Some particular cases of these polynomials were also considered, in the same context, by Van Dam and Haemers in [13].

In terms of the alternating polynomials, and for not necessarily regular graphs, (5) becomes

$$P_k(\lambda_0) > \|\boldsymbol{\nu}\|^2 - 1 \;\Rightarrow\; D(\Gamma) \le k, \tag{7}$$

where $\boldsymbol{\nu}$ is the normalized positive eigenvector, that is the eigenvector corresponding to λ_0 with smallest component equal to one. In the case of regular graphs, $\boldsymbol{\nu} = \boldsymbol{j}$, the all-1 vector, and this simplifies to

$$P_k(\lambda_0) > n - 1 \;\Rightarrow\; D(\Gamma) \leq k. \tag{8}$$

In this work we improve upon the above results by assuming that some extra information about the structure of Γ is known. We begin this task in the next section, where some applications of a result on the '(s,t)-diameter', given in [19], are derived; and some other 'conditional diameters' are considered. Then, in Section 3, we introduce a new family of polynomials which are defined in terms of the adjacency matrix $\boldsymbol{A}$, and hence they are called the *adjacency polynomials* of Γ. Some first applications of these polynomials are also discussed. Finally, in Section 4 we give results involving both the alternating and the adjacency polynomials, which improve and generalize the previous results.

We devote the rest of this section to recall the main terminology and known results used throughout the paper. In particular we pay attention to the *local spectrum* of a graph, a concept introduced by the authors in [21].

Let $\boldsymbol{A}$ be the *adjacency matrix* of $\Gamma = (V, E)$, that has $d+1$ distinct eigenvalues $\lambda_0 > \lambda_1 > \cdots > \lambda_d$. The spectrum of Γ, which is the set of the eigenvalues of $\boldsymbol{A}$ together with their multiplicities $m_l = m(\lambda_l)$, $0 \leq l \leq d$, is denoted by $\mathrm{S}(\Gamma) = \{\lambda_0^{m_0}, \lambda_1^{m_1}, \ldots, \lambda_d^{m_d}\}$. Because of its special role, the largest eigenvalue λ_0 will also be denoted by λ. As a consequence of Perron-Frobenius' theorem, λ is simple and positive, with positive eigenvector $\boldsymbol{\nu} = (\nu_1, \nu_2, \ldots, \nu_n)^\top$. As stated above, we will suppose that $\boldsymbol{\nu}$ is 'normalized' in such a way that its minimum component equals 1. As usual, we identify $\boldsymbol{A}$ with an endomorphism of the 'vertex-space' of Γ, $\ell^2(V)$, which, for any given indexing of the vertices, is isomorphic to $\mathbb{R}^n$. Thus, for a given ordering of its vertices, we only distinguish between a vertex e_i and the corresponding vector $\boldsymbol{e}_i$ of the canonical base of $\mathbb{R}^n$ by the bold type used. The *adjacency algebra* of $\boldsymbol{A}$, denoted by $\mathcal{A}(\boldsymbol{A})$, is the algebra of all the matrices which are polynomials in $\boldsymbol{A}$.

For a given vertex $e_i \in V$ we can consider its 'spectral decomposition'

$$\boldsymbol{e}_i = \sum_{l=0}^{d} \boldsymbol{z}_{il} = \frac{\nu_i}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_i \tag{9}$$

where $\boldsymbol{z}_{il} \in \mathrm{Ker}(x - \lambda_l)$ and $\boldsymbol{z}_i \in \boldsymbol{\nu}^\perp$. We let a polynomial p operate on $\mathbb{R}^n$ by the rule $p\boldsymbol{w} = p(\boldsymbol{A})\boldsymbol{w}$, and the matrix is not specified unless some confusion may arise. For instance, using (9), $p\boldsymbol{e}_i = p(\boldsymbol{A})\boldsymbol{e}_i = \frac{p(\lambda)\nu_i}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + p(\lambda_1)\boldsymbol{z}_{i1} + \cdots + p(\lambda_d)\boldsymbol{z}_{id}$.

The *(e_i-)local multiplicity* of an eigenvalue λ_l, $0 \leq l \leq d$ was defined in [21] as

$$m_{e_i}(\lambda_l) \equiv m_i(\lambda_l) = \|\boldsymbol{z}_{il}\|^2. \tag{10}$$

For example, the e_i-local multiplicity of λ is $m_i(\lambda) = \frac{\nu_i^2}{\|\boldsymbol{\nu}\|^2} > 0$. Notice that the local multiplicity $m_i(\lambda_l)$ corresponds in fact to $\cos^2 \beta_{il}$, where β_{il} is the angle between $\boldsymbol{e}_i$ and the eigenspace $\mathrm{Ker}(x-\lambda_l)$. The cosines $\cos\beta_{il}$, $1\le i\le n$, $0\le l\le d$, were formally introduced by Cvetković as the *'angles'* of Γ (see, for instance, [9, 10].)

Let $\lambda>\lambda_{i_1}>\cdots>\lambda_{i_m}$ be those eigenvalues of Γ having nonnull e_i-local multiplicities (note that $m_i(\lambda_l)=0$ iff $\boldsymbol{z}_{il}=\boldsymbol{0}$.) Denoting them by $\mu_0(=\lambda)>\mu_1>\cdots>\mu_m$, we can define the *($e_i$-)local spectrum* of Γ as

$$\mathrm{S}_i(\Gamma)=\{\lambda^{m_i(\lambda)},\mu_1^{m_i(\mu_1)},\ldots,\mu_m^{m_i(\mu_m)}\}$$

and so they will be referred to as the (e_i)-*local eigenvalues* of Γ. As was discussed in [21], when Γ is 'seen' from a given vertex, its local spectrum plays a similar role as the ('global') spectrum. In the following proposition we survey some of the results supporting this claim.

Proposition 1.1 *Let Γ be a graph on n vertices. Let $e_i\in V$ be a generic vertex with local eigenvalues $\mu_0>\mu_1>\cdots>\mu_m$, and let p denote a polynomial. Then,*

- *(a)* $(p(\boldsymbol{A}))_{ii}=\sum_{l=0}^{m}m_i(\mu_l)p(\mu_l)$;
- *(b)* $\sum_{l=0}^{m}\mu_l m_i(\mu_l)=0$, *and the degree of vertex e_i is* $\delta(e_i)=\sum_{l=0}^{m}\mu_l^2 m_i(\mu_l)$;
- *(c) The e_i-local multiplicities of all the eigenvalues add up to 1:* $\sum_{l=0}^{m}m_i(\mu_l)=1$ $(1\le i\le n)$;
- *(d) The multiplicity of an eigenvalue of Γ is the sum, extended to all vertices, of its local multiplicities:* $m(\lambda_l)=\sum_{i=1}^{n}m_i(\lambda_l)$ $(0\le l\le d)$;
- *(e) The eccentricity of vertex e_i satisfies $\varepsilon_i\le m$.* $\square$

In [20] Yebra and the authors introduced the following polynomial which, for non-regular graphs, plays a similar role as the well-known Hoffman polynomial [25].

$$H=\frac{\|\boldsymbol{\nu}\|^2}{\pi_0}\prod_{l=1}^{d}(x-\lambda_l),\quad \text{with } \pi_0=\prod_{l=1}^{d}(\lambda-\lambda_l). \tag{11}$$

Notice that $H(\lambda)=\|\boldsymbol{\nu}\|^2$ and $H(\lambda_l)=0$, $1\le l\le d$. Moreover, it was proved that H is the unique polynomial of degree $\le d$ satisfying $H(\boldsymbol{A})_{ij}=\nu_i\nu_j$, $1\le i,j\le n$. Notice that, when Γ is regular, $\boldsymbol{\nu}=\boldsymbol{j}$ gives $H(\boldsymbol{A})=\boldsymbol{J}$, so that H is the Hoffman polynomial.

2 Diameters of a graph and its eigenvalues

In this section we present some results bounding the diameter of a graph in terms of its eigenvalues, and some additional information about its structure. The results improve those of Quenell [29], and they are based on a theorem concerning the so-called (s,t)-diameter, which is a generalization of the standard diameter. Other recent generalizations of such a concept are also investigated.

2.1 The (s,t)-diameter

The distance between two subsets of vertices $U_1, U_2 \subset V$, denoted by $\partial(U_1, U_2)$, is defined as $\partial(U_1, U_2) = \min\{\partial(e_i, e_j) : e_i \in U_1, e_j \in U_2\}$. For some given integers $1 \le s, t \le n$, the *(s,t)-diameter* $D_{(s,t)}$, used in [2, 19], measures the maximum distance between two subsets of s and t vertices, that is,

$$D_{(s,t)} = \max_{V_1, V_2 \subset V} \{\partial(V_1, V_2) : |V_1| = s, |V_2| = t\}.$$

Thus, $D_{(1,1)}$ coincides with the standard diameter D. In [19] the authors proved the following result concerning the (s,t)-diameter:

Theorem 2.1 *Let $\Gamma = (V, E)$ be a graph with eigenvalues $\lambda > \lambda_1 > \cdots > \lambda_d$, and let P_k denote the k-alternating polynomial on the mesh $\{\lambda_1, \ldots, \lambda_d\}$. Let $\boldsymbol{\nu}$ be the positive eigenvector associated to λ. Then,*

$$P_k(\lambda) > \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{s} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{t} - 1\right)} \;\Rightarrow\; D_{(s,t)}(\Gamma) \le k. \quad \square \tag{12}$$

In the case of regular graphs, the above result was also implicitly proved by Van Dam and Haemers in [13] (using a generic polynomial and without mention to the conditional diameters.) For regular graphs also, and using the Chebychev polynomials T_k, Kahale [26] managed to prove that

$$D_{(s,t)} \le \left\lfloor \frac{\cosh^{-1}\sqrt{(ns^{-1} - 1)(nt^{-1} - 1)}}{\cosh^{-1}(\lambda_0/\lambda_*)} \right\rfloor + 1. \tag{13}$$

Since $\|T_k\|_\infty = 1$ in $[-1, 1]$, we have that $P_k(x) \ge T_k(x/\lambda_1)$ for any $x \ge \lambda_*$. Hence, a result like (13) for general graphs, with $\|\boldsymbol{\nu}\|^2$ instead of n, can be obtained by substituting $T_k(\lambda/\lambda_*)$ for $P_k(\lambda)$ in (12). Moreover, the use of the polynomial $T_k(x)$ 'shifted' to the interval $[\lambda_d, \lambda_1]$, that is $T_k((2x - \lambda_1 - \lambda_d)/(\lambda_1 - \lambda_d))$, gives the further improvement

$$D_{(s,t)} \le \left\lfloor \frac{\cosh^{-1}\sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{s} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{t} - 1\right)}}{\cosh^{-1}\left(\frac{2\lambda_0 - \lambda_1 - \lambda_d}{\lambda_1 - \lambda_d}\right)} \right\rfloor + 1. \tag{14}$$

Similar results (for general graphs) using the Laplacian matrix has been independently obtained in [19, 11, 12] (with the alternating polynomials), and in [6, 8] (with the shifted Chebychev polynomials.)

In the above-mentioned paper [19], the authors showed that Theorem 2.1 has some applications to the study of other parameters, such as the (vertex-)connectivity of Γ. Following this work, we next derive two new applications bounding the k-independence number and the (standard) diameter of Γ.

2.2 The k-independence number

For a graph Γ with diameter D, the *k-independence number* α_k, $0 \leq k \leq D-1$, is defined as the maximum number of vertices which are mutually at distance greater than k. Thus, trivially $\alpha_0 = n$, and $\alpha_1 \equiv \alpha$ is the standard *independence* or *stability* number. Notice also that α_k is, in fact, the independence number of the k-th power of Γ.

Proposition 2.2 *Let Γ be a graph as above. Then, for any $0 \leq k \leq D-1$, its k-independence number satisfies*

$$\alpha_k < \frac{2\|\boldsymbol{\nu}\|^2}{P_k(\lambda)+1} + 1. \tag{15}$$

Proof. The proof is based on the fact that the bound in Theorem 2.1, under the conditions $s+t = \alpha_k$ and $s,t \geq 1$, attains its minimum at $s = t$. Assume first that α_k is even. Then, taking $s = t = \frac{\alpha_k}{2}$, we clearly have $D_{(s,t)}(\Gamma) > k$. Consequently, Theorem 2.1 gives $P_k(\lambda) \leq \frac{2\|\boldsymbol{\nu}\|^2}{\alpha_k} - 1$, and so

$$\alpha_k \leq \frac{2\|\boldsymbol{\nu}\|^2}{P_k(\lambda)+1}. \tag{16}$$

Otherwise, if α_k is odd, we can take $s = \frac{\alpha_k+1}{2}$ and $t = \frac{\alpha_k-1}{2}$ to get

$$P_k^2(\lambda) \leq \left(\frac{2\|\boldsymbol{\nu}\|^2}{\alpha_k+1} - 1\right)\left(\frac{2\|\boldsymbol{\nu}\|^2}{\alpha_k-1} - 1\right)$$

which, solving for α_k, gives

$$\alpha_k \leq \frac{-2\|\boldsymbol{\nu}\|^2 + \sqrt{(P_k^2(\lambda)-1)^2 + 4\|\boldsymbol{\nu}\|^4 P_k^2(\lambda)}}{P_k^2(\lambda)-1} < \frac{2\|\boldsymbol{\nu}\|^2}{P_k(\lambda)+1} + 1, \tag{17}$$

where the second inequality has been deduced by adding $2(2\|\boldsymbol{\nu}\|^2 P_k(\lambda))(P_k^2(\lambda)-1)$ to the term inside the root. $\square$

In fact, a more detailed study of the odd case allow us to conclude that

$$\alpha_k < \frac{2\|\boldsymbol{\nu}\|^2}{P_k(\lambda)+1} + \sqrt{5} - 2, \tag{18}$$

see [22]. Notice that, when $\frac{2\|\boldsymbol{\nu}\|^2}{P_k(\lambda)+1}$ is an integer, we have (16). For instance, if Γ is a k-'boundary graph' as defined in [20], that is $P_k(\lambda) = \|\boldsymbol{\nu}\|^2 - 1$, the above result gives $\alpha_k \leq 2$. Hence, if $D(\Gamma) = k+1$ the obtained bound is tight. Another example is when we consider an r-*antipodal distance-regular* graph Γ (see, for instance, Biggs [3]), characterized by the fact that, given any vertex $e_i \in V$, the set $\{e_i\} \cup \Gamma_D(e_i)$ (with $\Gamma_D(e_i)$ defined below) has r vertices which are mutually at distance $D(= d.)$ In [20], the authors showed that the $(d-1)$-alternating polynomial of a such graph with n vertices satisfies $P_{d-1}(\lambda) = \frac{2}{r}n - 1$. Hence, (16) gives again the sharp bound $\alpha_{d-1} \leq r$.

2.3 The diameter

Given $e_i \in V$ and any integer ρ, $0 \le \rho \le D$, let $\Gamma_\rho(e_i)$ denote the set of vertices which are at distance ρ from e_i. For any integer $0 \le \tau \le D$, let us define the τ-*superdegree* of a vertex e_i as

$$\delta^*_\tau(e_i) = |\{e_j : \partial(e_i, e_j) \le \tau\}| = |\cup_{\rho=0}^{\tau} \Gamma_\rho(e_i)|.$$

Thus, $\delta^*_0(e_i) = 1$, $\delta^*_1(e_i) = 1 + \delta(e_i)$ and $\delta^*_D(e_i) = n$. The *minimum* τ-*superdegree* is then defined as $\delta^*_\tau = \min\{\delta^*_\tau(e_i) : e_i \in V\}$. Notice that, if Γ has minimum degree δ and girth g, then

$$\delta^*_\ell \ge 1 + \delta + \delta(\delta-1) + \cdots + \delta(\delta-1)^{\ell-1} \equiv n(\delta, \ell),$$

that is the 'Moore bound' for a δ-regular graph with diameter $\ell = \lfloor \frac{g-1}{2} \rfloor$, or odd girth $2\ell + 1$, see Biggs [3].

The following consequence of Theorem 2.1 takes into consideration the minimum τ-superdegree.

Proposition 2.3 *Let Γ be a graph as above. Then,*

$$P_k(\lambda) > \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{\delta^*_\sigma} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{\delta^*_\tau} - 1\right)} \;\Rightarrow\; D(\Gamma) \le k + \sigma + \tau. \tag{19}$$

Proof. Let e_i, e_j be two generic vertices. Then, since $|\cup_{\rho=0}^{\sigma} \Gamma_\rho(e_i)| \ge \delta^*_\sigma$ and $|\cup_{\rho=0}^{\tau} \Gamma_\rho(e_j)| \ge \delta^*_\tau$, we can always consider two subsets, S and T, of $s = \delta^*_\sigma$ and $t = \delta^*_\tau$ vertices respectively, such that

$$\partial(e_i, e_j) \le \sigma + \partial(S, T) + \tau \le \sigma + D_{(s,t)} + \tau.$$

Hence, $D(\Gamma) \equiv D_{(1,1)} \le \sigma + D_{(s,t)} + \tau$, and the result follows from Theorem 2.1. □

In particular, if Γ has minimum degree δ and girth g we can take $\sigma = \tau = \ell$, thus obtaining the following implication:

$$P_k(\lambda) > \frac{\|\boldsymbol{\nu}\|^2}{n(\delta, \ell)} - 1 \;\Rightarrow\; D(\Gamma) \le k + 2\ell. \tag{20}$$

This result improves, and generalizes for non-regular graphs, the result (6) of Quenell [29]. Moreover, it seems that the result in (20) is stronger as the value of ℓ increases. For example, the 'twisted odd graph' $\Gamma = O_4^{(12)}$, see [20], is a 4-regular graph on $n = 35$ vertices, with girth 5, and eigenvalues

$$\lambda = 4,\ \lambda_1 = 3,\ \lambda_2 = 2,\ \lambda_3 = 1,\ \lambda_4 = -1,\ \lambda_5 = -2,\ \lambda_6 = -3.$$

Then, the corresponding k-alternating polynomials have the following values at λ

$$P_5(4) = 34,\ P_4(4) = 15,\ P_3(4) = 6,\ P_2(4) = \frac{11}{4},\ P_1(4) = \frac{4}{3}.$$

Hence, since $P_5(4) = n-1$ (regular boundary graph [20]) we can not infer that $D(\Gamma) \le 5$. Similarly, since $n(4,1) = 5$, we get $P_3(4) = \frac{n}{n(4,1)} - 1$, and (20) neither allows us to conclude that $D(\Gamma) \le 5$. However, as $\ell = 2$ and $n(4,2) = 17$, we have $P_1(4) > \frac{n}{n(4,2)} - 1$, and (20) gives $D(\Gamma) \le 5$. (In fact, $D(\Gamma) = 4$.)

2.4 The $(s_1, \dots, s_r)$-diameter

A natural generalization of the (s,t)-diameter is obtained when we take into consideration some, say $r \ge 2$, vertex subsets of given cardinalities. Thus, for some integers $s_1, s_2, \dots, s_r$, $1 \le s_i \le n$, the $(s_1, s_2, \dots, s_r)$-*diameter* is defined as

$$D_{(s_1,s_2,\dots,s_r)} = \max_{U_1,\dots,U_r \subset V} \{ \min_{1 \le i < j \le r} \partial(U_i, U_j) : |U_i| = s_i, 1 \le i \le r \}. \tag{21}$$

In particular, if all the subsets have the same size, say s, we simply write $D_{r\times s}$ instead of $D_{(s,s,\dots,s)}$. Notice that, if $s = s_1 + \cdots + s_i$ and $t = s_{i+1} + \cdots + s_r$ for some $1 \le i \le r-1$, then $D_{(s_1,s_2,\dots,s_r)} \le D_{(s,t)}$, so that Theorem 2.1 gives

$$P_k(\lambda) > \frac{\|\boldsymbol{\nu}\|^2}{s} - 1 \;\Rightarrow\; D_{2s\times 1} \le k. \tag{22}$$

More generally, it was shown in [17], by using a different approach, that

$$P_k(\lambda) > \frac{2\|\boldsymbol{\nu}\|^2}{r} - 1 \Rightarrow\; D_{r\times 1} \le k \tag{23}$$

for any integer $r \ge 2$.

In [26], Kahale proved that if Γ is a regular graph on n vertices, and $\vartheta_0 (= \lambda_0), \vartheta_1 (= \lambda_*), \vartheta_2, \dots, \vartheta_{n-1}$ represent its eigenvalues (including multiplicities) with absolute value in nonincreasing order, $|\vartheta_0| > |\vartheta_1| \ge \cdots \ge |\vartheta_{n-1}|$, then

$$D_{r\times s} \le \left\lceil \frac{\cosh^{-1}\left(\frac{n}{s} - 1\right)}{\cosh^{-1}(\vartheta_0/\vartheta_{r-1})} \right\rceil + 1. \tag{24}$$

In [8], Chung, Delorme, and Solé prove, by using again the (normalized) Laplacian matrix (the *'Laplace operator'*) and the Chebychev polynomials, a result for general graphs, whose counterpart for the adjacency matrix is:

$$D_{(s_1,s_2,\dots,s_r)} \le \max_{1\le i<j\le r} \left\lfloor \frac{\cosh^{-1}\sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{s_i} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{s_j} - 1\right)}}{\cosh^{-1}\left(\frac{2\theta_0 - \theta_{r-1} - \theta_{n-1}}{\theta_{r-1} - \theta_{n-1}}\right)} \right\rfloor + 1, \tag{25}$$

where $\theta_0 (= \lambda_0) > \theta_1 \ge \cdots \ge \theta_{n-1}$ are the n eigenvalues of $\boldsymbol{A}$ (see also Chung, Grigor'yan, and Yau [7].) The proof is based in a geometric lemma given in [6] stating that, for any $r \ge 2$ arbitrary vectors of a $(r-2)$-dimensional Euclidean space, at least two of them have a nonnegative scalar product. Again, a better result can be obtained here if we use the alternating polynomials, as shown in the next theorem. Although its proof goes along the same lines as in [6, 8], we will give it in detail to illustrate the use of both, the alternating polynomials and the referred geometrical lemma.

Theorem 2.4 *Let $\Gamma = (V, E)$ be a graph with adjacency matrix $\boldsymbol{A}$, and n eigenvalues $\theta_0(= \lambda_0) > \theta_1 \geq \cdots \geq \theta_{n-1}$. Let $\boldsymbol{\nu}$ be the positive eigenvector associated to λ_0. Let $P_{k,r}$ denote the k-alternating polynomial on the mesh obtained by taking the different eigenvalues among $\theta_{r-1}, \theta_r, \ldots, \theta_{n-1}$ (that is, $\lambda_{i(r)} > \lambda_{i(r)+1} > \cdots > \lambda_d$; where $i(r) = 1$ if $m_1 > r-2$, and $i(r)$ is the maximum integer satisfying $m_1 + m_2 + \cdots + m_{i(r)-1} \leq r-2$, otherwise.) Then,*

$$P_{k,r}(\lambda) > \max_{1 \leq i < j \leq r} \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{s_i} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{s_j} - 1\right)} \Rightarrow D_{(s_1, s_2, \ldots, s_r)} \leq k. \tag{26}$$

Proof. Let us consider r generic subsets $U_i \subset V$ with given cardinalities $|U_i| = s_i$, $1 \leq i \leq r$. Then, for each $U_i \subset V$, consider the following spectral decomposition of its 'weighted characteristic vector':

$$\boldsymbol{f}_i = \sum_{e_l \in U_i} \nu_l \boldsymbol{e}_l = \frac{\|\boldsymbol{f}_i\|^2}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_i + \boldsymbol{w}_i \tag{27}$$

where $\boldsymbol{z}_i \in Z = \bigoplus_{i=1}^{r-2} \mathrm{Ker}(x - \theta_i)$ and $\boldsymbol{w}_i \in W = \bigoplus_{i=r-1}^{n-1} \mathrm{Ker}(x - \theta_i)$, so that

$$\|\boldsymbol{w}_i\|^2 = \|\boldsymbol{f}_i\|^2 - \frac{\|\boldsymbol{f}_i\|^4}{\|\boldsymbol{\nu}\|^2} - \|\boldsymbol{z}_i\|^2 \leq s_i\left(1 - \frac{s_i}{\|\boldsymbol{\nu}\|^2}\right).$$

As $\dim Z = r-2$, by the above-mentioned geometric lemma we can choose two sets, say U_i and U_j, such that $\langle \boldsymbol{z}_i, \boldsymbol{z}_j \rangle \geq 0$. Then, we get

$$\begin{aligned}
\sum_{e_l \in U_i, e_m \in U_j} (P_{k,r}(\boldsymbol{A}))_{lm} &= \langle P_{k,r}\boldsymbol{f}_i, \boldsymbol{f}_j \rangle \\
&= \left\langle P_{k,r}\left(\frac{\|\boldsymbol{f}_i\|^2}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_i + \boldsymbol{w}_i\right), \frac{\|\boldsymbol{f}_j\|^2}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_j + \boldsymbol{w}_j \right\rangle \\
&= P_{k,r}(\lambda)\frac{\|\boldsymbol{f}_i\|^2\|\boldsymbol{f}_j\|^2}{\|\boldsymbol{\nu}\|^2} + \langle P_{k,r}\boldsymbol{z}_i, \boldsymbol{z}_j \rangle + \langle P_{k,r}\boldsymbol{w}_i, \boldsymbol{w}_j \rangle \\
&\geq P_{k,r}(\lambda)\frac{s_i s_j}{\|\boldsymbol{\nu}\|^2} + P_{k,r}(\theta_{r-2})\langle \boldsymbol{z}_i, \boldsymbol{z}_j \rangle - \|P_{k,r}\boldsymbol{w}_i\|\|\boldsymbol{w}_j\| \\
&\geq P_{k,r}(\lambda)\frac{s_i s_j}{\|\boldsymbol{\nu}\|^2} - \|\boldsymbol{w}_i\|\|\boldsymbol{w}_j\| \\
&\geq \frac{s_i s_j}{\|\boldsymbol{\nu}\|^2}\left(P_{k,r}(\lambda) - \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{s_i} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{s_j} - 1\right)}\right) > 0.
\end{aligned}$$

Hence, $\partial(U_i, \boldsymbol{e}_j) \le k$, and the result follows. $\square$

For instance, as a corollary of the above theorem, we have that

$$P_{k,r}(\lambda) > \|\boldsymbol{\nu}\|^2 - 1 \Rightarrow \ D_{r\times 1} \le k, \tag{28}$$

a result to be compared with (23).

3 The adjacency polynomials

In order to improve further the previous results, we can use a new family of polynomials, related to the adjacency matrix of a graph, whose study is the topic of this section. Although the study can be done in general for the conditional diameters, we restrict ourselves to the simplest case of the standard diameter (so considering only distances between pairs of vertices.)

Let $\boldsymbol{A}$ be the adjacency matrix of some graph Γ with n vertices, diameter D and eigenvalues $\lambda > \lambda_1 > \cdots > \lambda_d$. Let $\mathbb{R}_k[x]$ denote the $(k+1)$-dimensional vector space of polynomials with degree at most k. Then, for each $k = 0, 1, \ldots, d$, the mapping from $\mathbb{R}_k[x]$ to $\mathbb{R}$ defined by $p \mapsto \|p\|_A = \max_{1\le i\le n}\{\|p\boldsymbol{e}_i\|\}$ is a norm of $\mathbb{R}_k[x]$. Notice that, using Proposition 1.1(a),

$$\|p\boldsymbol{e}_i\|^2 = \langle p^2\boldsymbol{e}_i, \boldsymbol{e}_i\rangle = (p^2(\boldsymbol{A}))_{ii} = \sum_{l=0}^{m} m_i(\mu_l)p^2(\mu_l) = \sum_{l=0}^{d} m_i(\lambda_l)p^2(\lambda_l) \tag{29}$$

and then

$$\|p\|_A^2 = \max_{1\le i\le n}\left\{\sum_{l=0}^{d} m_i(\lambda_l)p^2(\lambda_l)\right\}. \tag{30}$$

Using this norm, we can derive an upper bound for the eccentricity of a vertex.

Theorem 3.1 *Let $\Gamma = (V, E)$ be a graph with adjacency matrix $\boldsymbol{A}$ and eigenvalues $\lambda > \lambda_1 > \cdots > \lambda_d$. Let $\boldsymbol{\nu}$ be the positive eigenvector associated to λ. Let $P \in \mathbb{R}_d[x]$, and $e_i \in V$ with eccentricity $\varepsilon(e_i)$. Then,*

$$\frac{P(\lambda)}{\|P\|_A} > \frac{\sqrt{\|\boldsymbol{\nu}\|^2 - 1}}{\nu_i} \ \Rightarrow \ \varepsilon(e_i) \le \operatorname{dgr} P. \tag{31}$$

Proof. Let us first study the angle α_i between the vectors $P\boldsymbol{e}_i$ and $\boldsymbol{\nu}$. To this end, note that

$$P(\lambda)\nu_i = \langle P(\lambda)\boldsymbol{\nu}, \boldsymbol{e}_i\rangle = \langle \boldsymbol{e}_i, P\boldsymbol{\nu}\rangle = \langle P\boldsymbol{e}_i, \boldsymbol{\nu}\rangle = \|P\boldsymbol{e}_i\|\|\boldsymbol{\nu}\|\cos\alpha_i \le \|P\|_A\|\boldsymbol{\nu}\|\cos\alpha_i.$$

Hence,

$$\cos\alpha_i \geq \frac{P(\lambda)\nu_i}{\|P\|_A\|\boldsymbol{\nu}\|}\ , \quad \alpha_i \leq \cos^{-1}\left(\frac{P(\lambda)\nu_i}{\|P\|_A\|\boldsymbol{\nu}\|}\right) \tag{32}$$

Moreover, we claim that the cone with axis $\boldsymbol{\nu}$ and semi-angle $\beta = \cos^{-1}\left(\frac{\sqrt{\|\boldsymbol{\nu}\|^2-1}}{\|\boldsymbol{\nu}\|}\right)$ is contained in the 'positive region' $x_j \geq 0$, $1 \leq j \leq n$. Indeed, if β_j denotes the angle between $\boldsymbol{\nu}$ and the subspace $x_j = 0$, we have

$$\cos\beta_j = \frac{\sqrt{\|\boldsymbol{\nu}\|^2 - \nu_j^2}}{\|\boldsymbol{\nu}\|} \leq \frac{\sqrt{\|\boldsymbol{\nu}\|^2 - 1}}{\|\boldsymbol{\nu}\|} = \cos\beta$$

whence $\beta_j \geq \beta$ for any $1 \leq j \leq n$. Hence, the result follows from the fact that, if the lefthand inequality of (31) holds, then

$$\cos\alpha_i \geq \frac{P(\lambda)\nu_i}{\|P\|_A\|\boldsymbol{\nu}\|} > \frac{\sqrt{\|\boldsymbol{\nu}\|^2 - 1}}{\|\boldsymbol{\nu}\|} = \cos\beta,$$

so that $P\boldsymbol{e}_i$ is in the cone and hence all its components are positive. Consequently, $\varepsilon(e_i) \leq \operatorname{dgr} P$. $\square$

As two straightforward consequences of this theorem, we have the following new results concerning both the radius and the diameter of a graph.

Corollary 3.2 *Let Γ be a graph as above. Let $\nu_M = \max_{1\leq i\leq n} \nu_i$. Then,*

(a) $\frac{P(\lambda)}{\|P\|_A} > \frac{1}{\nu_M}\sqrt{\|\boldsymbol{\nu}\|^2 - 1} \ \Rightarrow\ r(\Gamma) \leq \operatorname{dgr} P;$

(b) $\frac{P(\lambda)}{\|P\|_A} > \sqrt{\|\boldsymbol{\nu}\|^2 - 1} \ \Rightarrow\ D(\Gamma) \leq \operatorname{dgr} P.$ $\square$

As above, to optimize these results, we must try to maximize $P(\lambda)$ when the considered polynomials are normalized by $\|P\|_A = 1$. Thus, let us consider the closed unit ball $\mathcal{B}_k = \{p \in \mathbb{R}_k[x] : \|p\|_A \leq 1\}$. On this compact set, the continuous function $\Psi : p \to p(\lambda)$ attains its maximum at a point Q_k that, according to Proposition 3.3 below, will be called the *k-adjacency polynomial* of Γ. Notice that, since Ψ is linear, such a point must be on the border of $\mathcal{B}_k$, that is $\|Q_k\|_A = 1$. Then, as a first property of these polynomials, the first inequality in (32) gives $Q_k(\lambda) \leq \|\boldsymbol{\nu}\|/\nu_i$ for any $1 \leq i \leq n$, that is,

$$Q_k(\lambda) \leq \frac{\|\boldsymbol{\nu}\|}{\nu_M} \quad (0 \leq k \leq d). \tag{33}$$

The following result proves the uniqueness of the k-adjacency polynomial for every k not greater than the radius of the graph.

Proposition 3.3 *Let Γ be a graph with adjacency matrix $\boldsymbol{A}$ and radius r. Then, for any $0 \leq k \leq r$, there is a unique k-adjacency polynomial Q_k.*

Proof. By contradiction, assume that there exists a polynomial of degree k, $R_k \neq Q_k$, such that $\|R_k\|_A \leq 1$ and $R_k(\lambda) = Q_k(\lambda)$. Then, let us consider the polynomial $T_k = \frac{1}{2}(Q_k + R_k) \in \mathbb{R}_k[x]$, satisfying $T_k(\lambda) = Q_k(\lambda)$ and

$$\begin{aligned}\|T_k \boldsymbol{e}_i\|^2 &= \tfrac{1}{4}\langle Q_k\boldsymbol{e}_i + R_k\boldsymbol{e}_i, Q_k\boldsymbol{e}_i + R_k\boldsymbol{e}_i\rangle = \tfrac{1}{4}\|Q_k\boldsymbol{e}_i\|^2 + \tfrac{1}{4}\|R_k\boldsymbol{e}_i\|^2 + \tfrac{1}{2}\langle Q_k\boldsymbol{e}_i, R_k\boldsymbol{e}_i\rangle \\ &\leq \tfrac{1}{2} + \tfrac{1}{2}\cos\gamma_i \quad (1 \leq i \leq n)\end{aligned}$$

where γ_i stands for the angle between $Q_k\boldsymbol{e}_i$ and $R_k\boldsymbol{e}_i$. If $\gamma_i \neq 0$ for any $1 \leq i \leq n$, then we would have $\|T_k\boldsymbol{e}_i\| < 1$ for any i, and hence $\|T_k\|_A < 1$, contradicting that the maximum is attained at some point on the border of $\mathcal{B}_k$. The same contradiction is reached even if, for some i, $\gamma_i = 0$ but either $\|Q_k\boldsymbol{e}_i\| < 1$ or $\|R_k\boldsymbol{e}_i\| < 1$. Therefore, we only need to consider the case where, for some i, $\|Q_k\boldsymbol{e}_i\| = \|R_k\boldsymbol{e}_i\| = 1$ and $\gamma_i = 0$, that is $Q_k\boldsymbol{e}_i = R_k\boldsymbol{e}_i$. Then, using decomposition (9) $\boldsymbol{e}_i = \frac{\nu_i}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \sum_{l=1}^{d}\boldsymbol{z}_{il}$, $\boldsymbol{z}_{il} \in \mathrm{Ker}(x-\lambda_l)$, we get

$$\sum_{l=1}^{d} Q_k(\lambda_l)\boldsymbol{z}_{il} = \sum_{l=1}^{d} R_k(\lambda_l)\boldsymbol{z}_{il}$$

since $Q_k(\lambda) = R_k(\lambda)$. If $\boldsymbol{z}_{il} \neq \mathbf{0}$ for some k values of l, the polynomials Q_k and R_k should coincide at not less than $k+1$ points, and hence $Q_k = R_k$. Otherwise, if $\boldsymbol{z}_{il} \neq \mathbf{0}$ for only $m \leq k-1$ values of l, Proposition 1.1(e) would imply that vertex $\boldsymbol{e}_i$ has eccentricity $\varepsilon(\boldsymbol{e}_i) \leq k-1$, and then $r \leq k-1$, a contradiction. □

In particular, since $2r \geq D$, the above result assures that there exists a unique k-adjacency polynomial Q_k for any $0 \leq k \leq \lceil \frac{D}{2} \rceil$.

For example, the 0-adjacency polynomial is clearly $Q_0 = 1$. To compute the 1-adjacency polynomial, let Γ have maximum degree Δ, and consider a generic polynomial of degree 1, $p = a_0 + a_1 x$. Then we want to maximize the function $\psi(a_0, a_1) = p(\lambda) = a_0 + a_1\lambda$, under the condition $\|p\|_A^2 = a_0^2 + a_1^2\Delta = 1$. This gives:

$$Q_1 = \frac{\Delta + \lambda x}{\sqrt{\Delta^2 + \lambda^2\Delta}} = \frac{1 + \frac{\lambda}{\Delta}x}{\sqrt{1 + \frac{\lambda}{\Delta}\lambda}}. \tag{34}$$

Example 3.4 *Let Γ be the graph obtained from K_4 by deleting an edge. Then $\mathrm{S}(\Gamma) = \{\frac{1+\sqrt{17}}{2}, 0, -1, \frac{1-\sqrt{17}}{2}\}$, $\boldsymbol{\nu} = (1, \frac{1+\sqrt{17}}{2}, 1, \frac{1+\sqrt{17}}{2})^\top$ (the 1 entries corresponding to the vertices of degree 2), $\|\boldsymbol{\nu}\|^2 = \frac{17+\sqrt{17}}{4}$ and, from the above,*

$$Q_1 = \frac{(\sqrt{17}+1)x + 12}{\sqrt{198 + 6\sqrt{17}}}$$

giving $Q_1(\lambda) = 1.6833\ldots$. Then, since $\sqrt{\|\boldsymbol{\nu}\|^2 - 1}/\nu_1 = 2.0690\ldots$ and $\sqrt{\|\boldsymbol{\nu}\|^2 - 1}/\nu_2 = 1.6154\ldots$, Corollary 3.2(a) gives $r(\Gamma) = 1$.

At the other extreme, let us see that a d-adjacency polynomial (not necessarily unique) is

$$Q_d = \frac{\|\boldsymbol{\nu}\|}{\nu_M \pi_0} \prod_{l=1}^{d} (x - \lambda_l) = \frac{H}{\nu_M \|\boldsymbol{\nu}\|} \ ,$$

where H is the polynomial given in (11). Indeed, since $Q_d \boldsymbol{e}_i = \frac{1}{\nu_M\|\boldsymbol{\nu}\|} H\boldsymbol{e}_i = \frac{\nu_i}{\nu_M\|\boldsymbol{\nu}\|}\boldsymbol{\nu}$, we have $\|Q_d\boldsymbol{e}_i\| = \frac{\nu_i}{\nu_M} \leq 1$ for $1 \leq i \leq n$, as required. Moreover,

$$Q_d(\lambda) = \frac{H(\lambda)}{\nu_M\|\boldsymbol{\nu}\|} = \frac{\|\boldsymbol{\nu}\|}{\nu_M}$$

which, according to (33), is the maximum possible value.

3.1 Partially walk-regular graphs

To compute Q_k for $1 < k < d$ we need to know some additional information about the structure of the graph. This is the case, for instance, when we are dealing with 'partially walk-regular' graphs. We say that, for some positive integer d', a graph Γ is *d'-partially walk-regular* if the number of closed walks (or circuits) of length k, $0 \leq k \leq d'$, through a vertex $\boldsymbol{e}_i$, that is $(\boldsymbol{A}^k)_{ii}$, does not depend on i. For instance, every δ-regular graph with girth g is $(g-1)$-partially walk-regular, since in this case, for any $1 \leq i \leq n$ and $0 \leq k \leq g-1$, we have $(\boldsymbol{A}^k)_{ii} = 0$ (k odd) and $(\boldsymbol{A}^k)_{ii} = \phi(k)$ (k even), where $\phi(k)$ denotes the number of circuits of length k which go through the root of an (internally) δ-regular tree of depth $\geq k/2$. Notice that, since $\boldsymbol{I}, \boldsymbol{A}, \ldots, \boldsymbol{A}^d$ is a basis of $\mathcal{A}(\boldsymbol{A})$, if $d' \geq d$ then Γ is τ-partially walk-regular for any integer τ. In this case Γ is simply called *walk-regular* (see Godsil and McKay [23, 24].) Examples of walk-regular graphs are the vertex-transitive and/or distance-regular graphs.

The interest of considering partially walk-regular graphs stems from the following result.

Lemma 3.5 *Let Γ be a d'-partially walk-regular graph, with adjacency matrix $\boldsymbol{A}$ and eigenvalues $\lambda(=\lambda_0) > \lambda_1 > \cdots > \lambda_d$. Let $m(\lambda_l)$ be the multiplicity of λ_l. Then, for any polynomial p of degree k ($k \leq \lfloor \frac{d'}{2} \rfloor$ if $d' < d$),*

$$\|p\|_A^2 = \frac{1}{n} \sum_{l=0}^{d} m(\lambda_l) p^2(\lambda_l).$$

Proof. Assume $d' < d$, the other case being similar, and consider the polynomial p^2, of degree $2k \leq d'$. Then, since $(\boldsymbol{A}^h)_{ii} = \langle x^h \boldsymbol{e}_i, \boldsymbol{e}_i \rangle$, $0 \leq h \leq 2k$, does not depend on i, neither does $\|p\boldsymbol{e}_i\|^2 = \langle p^2 \boldsymbol{e}_i, \boldsymbol{e}_i\rangle = (p^2(\boldsymbol{A}))_{ii}$. Hence, we have

$$\sum_{l=0}^{d} m(\lambda_l) p^2(\lambda_l) = \mathrm{tr}\ p^2(\boldsymbol{A}) = \sum_{i=1}^{n} \|p\boldsymbol{e}_i\|^2 = n\|p\|_A^2. \quad \square$$

As a by-product of these results, note that, from the above lemma and equation (29) we get, for any $1 \le i \le n$,

$$\sum_{l=0}^{d} m_i(\lambda_l) p^2(\lambda_l) = \|p\boldsymbol{e}_i\|^2 = \|p\|_A^2 = \frac{1}{n}\sum_{l=0}^{d} m(\lambda_l)p^2(\lambda_l).$$

Then,

$$\sum_{l=1}^{d}\left(m_i(\lambda_l) - \frac{m(\lambda_l)}{n}\right)p^2(\lambda_l) = 0$$

since, as Γ is regular, $m_i(\lambda) = \frac{1}{n} = \frac{m(\lambda)}{n}$. Consequently, if $d \le \operatorname{dgr} p^2 = 2k \le d'$ or, equivalently, $d' = d$, the graph Γ is *multiplicity-regular* [21]:

$$m_i(\lambda_l) = \frac{m(\lambda_l)}{n} \quad (0 \le l \le d).$$

This result was proved for distance-regular graphs in [21] although, by sure, it was already known in the literature (without mentioning local multiplicities.) The more general result for walk-regular graphs is also a direct consequence of the results in [15].

In our context, an important consequence of Lemma 3.5 is that, for a d'-partially walk-regular graph, the adjacency polynomial Q_k ($k \le \lfloor \frac{d'}{2} \rfloor$ if $d' < d$) has as coefficients the solution of the following optimization problem: Let $Q_k = a_0 + a_1x + \cdots + a_kx^k$. Then,

`maximize` $Q_k(\lambda)$

`subject to` $\sum_{l=0}^{d} m(\lambda_l)Q_k^2(\lambda_l) = n$.

The following result gives a solution to this problem.

Proposition 3.6 *Let Γ be a d'-partially walk-regular graph as above. Let $\{p_k\}$ be a sequence of orthogonal polynomials, with respect to the scalar product $\langle f, g\rangle_A = \sum_{l=0}^{d} \frac{m(\lambda_l)}{n} f(\lambda_l)g(\lambda_l)$, normalized in such a way that $\|p_k\|_A^2 = p_k(\lambda)$, $0 \le k \le d$. Let $q_k = \sum_{\tau=0}^{k} p_\tau$. Then, the k-adjacency polynomial of Γ is*

$$Q_k = \frac{q_k}{\sqrt{q_k(\lambda)}}$$

for any $0 \le k \le \lfloor \frac{d'}{2} \rfloor$ (whenever $d' < d$), or $0 \le k \le d$ (if $d' = d$.)

Proof. Consider a generic polynomial $p \in \mathbb{R}_k[x]$ given in terms of the basis $\{p_k\}$, that is $p = \sum_{\tau=0}^{k} a_\tau p_\tau$. Let $k_\tau = \|p_\tau\|_A^2 = p_\tau(\lambda)$. Then the maximization of the function

$$\psi(a_0, a_1, \ldots, a_k) = p(\lambda) = \sum_{\tau=0}^{k} a_\tau p_\tau(\lambda) = \sum_{\tau=0}^{k} a_\tau k_\tau$$

under the condition

$$\|p\|_A^2 = \sum_{\tau=0}^{k} \|a_\tau p_\tau\|_A^2 = \sum_{\tau=0}^{k} a_\tau^2 k_\tau = 1,$$

gives $a_\tau = 1/\sqrt{q_k(\lambda)}$, $0 \le \tau \le k$. $\square$

Moreover, in [21] it was shown that the polynomials $q_k = \sum_{\tau=0}^{d} p_\tau$, $(0 \le k \le d)$ of Proposition 3.6 form an orthogonal system with respect to the scalar product

$$\langle f, g\rangle^* = \sum_{l=1}^{d} \frac{(\lambda_0 - \lambda_l)m(\lambda_l)}{n} f(\lambda_l)g(\lambda_l) = \lambda_0 \langle f, g\rangle_A - \langle xf, g\rangle_A. \tag{35}$$

Hence, the same properties are shared by the k-adjacency polynomials Q_k of a d'-partially walk-regular graph Γ (assuming that $k \le \lfloor \frac{d'}{2} \rfloor$ if $d' < d$.)

The following result, to be compared with (8), is a consequence of Corollary 3.2 and the above proposition.

Corollary 3.7 *Let Γ be a d'-partially walk-regular graph as above. Then,*

$$q_k(\lambda) > n - 1 \;\Rightarrow\; D(\Gamma) \le k. \quad \square$$

Example 3.8 *Let O denote the graph of the octahedron. Then the graph $\Gamma = L^2 O$ (that is, the line graph of the line graph of O) is a vertex symmetric graph with spectrum $\mathrm{S}(\Gamma) = \{10^1, 6^3, 4^2, 2^6, -2^{24}\}$ Then, its corresponding polynomials $q_k = \sqrt{q_k(\lambda)}Q_k$, $0 \le k \le 4$, and their values at $\lambda = 10$ are:*

- $q_0 = 1$, *1;*
- $q_1 = x + 1$, *11;*
- $q_2 = \frac{1005}{2426}\left(x^2 - \frac{142}{67}x - \frac{7624}{1005}\right)$, *29.50...;*
- $q_3 = \frac{5907}{65104}\left(x^3 - \frac{11820}{1969}x^2 - \frac{6100}{1969}x + \frac{50640}{1969}\right)$, *35.78...;*
- $q_4 = \frac{1}{64}\left(x^4 - 10x^3 + 20x^2 + 40x - 96\right)$, *36;*

Therefore, since $q_3(\lambda) > n - 1$, Corollary 3.7 gives $D(\Gamma) \le 3$, which is the exact value of the diameter. Note also that, according to previous comments, q_4 is, in fact, the Hoffman polynomial H.

3.2 Partially distance-regular graphs

An example of partially walk-regular graphs are those graphs having a 'partial distance-regularity' around every of their vertices. More precisely, let Γ be a regular graph with adjacency matrix $\boldsymbol{A}$ and diameter D, and let $D' \leq D$ be the maximum integer such that, for any $0 \leq \tau \leq D'$ there exist a polynomial v_τ of degree τ such that $v_\tau(\boldsymbol{A})$ is the so-called *τ-distance matrix*, defined by

$$(v_\tau(\boldsymbol{A}))_{ij} = \begin{cases} 1 & \text{if } \partial(e_i, e_j) = \tau, \\ 0 & \text{otherwise.} \end{cases}$$

Then it is said that Γ is a *D'-partially distance-regular* graph. For instance, note that every regular graph is 1-partially distance-regular, since two obvious examples of τ-distance matrices are $\boldsymbol{I}$ ($v_0 = 1$) and $\boldsymbol{A}$ itself ($v_1 = x$.) In fact, if Γ has girth g, simple reasoning shows that $D' \geq \lfloor (g-1)/2 \rfloor$, with $v_0 = 1$, $v_1 = x$, $v_2 = x^2 - \delta$, and $v_\tau = x v_{\tau-1} - (\delta - 1) v_{\tau-2}$ ($3 \leq \tau \leq D'$), see Biggs [3]. The *distance polynomials* v_τ, $0 \leq \tau \leq D'$, of a D'-partially distance-regular graph, are orthogonal with respect to the scalar product $\langle f, g \rangle_A$ defined above since, for $\sigma \neq \tau$,

$$0 = \operatorname{tr}(v_\sigma(\boldsymbol{A}) v_\tau(\boldsymbol{A})) = \sum_{l=0}^{d} m(\lambda_l) v_\sigma(\lambda_l) v_\tau(\lambda_l) = n \langle v_\sigma, v_\tau \rangle_A.$$

Furthermore, for $\sigma = \tau$ we get

$$\|v_\tau\|_A^2 = \langle v_\tau, v_\tau \rangle_A = \frac{1}{n} \operatorname{tr}(v_\tau^2(\boldsymbol{A})) = \frac{1}{n} \sum_{i=1}^{n} |\Gamma_\tau(e_i)|,$$

but the number of vertices at distance τ from e_i does not depend on i since $|\Gamma_\tau(e_i)| = \langle v_\tau \boldsymbol{e}_i, \boldsymbol{j} \rangle = \langle \boldsymbol{e}_i, v_\tau \boldsymbol{j} \rangle = \langle \frac{1}{n}\boldsymbol{j} + \boldsymbol{z}_i, v_\tau(\lambda)\boldsymbol{j} \rangle = v_\tau(\lambda)$. Hence $\|v_\tau\|_A^2 = v_\tau(\lambda) \equiv k_\tau$, and $\{v_\tau\}$ is the sequence of polynomials satisfying the hypotheses of Proposition 3.6.

In fact any D'-partially distance-regular graph is also $2D'$-partially walk-regular since, for any $k = s + t \leq 2D'$, $s \leq t \leq D'$, we have:

$$(\boldsymbol{A}^k)_{ii} = \langle x^k \boldsymbol{e}_i, \boldsymbol{e}_i \rangle = \langle x^s \boldsymbol{e}_i, x^t \boldsymbol{e}_i \rangle = \langle \sum_{\sigma=0}^{s} a_\sigma v_\sigma \boldsymbol{e}_i, \sum_{\tau=0}^{t} b_\tau v_\tau \boldsymbol{e}_i \rangle = \sum_{\sigma=0}^{s} a_\sigma b_\sigma \|v_\sigma \boldsymbol{e}_i\|^2$$

where a_σ and b_σ are the Fourier coefficients of x^s and x^t with respect to the basis $\{v_\tau\}$, respectively (and so they do not depend on i) and, from the above, $\|v_\sigma \boldsymbol{e}_i\|^2 = \|v_\sigma\|_A^2 = k_\sigma$. Thus, a more explicit formula for $(\boldsymbol{A}^k)_{ii}$ is:

$$(\boldsymbol{A}^k)_{ii} = \sum_{\sigma=0}^{s} \frac{\langle x^s, v_\sigma \rangle_A}{\|v_\sigma\|_A^2} \frac{\langle x^t, v_\sigma \rangle_A}{\|v_\sigma\|_A^2} k_\sigma = \sum_{\sigma=0}^{s} \frac{\langle x^k, v_\sigma \rangle_A}{\|v_\sigma\|_A^2} = \frac{1}{n} \sum_{\sigma=0}^{s} \sum_{l=0}^{d} m(\lambda_l) \lambda_l^k \frac{v_\sigma(\lambda_l)}{k_\sigma}.$$

Corollary 3.9 *Let* Γ *be a* D'*-partially distance-regular graph. Then, the* k*-adjacency polynomial is*

$$Q_k = \frac{w_k}{\sqrt{w_k(\lambda)}} \quad (0 \le k \le D')$$

where $w_k = \sum_{\tau=0}^{k} v_\tau$. $\square$

4 The diameter of a graph and its spectrum

Here we present a unified approach to the previous results, by considering both the alternating and the adjacency polynomials.

Theorem 4.1 *Let* $\Gamma = (V, E)$ *be a graph with adjacency matrix* $\boldsymbol{A}$*, and eigenvalues* $\lambda > \lambda_1 > \cdots > \lambda_d$*. Let* $\boldsymbol{\nu}$ *be the positive eigenvector associated to* λ*. Let* P_k *denote the* k*-alternating polynomial on the mesh* $\{\lambda_1, \ldots, \lambda_d\}$*. Let* Q_σ *and* Q_τ *be the corresponding adjacency polynomials of* Γ*. Then,*

$$P_k(\lambda) > \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{Q_\sigma^2(\lambda)} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{Q_\tau^2(\lambda)} - 1\right)} \Rightarrow \; D(\Gamma) \le k + \sigma + \tau. \tag{36}$$

Proof. Let $\boldsymbol{A}$ be the adjacency matrix of Γ. Let $\boldsymbol{e}_i$ be the ith coordinate vector. Then, using again decomposition (9),

$$\|Q_\sigma \boldsymbol{e}_i\|^2 = \left\| Q_\sigma \left(\frac{\nu_i}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_i \right) \right\|^2 = \frac{\nu_i^2}{\|\boldsymbol{\nu}\|^2} Q_\sigma^2(\lambda) + \|Q_\sigma \boldsymbol{z}_i\|^2$$

Thus, we get

$$\begin{aligned}
(P_k Q_\sigma Q_\tau(\boldsymbol{A}))_{ij} &= \langle P_k Q_\sigma \boldsymbol{e}_i, Q_\tau \boldsymbol{e}_j \rangle \\
&= \left\langle P_k Q_\sigma \left(\frac{\nu_i}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_i \right), Q_\tau \left(\frac{\nu_j}{\|\boldsymbol{\nu}\|^2}\boldsymbol{\nu} + \boldsymbol{z}_j \right) \right\rangle \\
&= P_k(\lambda) \frac{\nu_i \nu_j}{\|\boldsymbol{\nu}\|^2} Q_\sigma(\lambda) Q_\tau(\lambda) + \langle P_k Q_\sigma \boldsymbol{z}_i, Q_\tau \boldsymbol{z}_j \rangle \\
&\ge P_k(\lambda) \frac{Q_\sigma(\lambda) Q_\tau(\lambda)}{\|\boldsymbol{\nu}\|^2} + \langle P_k Q_\sigma \boldsymbol{z}_i, Q_\tau \boldsymbol{z}_j \rangle.
\end{aligned}$$

Moreover, since $\|Q_\sigma \boldsymbol{e}_i\| \le \|Q_\sigma\|_A = 1$ and $\nu_i \ge 1$, we have $\|Q_\sigma \boldsymbol{z}_i\|^2 \le 1 - \frac{Q_\sigma^2(\lambda)}{\|\boldsymbol{\nu}\|^2}$, and hence

$$\begin{aligned}
|\langle P_k Q_\sigma \boldsymbol{z}_i, Q_\tau \boldsymbol{z}_j \rangle| &\le \|P_k Q_\sigma \boldsymbol{z}_i\| \|Q_\tau \boldsymbol{z}_j\| \le \|P_k\|_\infty \|Q_\sigma \boldsymbol{z}_i\| \|Q_\tau \boldsymbol{z}_j\| \\
&\le \sqrt{\left(1 - \frac{Q_\sigma^2(\lambda)}{\|\boldsymbol{\nu}\|^2}\right)\left(1 - \frac{Q_\tau^2(\lambda)}{\|\boldsymbol{\nu}\|^2}\right)} \\
&\le \frac{Q_\sigma(\lambda) Q_\tau(\lambda)}{\|\boldsymbol{\nu}\|^2} \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{Q_\sigma^2(\lambda)} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{Q_\tau^2(\lambda)} - 1\right)}
\end{aligned}$$

since $\|P_k(\boldsymbol{A})|_{\boldsymbol{\nu}^\perp}\| = \|P_k\|_\infty = 1$. Therefore,

$$(P_k Q_\sigma Q_\tau(\boldsymbol{A}))_{ij} \geq \frac{Q_\sigma(\lambda) Q_\tau(\lambda)}{\|\boldsymbol{\nu}\|^2} \left(P_k(\lambda) - \sqrt{\left(\frac{\|\boldsymbol{\nu}\|^2}{Q_\sigma^2(\lambda)} - 1\right)\left(\frac{\|\boldsymbol{\nu}\|^2}{Q_\tau^2(\lambda)} - 1\right)} \right) > 0$$

so that $\partial(e_i, e_j) \leq k + \sigma + \tau$, and hence $D(\Gamma) \leq k + \sigma + \tau$ as claimed. □

In particular, for $\sigma = \tau$, we get

$$P_k(\lambda) > \frac{\|\boldsymbol{\nu}\|^2}{Q_\tau^2(\lambda)} - 1 \Rightarrow D(\Gamma) \leq k + 2\tau. \tag{37}$$

As, for any graph, the 1-adjacency polynomial is given by (34), we have $Q_1^2(\lambda) = \frac{\Delta+\lambda^2}{\Delta}$, and hence:

Corollary 4.2 *Let* Γ *be a graph as above. Then,*

$$P_k(\lambda) > \frac{\|\boldsymbol{\nu}\|^2}{1 + (\lambda^2/\Delta)} - 1 \Rightarrow D(\Gamma) \leq k + 2. \quad \square \tag{38}$$

In particular, taking $k = 0$ ($P_0 = 1$), we obtain the following condition for Γ to have diameter at most two:

$$\lambda > \sqrt{\Delta\left(\frac{\|\boldsymbol{\nu}\|^2}{2} - 1\right)} \Rightarrow D(\Gamma) \leq 2 \tag{39}$$

which, for δ-regular graphs, reads $\lambda = \delta \geq \lfloor n/2 \rfloor \Rightarrow D(\Gamma) \leq 2$ (trivial.)

Another consequence of Theorem 4.1, corresponding to Corollary 3.2(b), is obtained when we take $k = \tau = 0$ ($P_0 = Q_0 = 1$):

Corollary 4.3 *Let* Γ *be a graph as above. Then,*

$$Q_\sigma(\lambda) > \sqrt{\|\boldsymbol{\nu}\|^2 - 1} \Rightarrow D(\Gamma) \leq \sigma. \quad \square \tag{40}$$

The similarity between the results (7) and (40) deserves a comparative study. With this aim, note first that the value of $P_k(\lambda)$ is obtained using only the eigenvalues of the graph. Thus, intuitively speaking, the successive steps

$$\boldsymbol{A} \rightarrow \mathrm{S}(\Gamma) \rightarrow \{\lambda > \lambda_1 > \cdots > \lambda_d\} \rightarrow P_k(\lambda)$$

progressively weaken the precision that a result about some property of Γ, deduced from some condition on $P_k(\lambda)$, can have. Consequently, it seems that the corresponding condition on the value $Q_k(\lambda)$, obtained from the whole spectrum of Γ, should lead to a stronger result. The following proposition shows that, at least for regular graphs, this is the case for (7) and (40).

Proposition 4.4 *Let Γ be a regular graph on n vertices, with eigenvalues $\lambda > \lambda_1 > \cdots > \lambda_d$. Then, for any $1 \le k \le d$,*

$$P_k(\lambda) > n-1 \Rightarrow Q_k^2(\lambda) > n-1.$$

Proof. Let e_i be a vertex such that $\|P_k \boldsymbol{e}_i\| = \|P_k\|_A = \max_{1\le j\le n}\{\|P_k \boldsymbol{e}_j\|\}$. Since

$$\|P_k \boldsymbol{e}_i\|^2 = \frac{P_k^2(\lambda)}{n} + \|P_k \boldsymbol{z}_i\|^2 \le \frac{P_k^2(\lambda)}{n} + 1 - \frac{1}{n}\,,$$

the vector

$$\frac{\sqrt{n}}{\sqrt{P_k^2(\lambda)+n-1}} P_k \boldsymbol{e}_i$$

has norm ≤ 1. Hence, from the choice of $\boldsymbol{e}_i$ and the definition of Q_k,

$$Q_k(\lambda) \ge \frac{\sqrt{n}P_k(\lambda)}{\sqrt{P_k^2(\lambda)+n-1}}$$

and so, using the hypothesis,

$$Q_k^2(\lambda) \ge \frac{nP_k^2(\lambda)}{P_k^2(\lambda)+n-1} = n - \frac{n^2-n}{P_k^2(\lambda)+n-1} > n-1. \quad \square$$

To show that the converse of the above result does not hold, we can consider again the graph $\Gamma = L^2O$ in the example of Section 3. Indeed, we already saw that such a graph has $Q_3^2(\lambda) = q_3(10) = 35.78\ldots > n-1 = 35$, whereas its 3-alternating polynomial is $P_3 = \frac{3}{32}x^3 - \frac{5}{8}x^2 + \frac{1}{8}x + \frac{5}{2}$, which gives $P_3(10) = 35$ (L^2O is a boundary graph.)

Going back to the consequences of Theorem 4.1, we can use Corollary 3.9 to derive a result for D'-partially walk-regular graphs.

Corollary 4.5 *Let Γ be a D'-partially distance-regular graph on n vertices. Then, for any $0 \le \sigma, \tau \le D'$,*

$$P_k(\lambda) > \sqrt{\left(\frac{n}{q_\sigma(\lambda)} - 1\right)\left(\frac{n}{q_\tau(\lambda)} - 1\right)} \Rightarrow D(\Gamma) \le k + \sigma + \tau. \quad \square \tag{41}$$

In particular, if Γ has girth g and $\sigma = \tau = \ell$, we have $q_\ell(\lambda) = n(\delta, \ell)$ and the above corollary gives (20).

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