Some Families of Orthogonal Polynomials of a Discrete Variable and their Applications to Graphs and Codes *

M. Cámara, J. Fàbrega, M.A. Fiol and E. Garriga

Departament de Matemàtica Aplicada IV
Universitat Politècnica de Catalunya
Jordi Girona 1-3 , Mòdul C3, Campus Nord
08034 Barcelona, Catalonia (Spain).

September 15, 2008

Abstract

We present some related families of orthogonal polynomials of a discrete variable and survey some of their applications in the study of (distance-regular) graphs and (completely regular) codes. One of the main peculiarities of such orthogonal systems is their non-standard normalization condition, requiring that the square norm of each polynomial must equal its value at a given point of the mesh. For instance, when they are defined from the spectrum of a graph, one of these families is the system of the pre-distance polinomials which, in the case of distance-regular graphs, turns out to be the sequence of distance polinomials. The applications range from (quasi-spectral) characterizations of distance-regular graphs, walk-regular graphs, local distance-regularity and completely regular codes, to some results on representation theory.

1 Introduction

The theory of orthogonal polynomials is a well-developed area of mathematics and it has a large number of applications in the study of both theoretical and practical problems. Two standard references on this topic are the classic textbook of Szegö [25] and Chihara's work [4] which puts more emphasis on the discrete case.

In particular, different sequences of orthogonal polynomials have important applications in algebraic combinatorics. For instance, as described by Godsil [22], some examples of such sequences are the matching polynomials of the complete graphs and the rook polynomials of the complete bipartite graphs. Another example studied in the same reference is the application of orthogonal polynomials in the study of polynomial spaces.

In the area of graph theory, we find the Chebyshev polynomials (of the second kind) when studying the characteristic polynomials of the paths. Another recent application in this area has been done by Chung, Faber and Manteuffel [5], and Van Dam and Haemers [8], who gave upper bounds on the diameter of a graph in terms of its spectrum by using Chebyshev polynomials shifted to a proper interval.

In the same area, one of the most important applications of orthogonal polynomials, not always sufficiently exploited in opinion of the authors, is the study of distance-regularity of graphs and related codes. Since their introduction, distance-regular graphs and their main generalization, the association schemes, have proved to be a key concept in algebraic combinatorics. They have important connections with other branches of mathematics, such as geometry, coding theory, group theory, design theory, as well as with other areas of graph theory. As stated in the preface of the comprehensive textbook of Brouwer, Cohen and Neumaier [3], this is because most finite objects bearing "enough regularity" are closely related to certain distance-regular graphs. Other basic references on distance-regular graphs are Biggs [2], with a good introduction to distance-transitive graphs, and Bannai and Ito [1] where the connection with the theory of distance-regular graphs is emphasized.

The aim of this paper is to convince the reader of the importance and possibilities of some families of orthogonal polynomials in the study of different (local and global) concepts of distance-regularity in graphs. With this aim, we describe in detail three of such families and survey some of their recent applications. We believe that these applications do not exhaust all the possibilities and hope that much more will be given in the near future. Thus, one of the more recent application of one of these families, the so-called predistance polynomials, has been in the study of a kind of partial distance-regularity in graphs (the so-called k-walk-regular graphs), which as extreme cases includes both distance-regular and walk-regular graphs; see [6].

The plan of the paper is as follows. In the next section we present some new families of orthogonal polynomials of a discrete variable, which have recently shown very useful in the study of distance-regular graphs and their related concepts, such as local distance-regularity and completely regular codes. One of the main peculiarities of such orthogonal systems is their non-standard normalization condition, requiring that the square norm of each polynomial must equal its value at a given point of the mesh. Then, to illustrate the usefulness of such polynomials, we discuss in Section 3 some of their applications in the area of algebraic graph theory. More specially, we study some results concerning the concept of distance-regularity, defined in Subsection 3.3, and we will survey some results obtained from the study of two different meshes and its corresponding orthogonal canonical

system: the local spectrum of a given graph, defined in Subsection 3.2, and the spectrum of a subset of its vertex set, defined in Subsection 3.7.

2   On orthogonal polynomials of a discrete variable

In this section we begin by surveying some known results about orthogonal polynomials of a discrete variable. In order to do this paper more accessible to readers not familiarized with this topic, we have included all the proofs. Afterwards, we describe three new families of such polynomials: The canonical orthogonal system, their dual polynomials and their conjugate. We begin by presenting some notation and basic facts.

Let $\mathcal{M} := \{\lambda_0, \lambda_1, \cdots, \lambda_d\}$, $\lambda_0 > \lambda_1 > \cdots > \lambda_d$, be a mesh of real numbers. A real function of a discrete variable $f : \mathcal{M} \longrightarrow \mathbb{R}$ can be seen as the restriction on $\mathcal{M}$ of a number of functions of real variable. Moreover, if we only consider polynomial functions, the class of possible extensions of one discrete function on $\mathcal{M}$ constitute an element of the quotient algebra $\mathbb{R}[x]/(Z)$ where (Z) is the ideal generated by the polynomial $Z := \prod_{l=0}^{d}(x - \lambda_l)$. Each class has a unique canonical representative of degree at most d. Denoting by $\mathcal{F}(\mathcal{M})$ the set of functions on the mesh, we then have the following natural identifications:

$$\mathcal{F}(\mathcal{M}) \longleftrightarrow \mathbb{R}[x]/(Z) \longleftrightarrow \mathbb{R}_d[x]. \tag{1}$$

For simplicity, we represent by the same symbol, say p, any of the three mathematical objects identified in (1). When we need to point out some of the above three sets, we will make it explicit.

A positive function $g : \mathcal{M} \longrightarrow \mathbb{R}$ will be called a *weight function* on $\mathcal{M}$. We say that it is *normalized* when $g(\lambda_0) + g(\lambda_1) + \cdots + g(\lambda_d) = 1$. We shall write, for short, $g_l := g(\lambda_l)$. From the pair $(\mathcal{M}, g)$ we can define an inner product in $\mathbb{R}_d[x]$ (indistinctly in $\mathcal{F}(\mathcal{M})$ or in $\mathbb{R}[x]/(Z)$) as

$$\langle p, q \rangle := \sum_{l=0}^{d} g_l p(\lambda_l) q(\lambda_l), \qquad p, q \in \mathbb{R}_d[x], \tag{2}$$

with corresponding norm $\| \cdot \|$. From now on, this will be referred to as *the scalar product associated to* $(\mathcal{M}, g)$. Note that $\langle 1, 1 \rangle = 1$ is the condition concering the normalized character of the weight function g, which will be hereafter assumed.

In order to simplify some expressions, it is useful to introduce the following moment-like parameters, computed from the points of the mesh $\mathcal{M}$,

$$\pi_k := \prod_{l=0\,(l \neq k)}^{d} |\lambda_k - \lambda_l| = (-1)^k \prod_{l=0\,(l \neq k)}^{d} (\lambda_k - \lambda_l) \qquad (0 \leq k \leq d); \tag{3}$$

and the family of interpolating polynomials (with degree d):

$$Z_k := \frac{(-1)^k}{\pi_k} \prod_{l=0 \, (l \neq k)}^{d} (x - \lambda_l) \qquad (0 \leq k \leq d), \tag{4}$$

which satisfy:

$$Z_k(\lambda_h) = \delta_{hk}, \qquad \langle Z_h, Z_k \rangle = \delta_{hk} g_k. \tag{5}$$

Then, using Lagrange interpolation, $p = \sum_{k=0}^{d} p(\lambda_k) Z_k$ for any $p \in \mathbb{R}_d[x]$. In particular, when $p = x^i$, $i = 0, 1, \ldots, d$, we get $x^i = \sum_{k=0}^{d} \lambda_k^i Z_k$ whence, equating the terms with degree d,

$$\sum_{k=0}^{d} \frac{(-1)^k}{\pi_k} \lambda_k^i = 0 \quad (0 \leq i \leq d-1), \qquad \sum_{k=0}^{d} \frac{(-1)^k}{\pi_k} \lambda_k^d = 1. \tag{6}$$

2.1 Forms and orthogonal systems

Each real number λ induces a linear form on $\mathbb{R}_d[x]$, defined by $[\lambda](p) := p(\lambda)$. Then, the first equality in (5) can be interpreted by saying that the forms $[\lambda_0]$, $[\lambda_1]$, ..., $[\lambda_d]$ are the dual basis of the polynomials Z_0, Z_1, ..., Z_d. The scalar product associated to $(\mathcal{M}, g)$ induces an isomorphism between the space $\mathbb{R}_d[x]$ and its dual, where each polynomial p corresponds to the form ω_p, defined as $\omega_p(q) := \langle p, q \rangle$ and, reciprocally, each form ω is associated to a polynomial p_ω through $\langle p_\omega, q \rangle = \omega(q)$. By observing how the isomorphism acts on the bases $\{[\lambda_l]\}_{0 \leq l \leq d}$, $\{Z_l\}_{0 \leq l \leq d}$, we get the expressions:

$$\omega_p = \sum_{l=0}^{d} g_l p(\lambda_l) [\lambda_l], \qquad p_\omega = \sum_{l=0}^{d} \frac{1}{g_l} \omega(Z_l) Z_l. \tag{7}$$

In particular, the polynomial corresponding to $[\lambda_k]$ is

$$\begin{aligned} H_k \quad &:= \quad p_{[\lambda_k]} = \sum_{l=0}^{d} \frac{1}{g_l} [\lambda_k](Z_l) Z_l = \sum_{l=0}^{d} \frac{1}{g_l} \delta_{lk} Z_l \\ &= \quad \frac{1}{g_k} Z_k = \frac{(-1)^k}{g_k \pi_k} (x - \lambda_0) \cdots (\widehat{x - \lambda_k}) \cdots (x - \lambda_d), \end{aligned}$$

and their scalar products are:

$$\langle H_h, H_k \rangle = [\lambda_h](H_k) = H_k(\lambda_h) = \frac{1}{g_h} \delta_{hk}, \tag{8}$$

where $(\widehat{x - \lambda_k})$ denotes that this factor is not present in the product. Moreover, property (6) is equivalent to stating that the form $\sum_{k=0}^{d} \frac{(-1)^k}{\pi_k} [\lambda_k]$ annihilates on the space $\mathbb{R}_{d-1}[x]$.

4

Lemma 2.1 *In the space $\mathbb{R}_d[x]$, let us consider the scalar product associated to $(\mathcal{M}, g)$. Then, the polynomial*

$$T := \sum_{k=0}^{d} \frac{(-1)^k}{\pi_k} H_k = \sum_{k=0}^{d} \frac{1}{g_k \pi_k^2} (x - \lambda_0) \cdots (\widehat{x - \lambda_k}) \cdots (x - \lambda_d)$$

verify the following:

(a) *T is orthogonal to $\mathbb{R}_{d-1}[x]$;*

(b) *$\|T\|^2 = \displaystyle\sum_{k=0}^{d} \frac{1}{g_k \pi_k^2}$;*

(c) *$T(\lambda_0) = \dfrac{1}{g_0 \pi_0}$.*

Proof. The proof of (a) is straightforward by considering the form ω_T associated to T, whereas (b) and (c) are proved by simple computations:

$$\|T\|^2 = \sum_{h,k=0}^{d} \frac{(-1)^{h+k}}{\pi_h \pi_k} \langle H_h, H_k \rangle = \sum_{k=0}^{d} \frac{1}{g_k \pi_k^2};$$

$$T(\lambda_0) = \sum_{k=0}^{d} \frac{(-1)^k}{\pi_k} H_k(\lambda_0) = \frac{1}{g_0 \pi_0}. \quad \square$$

A family of polynomials $r_0, r_1, \ldots, r_d$ is said to be an *orthogonal system* when each polynomial r_k is of degree k and $\langle r_h, r_k \rangle = 0$ for any $h \neq k$.

Proposition 2.2 *Every orthogonal system $r_0, r_1, \ldots, r_d$ satisfies the following properties:*

(a) *There exists a tridiagonal matrix $\boldsymbol{R}$ (called the recurrence matrix of the system) such that, in $\mathbb{R}[x]/(Z)$:*

$$x\boldsymbol{r} := x \begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ \vdots \\ r_{d-2} \\ r_{d-1} \\ r_d \end{pmatrix} = \begin{pmatrix} a_0 & c_1 & 0 & & & & \\ b_0 & a_1 & c_2 & 0 & & & \\ 0 & b_1 & a_2 & \ddots & \ddots & & \\ & 0 & \ddots & \ddots & \ddots & 0 & \\ & & \ddots & \ddots & a_{d-2} & c_{d-1} & 0 \\ & & & 0 & b_{d-2} & a_{d-1} & c_d \\ & & & & 0 & b_{d-1} & a_d \end{pmatrix} \begin{pmatrix} r_0 \\ r_1 \\ r_2 \\ \vdots \\ r_{d-2} \\ r_{d-1} \\ r_d \end{pmatrix} = \boldsymbol{R}\boldsymbol{r},$$

and this equality, in $\mathbb{R}[x]$, reads:

$$x\boldsymbol{r} = \boldsymbol{R}\boldsymbol{r} + \begin{pmatrix} 0 & 0 & \cdots & 0 & \dfrac{\|r_d\|^2}{r_d(\lambda_0)} \dfrac{1}{g_0 \pi_0} Z \end{pmatrix}^{\top}.$$

5

(b) *All the entries b_k, c_k, of matrix $\boldsymbol{R}$ are nonnull and satisfy $b_k c_{k+1} > 0$.*

(c) *The matrix $\boldsymbol{R}$ diagonalizes with eigenvalues the elements of $\mathcal{M}$. An eigenvector associated to λ_k is $(r_0(\lambda_k), r_1(\lambda_k), \ldots, r_{d-1}(\lambda_k), r_d(\lambda_k))^\top$.*

(d) *For every $k = 1, \ldots, d$ the polynomial r_k has real simple roots. If $\mathcal{M}_k$ denotes the mesh of the ordered roots of r_k, then (the points of) the mesh $\mathcal{M}_d$ interlaces $\mathcal{M}$ and, for each $k = 1, 2, \ldots, d-1$, $\mathcal{M}_k$ interlaces $\mathcal{M}_{k+1}$.*

Proof. (a) Working in $\mathbb{R}[x]/(Z)$, we have $\langle xr_k, r_h \rangle = 0$ provided that $k < h-1$ and, by symmetry, the result is also zero when $h < k-1$. Therefore we can write, for any $k = 0, 1, \ldots, d$,

$$xr_k = \sum_{h=0}^{d} \frac{\langle xr_k, r_h \rangle}{\|r_h\|^2} r_h = \sum_{h=\max\{0, k-1\}}^{\min\{k+1, d\}} \frac{\langle xr_k, r_h \rangle}{\|r_h\|^2} r_h = b_{k-1} r_{k-1} + a_k r_k + c_{k+1} r_{k+1},$$

where, in order to uniform the notation, we have introduced the null formal terms $b_{-1} r_{-1}$, and $c_{d+1} r_{d+1}$. Then, for any $k = 0, 1, \ldots, d$ the parameters b_k, a_k, c_k are defined by:

$$b_k = \frac{\langle xr_{k+1}, r_k \rangle}{\|r_k\|^2} \quad (0 \le k \le d-1), \qquad b_d = 0,$$

$$a_k = \frac{\langle xr_k, r_k \rangle}{\|r_k\|^2} \quad (0 \le k \le d),$$

$$c_0 = 0, \qquad c_k = \frac{\langle xr_{k-1}, r_k \rangle}{\|r_k\|^2} \quad (1 \le k \le d).$$

Given any $k = 0, 1, \ldots, d$ let $Z_k^* := \prod_{l=0, l \ne k}^{d}(x - \lambda_l) = \xi_0 r_d + \xi_1 r_{d-1} + \cdots$, where notice that ξ_0 does not depend on k. Thus,

$$\langle r_d, Z_k^* \rangle = g_k r_d(\lambda_k)(-1)^k \pi_k = \xi_0 \|r_d\|^2 = g_0 r_d(\lambda_0) \pi_0 \ne 0. \tag{9}$$

Moreover, for any $k = 0, 1, \ldots, d$, we get:

$$r_d - \frac{\|r_d\|^2}{r_d(\lambda_0)} \frac{1}{g_0 \pi_0} Z_k^* \in \mathbb{R}_{d-1}[x], \qquad \frac{r_d(\lambda_k)}{r_d(\lambda_0)} = (-1)^k \frac{g_0 \pi_0}{g_k \pi_k}. \tag{10}$$

Then, the equality $xr_d = b_{d-1} r_{d-1} + a_d r_d$, holding in $\mathbb{R}[x]/(Z)$, and the comparison of the degrees allows us to stablish the existence of $\psi \in \mathbb{R}$ such that $xr_d = b_{d-1} r_{d-1} + a_d r_d + \psi Z$ in $\mathbb{R}[x]$. Noticing that ψ is the first coefficient of r_d, we get, from (10),

$$\psi = \frac{\|r_d\|^2}{r_d(\lambda_0)} \frac{1}{g_0 \pi_0}.$$

(b) By looking again to the degrees, we realize that $c_1, c_2, \ldots, c_d$ are nonzero. For $k = 0, 1, \ldots, d-1$, we have, from the equality

$$b_k = \frac{\langle xr_{k+1}, r_k \rangle}{\|r_k\|^2} = \frac{\langle xr_k, r_{k+1} \rangle}{\|r_{k+1}\|^2} \frac{\|r_{k+1}\|^2}{\|r_k\|^2} = \frac{\|r_{k+1}\|^2}{\|r_k\|^2} c_{k+1},$$

6

that the parameters $b_0, b_1, \ldots, b_{d-1}$ are also nonnull and, moreover, $b_k c_{k+1} > 0$ for any $k = 0, 1, \ldots, d - 1$.

(c) This result follows immediately if we evaluate, in $\mathbb{R}[x]$ and for each λ_k, the matrix equation obtained in (a).

(d) From (10) we observe that r_d takes alternating signs on the points of $\mathcal{M}$. Hence, this polynomial has d simple roots whose mesh $\mathcal{M}_d$ interlaces $\mathcal{M}$. Noticing that Z takes alternating signs over the elements of $\mathcal{M}_d$, from the equality $b_{d-1} r_{d-1} = (x - a_d) r_d - \psi Z$ it turns out that r_{d-1} takes alternating signs on the elements of $\mathcal{M}_d$; whence $\mathcal{M}_{d-1}$ interlaces $\mathcal{M}_d$ and r_d has alternating signs on $\mathcal{M}_{d-1}$. Recursively, suppose that, for $k = 1, \ldots, d-2$, the polynomials r_{k+1} and r_{k+2} have simple real roots and that $\mathcal{M}_{k+1}$ interlaces $\mathcal{M}_{k+2}$, so that r_{k+2} takes alternating signs on $\mathcal{M}_{k+1}$. Then, the result follows by just evaluating the equality $b_k r_k = (x - a_{k+1}) r_{k+1} - c_{k+2} r_{k+2}$ at the points of $\mathcal{M}_{k+1}$. $\quad\square$

2.2   The canonical orthogonal system

Consider the space $\mathbb{R}_d[x]$ with the scalar product associated to $(\mathcal{M}, g)$. From the identification of such a space with its dual by contraction of the scalar product, the form $[\lambda_0] : p \to p(\lambda_0)$ is represented by the polynomial $H_0 = \frac{1}{g_0 \pi_0}(x - \lambda_1) \cdots (x - \lambda_d)$ through $\langle H_0, p \rangle = p(\lambda_0)$.

For any given $0 \le k \le d - 1$, let $q_k \in \mathbb{R}_k[x]$ denote the orthogonal projection of H_0 over $\mathbb{R}_k[x]$. Alternatively, the polynomial q_k can be defined as the unique polynomial in $\mathbb{R}_k[x]$ such that

$$\|H_0 - q_k\| = \min\{\|H_0 - q\| : q \in \mathbb{R}_k[x]\}.$$

(See Fig. 1.) Let $\mathcal{S}$ denote the sphere in $\mathbb{R}_d[x]$ such that 0 and H_0 are antipodal points on it; that is, the sphere with center $\frac{1}{2}H_0$ and radius $\frac{1}{2}\|H_0\|$. Notice that its equation $\|p - \frac{1}{2}H_0\|^2 = \frac{1}{4}\|H_0\|^2$ can also be written as $\|p\|^2 = \langle H_0, p \rangle = p(\lambda_0)$. Consequently,

$$\mathcal{S} = \{p \in \mathbb{R}_d[x] : \|p\|^2 = p(\lambda_0)\} = \{p \in \mathbb{R}_d[x] : \langle H_0 - p, p \rangle = 0\}.$$

Note also that the projection q_k is on the sphere $\mathcal{S}_k := \mathcal{S} \cap \mathbb{R}_k[x]$ since, in particular, $\langle H_0 - q_k, q_k \rangle = 0$.

Proposition 2.3 *The polynomial q_k, which is the orthogonal projection of H_0 on $\mathbb{R}_k[x]$, can be defined as the unique polynomial of $\mathbb{R}_k[x]$ satisfying*

$$\langle H_0, q_k \rangle = q_k(\lambda_0) = \max\{q(\lambda_0) : \text{ for all } q \in \mathcal{S}_k\},$$

where $\mathcal{S}_k$ is the sphere $\{q \in \mathbb{R}_k[x] : \|q\|^2 = q(\lambda_0)\}$. Equivalently, q_k is the antipodal point of the origin in $\mathcal{S}_k$.

Proof. Since q_k is orthogonal to $H_0 - q_k$, we have $\|q_k\|^2 + \|H_0 - q_k\|^2 = \|H_0\|^2 = \frac{1}{g_0}$. Then, as $q_k \in \mathcal{S}_k$ we get

$$
\begin{aligned}
q_k(\lambda_0) &= \|q_k\|^2 = \frac{1}{g_0} - \|H_0 - q_k\|^2 = \frac{1}{g_0} - \min\{\|H_0 - q\|^2 : \text{ for all } q \in \mathcal{S}_k\} = \\
&= \max\{\|q\|^2 : \text{ for all } q \in \mathcal{S}_k\} = \max\{q(\lambda_0) : \text{ for all } q \in \mathcal{S}_k\}.
\end{aligned}
$$

Considering the equivalent form $\|q_k\| = \max\{\|q\| : \text{ for all } q \in \mathcal{S}_k\}$, the proof is complete.
$\square$
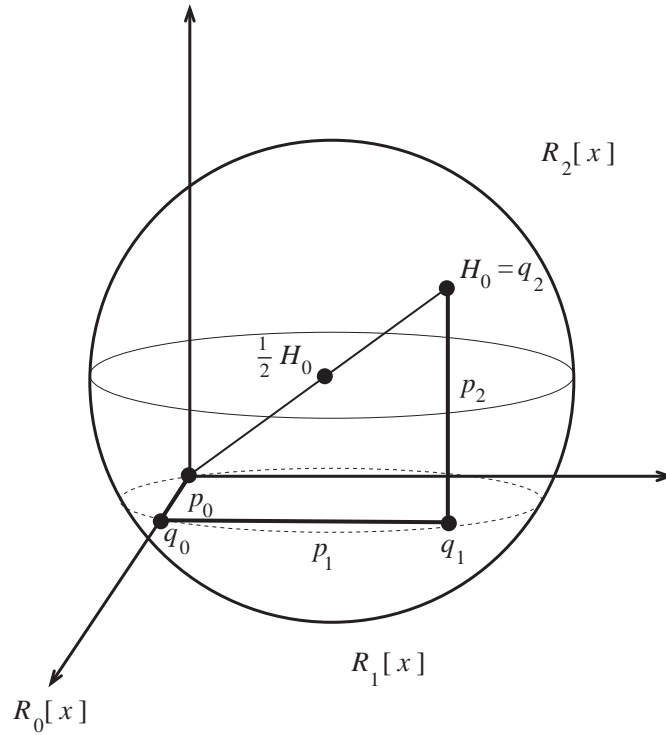
Figure 1: Obtaining the q's and the p's by projecting H_0.

With the notation $q_d := H_0$, we obtain the family of polynomials q_0, q_1, ..., q_{d-1}, q_d. Let us remark some of their properties.

Corollary 2.4 *The polynomials q_0, q_1, ..., q_{d-1}, q_d, satisfy the following:*

(a) *Each q_k has degree exactly k.*

(b) $1 = q_0(\lambda_0) < q_1(\lambda_0) < \cdots < q_{d-1}(\lambda_0) < q_d(\lambda_0) = \dfrac{1}{g_0}$.

(c) *The polynomials $q_0, q_1, \ldots, q_{d-1}$ constitute an orthogonal system with respect to the scalar product associated to the mesh $\{\lambda_1 > \lambda_2 > \cdots > \lambda_d\}$ and the weight function $\lambda_k \mapsto (\lambda_0 - \lambda_k) g_k$, $k = 1, \ldots, d$.*

Proof. (*a*) Notice that $\mathcal{S}_0 = \{0, 1\}$. Consequently, $q_0 = 1$. Assume that q_{k-1} has degree $k-1$, but q_k has degree lesser than k. Because of the uniqueness of the projection, $q_k = q_{k-1}$ and $H_0 - q_{k-1}$ would be orthogonal to $\mathbb{R}_k[x]$. In particular,

$$
\begin{aligned}
0 &= \langle H_0 - q_{k-1}, (x - \lambda_0) q_{k-1} \rangle = \langle (x - \lambda_0) H_0 - (x - \lambda_0) q_{k-1}, q_{k-1} \rangle \\
&= \langle (\lambda_0 - x) q_{k-1}, q_{k-1} \rangle = \sum_{l=0}^{d} g_l (\lambda_0 - \lambda_l) q_{k-1}^2 (\lambda_l).
\end{aligned}
$$

Hence, $q_{k-1}(\lambda_l) = 0$ for any $1 \le l \le d$ and q_{k-1} would be null.

(*b*) If $q_{k-1}(\lambda_0) = q_k(\lambda_0)$, from Proposition 2.3 we would get $q_{k-1} = q_k$, which is not possible because of (*a*).

(*c*) Let $0 \le h < k \le d - 1$. Since $H_0 - q_k$ is orthogonal to $\mathbb{R}_k[x]$ we have, in particular, that

$$
\begin{aligned}
0 &= \langle H_0 - q_k, (x - \lambda_0) q_h \rangle = \langle (x - \lambda_0) H_0 - (x - \lambda_0) q_k, q_h \rangle = \langle (\lambda_0 - x) q_k, q_h \rangle = \\
&= \sum_{l=0}^{d} g_l (\lambda_0 - \lambda_l) q_k(\lambda_l) q_h(\lambda_l) = \sum_{l=1}^{d} (\lambda_0 - \lambda_l) g_l q_k(\lambda_l) q_h(\lambda_l),
\end{aligned}
$$

stablishing the claimed orthogonality. $\square$

The polynomial q_k, as the orthogonal projection of H_0 over $\mathbb{R}_k[x]$, can also be seen as the orthogonal projection of q_{k+1} over $\mathbb{R}_k[x]$, as $q_{k+1} - q_k = H_0 - q_k - (H_0 - q_{k+1})$ is orthogonal to $\mathbb{R}_k[x]$. Consider the family of polynomials defined as

$$
p_0 := q_0 = 1, \ p_1 := q_1 - q_0, \ p_2 := q_2 - q_1, \ldots,
$$
$$
p_{d-1} := q_{d-1} - q_{d-2}, \ p_d := q_d - q_{d-1} = H_0 - q_{d-1}. \tag{11}
$$

Note that, then, $q_k = p_0 + p_1 + \cdots + p_k$ ($0 \le k \le d$), and, in particular, $p_0 + p_1 + \cdots + p_d = H_0$. Let us now begin the study of the polynomials $(p_k)_{0 \le k \le d}$.

Proposition 2.5 *The polynomials $p_0, p_1, \ldots, p_{d-1}, p_d$ constitute an orthogonal system with respect to the scalar product associated to $(\mathcal{M}, g)$.*

Proof. From $p_k = q_k - q_{k-1}$ we see that p_k has degree k. Moreover, we have already seen that $p_k = q_k - q_{k-1}$ is orthogonal to $\mathbb{R}_{k-1}[x]$, whence the polynomials p_k form an orthogonal system. $\square$

The sequence of polynomials $(p_k)_{0 \le k \le d}$, defined in (11), will be called the *canonical orthogonal system* associated to $(\mathcal{M}, g)$. The next result gives three different characterizations of such systems.

9

Proposition 2.6 *Let $r_0, r_1, \ldots, r_{d-1}, r_d$ be an orthogonal system with respect to the scalar product associated to $(\mathcal{M}, g)$. Then the following assertions are all equivalent:*

(a) *$(r_k)_{0 \leq k \leq d}$ is the canonical orthogonal system associated to $(\mathcal{M}, g)$;*

(b) *$r_0 = 1$ and the entries of the recurrence matrix $\boldsymbol{R}$ associated to $(r_k)_{0 \leq k \leq d}$, satisfy $a_k + b_k + c_k = \lambda_0$, for any $k = 0, 1, \ldots, d$;*

(c) *$r_0 + r_1 + \cdots + r_d = H_0$;*

(d) *$\|r_k\|^2 = r_k(\lambda_0)$ for any $k = 0, 1, \ldots, d$.*

Proof. Let $(p_k)_{0 \leq k \leq d}$ be the canonical orthogonal system associated to $(\mathcal{M}, g)$. The space $\mathbb{R}_k[x] \cap \mathbb{R}_{k-1}^{\perp}[x]$ has dimension one, and hence the polynomials r_k, p_k are proporcional: $r_k = \xi_k p_k$. Let $\boldsymbol{j} := (\ 1 \quad 1 \quad \cdots \quad 1\ )^{\top}$.

$(a) \Rightarrow (b)$: We have $r_0 = p_0 = 1$. Consider the recurrence matrix $\boldsymbol{R}$ (Proposition 2.2) associated to the canonical orthogonal system $(r_k)_{0 \leq k \leq d} = (p_k)_{0 \leq k \leq d}$. Then, computing xq_d en $\mathbb{R}[x]/(Z)$ in two different ways we get:

$$
\begin{aligned}
xq_d &= x\sum_{k=0}^{d} p_k = x\boldsymbol{j}^{\top}\boldsymbol{p} = \boldsymbol{j}^{\top}\boldsymbol{R}\boldsymbol{p} = (\ a_0 + b_0 \quad c_1 + a_1 + b_1 \quad \cdots \quad c_d + a_d\ )^{\top}\boldsymbol{p} = \\
&= \sum_{k=0}^{d}(a_k + b_k + c_k)p_k\ ; \\
xq_d &= xH_0 = \lambda_0 H_0 = \sum_{k=0}^{d} \lambda_0 p_k\ ,
\end{aligned}
$$

and, from the linear independence of the polynomials p_k, we get $a_k + b_k + c_k = \lambda_0$.

$(b) \Rightarrow (c)$: Working in $\mathbb{R}[x]/(Z)$ and from $x\boldsymbol{r} = \boldsymbol{R}\boldsymbol{r}$, we have:

$$
0 = \boldsymbol{j}^{\top}(x\boldsymbol{r} - \boldsymbol{R}\boldsymbol{r}) = x\sum_{k=0}^{d} r_k - \boldsymbol{j}^{\top}\boldsymbol{R}\boldsymbol{r} = x\sum_{k=0}^{d} r_k - \lambda_0 \boldsymbol{j}^{\top}\boldsymbol{r} = (x - \lambda_0)\sum_{k=0}^{d} r_k\ .
$$

Therefore there exists ξ such that $\sum_{k=0}^{d} r_k = \xi H_0 = \sum_{k=0}^{d} \xi p_k$. Since, also, $\sum_{k=0}^{d} r_k = \sum_{k=0}^{d} \xi_k p_k$, where $\xi_0 = 1$, it turns out that $\xi_0 = \xi_1 = \cdots = \xi_d = \xi = 1$. Consequently, $\sum_{k=0}^{d} r_k = H_0$.

$(c) \Rightarrow (d)$: $\|r_k\|^2 = \langle r_k, r_0 + r_1 + \cdots + r_d \rangle = \langle r_k, H_0 \rangle = r_k(\lambda_0)$.

$(d) \Rightarrow (a)$: From $r_k = \xi_k p_k$, we have $\xi_k^2 \|p_k\|^2 = \|r_k\|^2 = r_k(\lambda_0) = \xi_k p_k(\lambda_0) = \xi_k \|p_k\|^2$. Whence $\xi_k = 1$ and $r_k = p_k$. $\quad \square$

Corollary 2.7 *The highest degree polynomial p_d of the canonical orthogonal system associatet to $(\mathcal{M}, g)$ satisfies the following:*

(a) $p_d = \left(\sum_{l=0}^d \dfrac{g_0 \pi_0}{g_l \pi_l^2} \right)^{-1} \sum_{k=0}^d \dfrac{1}{g_k \pi_k^2} (x - \lambda_0) \cdots \widehat{(x - \lambda_k)} \cdots (x - \lambda_d)$;

(b) $p_d(\lambda_0) = \dfrac{1}{g_0} \left(\sum_{l=0}^d \dfrac{g_0 \pi_0^2}{g_l \pi_l^2} \right)^{-1}$; $\qquad p_d(\lambda_k) = (-1)^k \dfrac{g_0 \pi_0}{g_k \pi_k} p_d(\lambda_0) \quad (1 \le k \le d)$.

Proof. Recalling that the polynomial $T = \sum_{k=0}^d \frac{(-1)^k}{\pi_k} H_k$, introduced in Lemma 2.1, is orthogonal to $\mathbb{R}_{d-1}[x]$, there exists a constant ξ such that $p_d = \xi T$. From $\|p_d\|^2 = p_d(\lambda_0)$, we then obtain $p_d = \frac{T(\lambda_0)}{\|T\|^2} T$. Substituting into this formula the values of $T(\lambda_0)$ and $\|T\|^2$, given also in Lemma 2.1, we obtain the claimed expressions for p_d, $p_d(\lambda_0)$ and $p_d(\lambda_k)$. $\qquad \square$

From the last equality of Corollary 2.7 we get:

$$g_k = g_0 \frac{\pi_0}{\pi_k} \frac{p_d(\lambda_0)}{(-1)^k p_d(\lambda_k)} \qquad (0 \le k \le d) \tag{12}$$

which, together with the normalization of g, implies that, given $\mathcal{M}$, the knowledge of p_d allows us to reconstruct the weight function.

2.3   The conjugate canonical orthogonal system

Consider a given mesh $\mathcal{M} = \{\lambda_0 > \lambda_1 > \cdots > \lambda_d\}$. As we have seen, each normalized weight function $g : \mathcal{M} \to \mathbb{R}$ induces a scalar product and its corresponding canonical orthogonal system $(p_k)_{0 \le k \le d}$. Moreover, we know that its recurrence matrix $\boldsymbol{R}$, given in Proposition 2.2, satisfies:

$$x\boldsymbol{p} = \boldsymbol{R}\boldsymbol{p}, \qquad \boldsymbol{j}^\top \boldsymbol{R} = \lambda_0 \boldsymbol{j}^\top, \tag{13}$$

where $\boldsymbol{p}$ and $\boldsymbol{j}$ are the column matrices $(\, p_0 \quad p_1 \quad \cdots \quad p_d \,)^\top$ and $(\, 1 \quad 1 \quad \cdots \quad 1 \,)^\top$, respectively.

Given an $n \times m$ matrix $\boldsymbol{A} = (a_{ij})$ we denote by $\boldsymbol{A}^\star$ the $n \times m$ matrix with (i, j)-entry $a_{n-i+1, m-j+1}$, which results by applying a central symmetry to $\boldsymbol{A}$. It is immediate to check that $(\lambda \boldsymbol{A} + \mu \boldsymbol{B})^\star = \lambda \boldsymbol{A}^\star + \mu \boldsymbol{B}^\star$ and $(\boldsymbol{AB})^\star = \boldsymbol{A}^\star \boldsymbol{B}^\star$. The square $(d+1)$-matrix $\boldsymbol{S}$ with null entries excepting those on the principal antidiagonal which are 1's, satisfies $\boldsymbol{S}^\top = \boldsymbol{S}^{-1} = \boldsymbol{S}$ and, when $\boldsymbol{A}$ is any square $(d+1)$-matrix, $\boldsymbol{A}^\star = \boldsymbol{SAS}$.

The polynomial p_d has an inverse in $\mathbb{R}[x]/(Z)$ and, therefore, we can define $\tilde{p}_k := p_d^{-1} p_{d-k}$ for any $k = 0, 1, \ldots, d$. Then, with the notation

$$\tilde{\boldsymbol{p}} := (\, \tilde{p}_0 \quad \tilde{p}_1 \quad \cdots \quad \tilde{p}_d \,)^\top = p_d^{-1} \boldsymbol{p}^\star = (\, p_d^{-1} p_d \quad p_d^{-1} p_{d-1} \quad \cdots \quad p_d^{-1} p_0 \,)^\top$$

we obtain, from (13),

$$x\tilde{\boldsymbol{p}} = \boldsymbol{R}^\star \tilde{\boldsymbol{p}}, \qquad \boldsymbol{j}^\top \boldsymbol{R}^\star = \lambda_0 \boldsymbol{j}^\top. \tag{14}$$

The entries of the tridiagonal matrix $\boldsymbol{R}^\star$, which, according to the notation of Proposition 2.2, are denoted by $\tilde{a}_k, \tilde{b}_k, \tilde{c}_k$, are defined by: $\tilde{a}_k = a_{d-k}$, $\tilde{b}_k = c_{d-k}$, $\tilde{c}_k = b_{d-k}$ and $\tilde{a}_k + \tilde{b}_k + \tilde{c}_k = \lambda_0$, for $k = 0, 1, \ldots, d$. Since $\tilde{b}_k \tilde{c}_{k+1} = c_{d-k} b_{d-k-1} > 0$ and $\tilde{p}_0 = 1$ it turns out that each $\tilde{p}_k$ has degree k.

Let $\boldsymbol{P}$, respectively $\tilde{\boldsymbol{P}}$, denote the square $(d+1)$-matrix with (i,j)-entry $p_i(\lambda_j)$, respectively $\tilde{p}_i(\lambda_j)$, $0 \leq i, j \leq d$. Also, let us consider the following diagonal matrices $\boldsymbol{D} := \operatorname{diag}(\|p_0\|^2, \|p_1\|^2, \ldots, \|p_d\|^2)$, $\tilde{\boldsymbol{D}} := \operatorname{diag}(\tilde{p}_0(\lambda_0), \tilde{p}_1(\lambda_0), \ldots, \tilde{p}_d(\lambda_0))$, $\boldsymbol{P}_d := \operatorname{diag}(p_d(\lambda_0), p_d(\lambda_1), \ldots, p_d(\lambda_d))$, and $\boldsymbol{G} := \operatorname{diag}(g_0, g_1, \ldots, g_d)$. Now, we have the following facts:

(a) The sequence $(p_k)_{0 \leq k \leq d}$ is the canonical orthogonal system with respect to the inner product associated to $(\mathcal{M}, g)$ if and only if $\operatorname{dgr} p_k = k$, $0 \leq k \leq d$, and

$$\boldsymbol{P}\boldsymbol{G}\boldsymbol{P}^\top = \boldsymbol{D}; \tag{15}$$

(b) By the definition of $\tilde{\boldsymbol{P}}$ we immediately have $\tilde{\boldsymbol{P}} = \boldsymbol{S}\boldsymbol{P}\boldsymbol{P}_d^{-1}$;

(c) Similarly, from the definition of $\tilde{\boldsymbol{D}}$, we get $\tilde{\boldsymbol{D}} = p_d^{-1}(\lambda_0)\boldsymbol{S}\boldsymbol{D}\boldsymbol{S}$.

Then, the following computation

$$\begin{aligned} \tilde{\boldsymbol{P}}\left(p_d^{-1}(\lambda_0)\boldsymbol{P}_d\boldsymbol{G}\boldsymbol{P}_d\right)\tilde{\boldsymbol{P}}^\top &= p_d^{-1}(\lambda_0)\tilde{\boldsymbol{P}}\boldsymbol{P}_d\boldsymbol{G}\boldsymbol{P}_d\tilde{\boldsymbol{P}}^\top \\ &= p_d^{-1}(\lambda_0)\boldsymbol{S}\boldsymbol{P}\boldsymbol{P}_d^{-1}\boldsymbol{P}_d\boldsymbol{G}\boldsymbol{P}_d\boldsymbol{P}_d^{-1}\boldsymbol{P}^\top\boldsymbol{S} \\ &= p_d^{-1}(\lambda_0)\boldsymbol{S}\boldsymbol{P}\boldsymbol{G}\boldsymbol{P}^\top\boldsymbol{S} = p_d^{-1}(\lambda_0)\boldsymbol{S}\boldsymbol{D}\boldsymbol{S} = \tilde{\boldsymbol{D}}, \end{aligned}$$

stablishes that the family of polynomials $(\tilde{p}_k)_{0 \leq k \leq d}$, with $\operatorname{dgr} \tilde{p}_k = k$, $0 \leq k \leq d$, is the canonical orthogonal system with respect to the product $(\mathcal{M}, \tilde{g})$, where, using Corollary 2.7, $\tilde{g}_k := \tilde{g}(\lambda_k)$ corresponds to the expression:

$$\begin{aligned} \tilde{g}_k &= p_d^{-1}(\lambda_0)\left(\boldsymbol{P}_d\boldsymbol{G}\boldsymbol{P}_d\right)_{kk} = p_d^{-1}(\lambda_0)g_k p_d^2(\lambda_k) \\ &= g_0 \frac{g_0 \pi_0^2}{g_k \pi_k^2} p_d(\lambda_0) = \frac{g_0 \pi_0^2}{g_k \pi_k^2}\left(\sum_{l=0}^d \frac{g_0 \pi_0^2}{g_l \pi_l^2}\right)^{-1}. \end{aligned} \tag{16}$$

Note that, in particular, $\tilde{g} : \mathcal{M} \to \mathbb{R}$ is a normalized weight function on $\mathcal{M}$. All the above facts are summarized in the following result:

Proposition 2.8 *Given a mesh* $\mathcal{M} = \{\lambda_0 > \lambda_1 > \cdots > \lambda_d\}$, *we associate, to each normalized weight function* $g : \mathcal{M} \to \mathbb{R}$, *a new weight function* $\tilde{g} : \mathcal{M} \to \mathbb{R}$, *which is also normalized, defined as:*

$$\tilde{g}_k = \frac{g_0 \pi_0^2}{g_k \pi_k^2}\left(\sum_{l=0}^d \frac{g_0 \pi_0^2}{g_l \pi_l^2}\right)^{-1} \qquad (0 \leq k \leq d).$$

Then the respective canonical orthogonal systems:

$(p_k)_{0 \leq k \leq d}$ *with respect to* $\langle p, q \rangle = \sum_{l=0}^{d} g_l p(\lambda_l) q(\lambda_l)$; *and*

$(\tilde{p}_k)_{0 \leq k \leq d}$ *with respect to* $\langle p, q \rangle^{\check{}} := \sum_{l=0}^{d} \tilde{g}_l p(\lambda_l) q(\lambda_l)$;

are related by $\tilde{p}_k = p_d^{-1} p_{d-k}$, $0 \leq k \leq d$, *and the respective recurrence matrices,* $\boldsymbol{R}$ *and* $\tilde{\boldsymbol{R}}$, *coincide up to a central symmetry.*

Corollary 2.9 *The mapping* $g \mapsto \tilde{g}$, *defined on the set of normalized weight functions on* $\mathcal{M}$, *is involutive.*

Proof. The result follows immediately from the fact that $\tilde{\boldsymbol{R}}$ is the matrix obtained by applying a central symmetry to $\boldsymbol{R}$. Or, alternatively, since $\tilde{p}_d = p_d^{-1}$ we have: $\tilde{p}_d^{-1} \tilde{p}_{d-k} = p_d p_d^{-1} p_k = p_k$. Whence, using (12), it turns out that the conjugate weight function of $\tilde{g}$ is g itself. $\square$

We shall say that the weight functions g and $\tilde{g}$, the respective scalar products, and the corresponding canonical orthogonal systems are mutually *conjugate*.

2.4   The dual canonical polynomials

Associated to the canonical polynomials, there is another set of orthogonal polynomials, which are called the "dual (canonical) polynomials". In order to introduce them, notice that the orthogonality property in (15) can also be written as $\boldsymbol{P}^\top \boldsymbol{D}^{-1} \boldsymbol{P} = \boldsymbol{G}^{-1}$. This may be rewritten, in turn, as

$$\widehat{\boldsymbol{P}} \boldsymbol{D} \widehat{\boldsymbol{P}}^\top = \boldsymbol{G}^{-1}, \tag{17}$$

where we have introduced the new matrix $\widehat{\boldsymbol{P}} := \boldsymbol{P}^\top \boldsymbol{D}^{-1}$. Then, note that (17) can also be interpreted as an orthogonality property, with respect to the scalar product

$$\langle p, q \rangle^* := \sum_{l=0}^{d} \|p_l\|^2 p(\lambda_l) q(\lambda_l) \tag{18}$$

for the new polynomials $\hat{p}_k$, $0 \leq k \leq d$, defined as

$$\hat{p}_k(\lambda_l) := (\widehat{\boldsymbol{P}})_{kl} = \frac{p_l(\lambda_k)}{\|p_l\|^2} = \frac{p_l(\lambda_k)}{p_l(\lambda_0)} \qquad (0 \leq l \leq d), \tag{19}$$

and which will be called the *dual polynomials* of the p_k. Thus, (17) reads

$$\langle \hat{p}_k, \hat{p}_l \rangle^* = \delta_{kl} g_l^{-1} \qquad (0 \leq k, l \leq d), \tag{20}$$

whence, using (18), the values of the weight function can be computed from the polynomials $(p_k)_{0 \le k \le d}$ as:

$$g_l = \frac{1}{(\|\hat{p}_l\|^*)^2} = \left(\sum_{k=0}^{d} \frac{p_k(\lambda_l)^2}{p_k(\lambda_0)} \right)^{-1}. \tag{21}$$

This is an alternative formula to (12).

Moreover, we have already seen, in Proposition 2.2(c) that the l-th column of $\boldsymbol{P}$, namely $(p_0(\lambda_l), p_1(\lambda_l), \ldots, p_d(\lambda_l))^\top$, is an eigenvector of the tridiagonal recurrence matrix $\boldsymbol{R}$, with eigenvalue λ_l. That is,

$$\boldsymbol{R}\boldsymbol{P} = \boldsymbol{P}\boldsymbol{D}_\lambda, \tag{22}$$

where $\boldsymbol{D}_\lambda := \mathrm{diag}(\lambda_0, \lambda_1, \ldots, \lambda_d)$. Similarly, from (15) and the definition of $\widehat{\boldsymbol{P}}$ we see that $\boldsymbol{P}^{-1} = \boldsymbol{G}\boldsymbol{P}^\top \boldsymbol{D}^{-1} = \boldsymbol{G}\widehat{\boldsymbol{P}}$. Then, (22) yields

$$\widehat{\boldsymbol{P}}\boldsymbol{R} = \boldsymbol{D}_\lambda\widehat{\boldsymbol{P}}. \tag{23}$$

That is, the k-th row of $\widehat{\boldsymbol{P}}$,

$$(\hat{p}_k(\lambda_0), \hat{p}_k(\lambda_1), \ldots, \hat{p}_k(\lambda_d)) = \left(\frac{p_0(\lambda_k)}{p_0(\lambda_0)}, \frac{p_1(\lambda_k)}{p_1(\lambda_0)}, \ldots, \frac{p_d(\lambda_k)}{p_d(\lambda_0)} \right),$$

is a left eigenvector of $\boldsymbol{R}$ with eigenvalue λ_k.

The *number of sign-changes* in a given sequence of real numbers is the number of times that consecutive terms (after removing the null ones) have distinct sign. Thus, if $(p_k)_{0 \le k \le d}$ is a (canonical) orthogonal system, the fact that $\mathrm{dgr}\, p_k = k$ implies that the sequence $p_k(\lambda_0), p_k(\lambda_1), \ldots, p_k(\lambda_d)$ has exactly k sign-changes. Although the degrees of the dual polynomials $(\hat{p}_k)_{0 \le k \le d}$ does not necessarily coincide with their indexes, they keep the above property and the sequence $\hat{p}_l(\lambda_0), \hat{p}_l(\lambda_1), \ldots, \hat{p}_l(\lambda_d)$ also has exactly l sign-changes. This is a direct consequence of a known result about orthogonal polynomials (see e.g. [25, 22]), which we formally state in the the next lemma, and prove it by considering the "equivalent" sequence $p_0(\lambda_l), p_1(\lambda_l), \ldots, p_d(\lambda_l)$ (since $p_k(\lambda_0) > 0$ for any $0 \le k \le d$).

Lemma 2.10 *Let $(p_k)_{0 \le k \le d}$ be a sequence of orthogonal polynomials and let $\lambda_0 > \lambda_1 > \cdots > \lambda_d$ be the zeros of p_{d+1}. Then, for any given $0 \le l \le d$, the sequence $p_0(\lambda_l), p_1(\lambda_l), \ldots, p_d(\lambda_l)$ has exactly l sign-changes.*

Proof. We know that, between any two consecutive zeros of p_{k+1}, there lies one zero of p_k. With this in mind, this could be seen as a "proof without words"; consider Fig. 2: The number of sign-changes coincide with the crossed "staircases". $\square$

A "non-visual" proof of this result can be found in Godsil [22]. Moreover, since each column of the recurrence matrix sums to λ_0, we also have the following corollary:
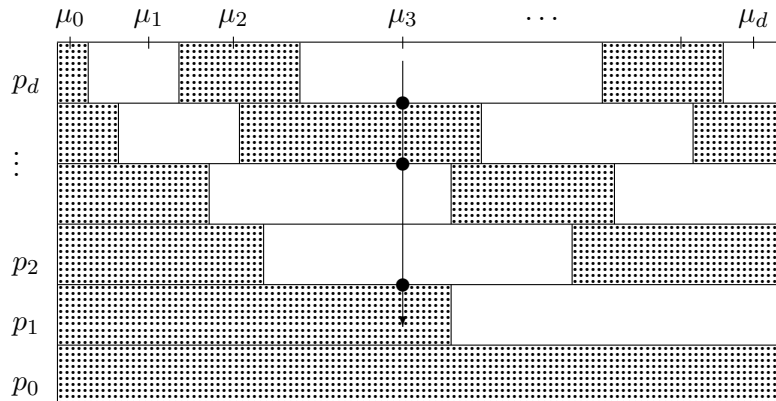
Figure 2: Proof of Lemma 2.10.

Corollary 2.11 *Let us consider a recurrence with coefficients satisfying $a_k + b_k + c_k = \mu_0$, $0 \le k \le d$. Then, for any $1 \le l \le d$, the sequence $\hat{p}_l(\lambda_0) - \hat{p}_l(\lambda_1), \ldots, \hat{p}_l(\lambda_{d-1}) - \hat{p}_l(\lambda_d)$ has exactly $l - 1$ sign-changes.*

Proof. Let $\boldsymbol{C}$ be the $(d+1) \times (d+1)$ matrix with 1's on the principal diagonal, -1's on the diagonal below the principal one, and 0's elsewhere. We know that $\widehat{\boldsymbol{P}}_l := (\hat{p}_l(\lambda_0), \hat{p}_l(\lambda_1), \ldots, \hat{p}_l(\lambda_d))$ is a (left) eigenvector of the recurrence matrix $\boldsymbol{R}$, so that $\widehat{\boldsymbol{P}}_l \boldsymbol{C}$ is an eigenvector of the (also tridiagonal) matrix $\boldsymbol{R}' := \boldsymbol{C}^{-1} \boldsymbol{R} \boldsymbol{C}$. From this, one deduces that $(\hat{p}_l(\lambda_0) - \hat{p}_l(\lambda_1), \ldots, \hat{p}_l(\lambda_{d-1}) - \hat{p}_l(\lambda_d))$ is a left eigenvector of the $d \times d$ principal submatrix of $\boldsymbol{R}'$:

$$\begin{pmatrix} \lambda_0 - b_0 - c_1 & c_1 & & & & \\ b_1 & \lambda_0 - b_1 - c_2 & c_2 & & & \\ & b_2 & \cdot & & & \\ & & \cdot & \cdot & & \\ & & & \cdot & \cdot & c_{d-1} \\ & & & & b_{d-1} & \lambda_0 - b_{d-1} - c_d \end{pmatrix}$$

with corresponding eigenvalue $\lambda_l \in \operatorname{ev} \boldsymbol{R} \setminus \{\lambda_0\}$. Then the result follows from Lemma 2.10. □

3 Applications to graphs and codes

This section is devoted to discuss some applications of the results about orthogonal polynomials given in Section 1 to the area of algebraic graph theory. We are specially interested in the notion of distance-regularity, defined in Subsection 3.3, and we will survey some results obtained from the study of two different meshes and its corresponding orthogonal canonical system: the local spectrum of a given graph G, defined in Subsection 3.2, and the spectrum of a subset of its vertex set, defined in Subsection 3.7.

Throughout this section $G = (V, E)$ denotes a simple undirected graph with vertex set $V = \{1, 2, \ldots, n\}$ and edge set E. Two vertices $i \in V$ and $j \in V$ are adjacent if $\{i, j\} \in E$ and we denote it by $i \sim j$. A walk of length k from $i \in V$ to $j \in V$ is a finite sequence of vertices of G, $i = u_0, u_1, u_2, \ldots, u_k = j$, such that $u_t \sim u_{t+1}, 0 \leq t \leq k - 1$, and the minimum length of such a walk is the distance $\operatorname{dist}(i, j)$ between i and j. If there is no walk from i to j we write $\operatorname{dist}(i, j) = \infty$. The *k-apart* from a vertex i, $\Gamma_k(i)$, is the set of vertices at distance k from i, and the *k-neighbourhood* of i, $N_k(i)$, is the set of vertices at distance at most k from i, that is, $N_k(i) = \Gamma_0(i) \cup \Gamma_1(i) \cup \cdots \cup \Gamma_k(i)$. The *degree* of a vertex i is $\delta_i = |\Gamma_1(i)|$ and its eccentricity is $\operatorname{ecc}(i) = \max_{1 \leq j \leq n} \operatorname{dist}(i, j)$. Finally, the *diameter* of G is $D = D(G) = \max_{1 \leq i \leq n} \operatorname{ecc}(i)$ and its *radius* $r = r(G) = \min_{1 \leq i \leq n} \operatorname{ecc}(i)$. Notice that the diameter can be equivalently defined as the maximum distance between two vertices and G is connected if and only if $D(G) < \infty$.

3.1   Some algebraic-graph results

One of the most important tools in the study of the algebraic properties of a graph G is its *adjacency matrix*, $\boldsymbol{A} = \boldsymbol{A}(G)$, which is the $n \times n$ matrix with entries

$$(\boldsymbol{A})_{ij} = \begin{cases} 1 & \text{if } i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Since G is taken to be a simple undirected graph, $\boldsymbol{A}(G)$ is a symmetric $(0,1)$-matrix with zero diagonal entries. We denote the characteristic polynomial of $\boldsymbol{A}(G)$ by $\phi_G(x)$ (since it is uniquely determined by the underlying graph G) and we will refer to it as the *characteristic polynomial of G*. The *spectrum* of G is the set of eigenvalues of $\boldsymbol{A}(G)$ together with their multiplicities, and we will write

$$\operatorname{sp} G := \operatorname{sp} \boldsymbol{A} = \{\lambda_0^{m(\lambda_0)}, \lambda_1^{m(\lambda_1)}, \ldots, \lambda_d^{m(\lambda_d)}\},$$

where $\lambda_0 > \lambda_1 > \ldots > \lambda_d$ and $m(\lambda_i)$ is the multiplicity of λ_i as a root of $\phi_G(x)$. Similarly,

$$\operatorname{ev} G := \{\lambda_0, \lambda_1, \ldots, \lambda_d\}$$

denotes the set of different eigenvalues of G. If we consider matrices and vectors indexed by the vertices of G and associate to any vertex $i \in V$ the i-th unitary vector $\boldsymbol{e}_i$ of the canonical basis of $\mathbb{R}^n$, we can interpret the adjacency matrix $\boldsymbol{A}$ as an endomorphism of $\mathbb{R}^n$, and the following equivalence holds:

$$\boldsymbol{A}\boldsymbol{u} = \lambda\boldsymbol{u} \quad \Longleftrightarrow \quad \sum_{j \sim i} u_j = \lambda u_i \qquad (1 \leq i \leq n).$$

Moreover, taking the mesh $\mathcal{M} = \operatorname{ev} G$ and proceeding as in (3) we can consider the moment-like parameters

$$\pi_l := \prod_{h=0, h \neq l}^{m} |\lambda_l - \lambda_h| \qquad (0 \leq l \leq d)$$

16

satisfying (6):

$$\sum_{l=0}^{m}(-1)^l\frac{\lambda_l^k}{\pi_l} = \begin{cases} 0 & \text{if } 0 \leq k < d \\ 1 & \text{if } k = d. \end{cases}$$

When G is connected, the Perron-Frobenius Theorem for nonnegative matrices guaranties that its largest eigenvalue, λ_0, is positive and simple and has an eigenvector $\boldsymbol{v} = (v_1, \ldots, v_n)$ with all its components positive. In particular we can normalize $\boldsymbol{v}$ in such a way that $\min_{1 \leq i \leq n} v_i = 1$. Given U a subset of the vertices of G, let $\boldsymbol{\rho}$ be the mapping defined by $\boldsymbol{\rho}U := \sum_{i \in U} v_i \boldsymbol{e}_i$. In what follows we suppose, for simplicity, that G is connected and δ-*regular*, that is $\delta_i = \delta$ for every $i \in V$. In this case, $\lambda_0 = \delta$ and $\boldsymbol{v} = \boldsymbol{j}$, the all-1 vector, and $\boldsymbol{\rho}U$ turns out to be the characteristic vector of U, that is, $(\boldsymbol{\rho}U)_i = 1$ if $i \in U$ and $(\boldsymbol{\rho}U)_i = 0$ otherwise.

The *adjacency algebra* $\mathcal{A}(G)$ of G is the algebra of polynomials in its adjacency matrix $\boldsymbol{A}$. A simple inductive argument proves that the number of walks of length k between vertices i and j is $(\boldsymbol{A}^k)_{ij}$ (see [2] for example). Therefore, if G has diameter D, then the set $\{\boldsymbol{I}, \boldsymbol{A}, \boldsymbol{A}^2, \ldots, \boldsymbol{A}^D\}$ is linearly independent in $\mathcal{A}(G)$, or to put it in another way, the dimension of $\mathcal{A}(G)$ is at least $D + 1$. Moreover, if G has $d + 1$ distinct eigenvalues, the minimum polynomial of $\boldsymbol{A}$ has degree d and the dimension of $\mathcal{A}(G)$ is $d+1$. This fact gives us an upper bound for the diameter of a connected graph G, namely $D \leq d = |\operatorname{ev} G| - 1$. When the equality holds, the diameter is spectrally maximal and we say that G is *extremal*.

3.2 Local spectrum

For each eigenvalue $\lambda_l \in \operatorname{sp} G$, let $\boldsymbol{U}_l$ be the matrix whose columns form an orthogonal basis for the eigenspace $\mathcal{E}_l := \operatorname{Ker}(\boldsymbol{A} - \lambda_l \boldsymbol{I})$ associated to λ_l. The *principal idempotents* of $\boldsymbol{A}$ are the matrices $\boldsymbol{E}_l := \boldsymbol{U}_i \boldsymbol{U}_l^\top$ representing the orthogonal projections onto $\mathcal{E}_l$. They can be obtainded by the formula $\boldsymbol{E}_l = Z_l(\boldsymbol{A})$, $0 \leq l \leq d$, where Z_l is the interpolating polynomial in (4) and $d = |\operatorname{ev} G| - 1$. In particular, $\boldsymbol{E}_0 = (\boldsymbol{v}\boldsymbol{v}^\top)/\|\boldsymbol{v}\|^2$. These matrices satisfy the following properties (see [22]):

(a) $\boldsymbol{E}_l \boldsymbol{E}_h = \begin{cases} \boldsymbol{E}_l, & \text{if } l = h \\ \boldsymbol{0}, & \text{otherwise}; \end{cases}$

(b) $\boldsymbol{A}\boldsymbol{E}_l = \lambda_l \boldsymbol{E}_l$;

(c) $p(\boldsymbol{A}) = \sum_{l=0}^{d} p(\lambda_l)\boldsymbol{E}_l$, for any $p \in \mathbb{R}[x]$.

By taking $p = 1$ in (c) we obtain $\sum_{l=0}^{d} \boldsymbol{E}_l = \boldsymbol{I}$, and for $p = x$ we get the so-called *Spectral Decomposition Theorem*:

$$\boldsymbol{A} = \sum_{l=0}^{d} \lambda_l \boldsymbol{E}_l.$$

17

More generally, taking $p = x^k$, each power of $\boldsymbol{A}$ can be expressed as a linear combination of the idempotents $\boldsymbol{E}_l$:

$$\boldsymbol{A}^k = \sum_{l=0}^{d} \lambda_l^k \boldsymbol{E}_l.$$

In [18], Fiol, Garriga and Yebra defined the *i-local multitplicity* of $\lambda_l \in \mathrm{ev}\, G$ as the square of the norm of the projection of $\boldsymbol{e}_i$ onto $\mathcal{E}_l$, $m_i(\lambda_l) = \|\boldsymbol{E}_l \boldsymbol{e}_i\|^2 \geq 0$ (in particular, $m_i(\lambda_0) = 1/\|\boldsymbol{v}\|^2$). Note that, since $\langle \boldsymbol{E}_l \boldsymbol{e}_i, \boldsymbol{E}_l \boldsymbol{e}_i \rangle = \langle \boldsymbol{E}_l \boldsymbol{e}_i, \boldsymbol{e}_i \rangle = (\boldsymbol{E}_l)_{ii}$, the i-local multiplicity coincides with the i-th entry of the diagonal of $\boldsymbol{E}_l$. Moreover, if $\mu_0 = \lambda_0 > \mu_1 > \ldots > \mu_{d_i}$ $(d_i \leq d)$ are the eigenvalues having not null i-local multiplicity, the above authors also defined the *i-local spectrum* as:

$$\mathrm{sp}_i\, G := \{\lambda_0^{m_i(\mu_0)}, \mu_1^{m_i(\mu_1)}, \ldots, \mu_m^{m_i(\mu_{d_i})}\}. \tag{24}$$

The name given to these parameters is justified by the fact that, when the graph "is seen" from a given vertex i, its local multiplicities play a role similar to that of the standard multiplicities. The following results from [18] support this claim.

Proposition 3.1 *The i-local multiplicities satisfy:*

(a) *For any vertex i,*

$$\sum_{l=0}^{d_i} m_i(\mu_l) = 1.$$

(b) *The multiplicity of an eigenvalue of G is the sum, extended to all vertices, of its local multiplicities:*

$$m(\lambda_l) = \sum_{i=1}^{n} m_i(\lambda_l) \quad (0 \leq l \leq d).$$

Proposition 3.2 *Let $i \in V$ be a vertex and let p denote a polynomial. Then,*

$$(p(\boldsymbol{A}))_{ii} = \sum_{l=0}^{d_i} m_i(\mu_l) p(\mu_l).$$

By taking $p = x^k$ we obtain the number of circuits of length k through (or rooted at) vertex i, namely $\mathcal{C}_i(k) = \sum_{l=0}^{d_i} m_i(\mu_l)\mu_l^k$.

Other facts support this interpretation of the local spectrum. Given a vertex i, its degree satisfies $\delta_i = \sum_{l=0}^{d_i} m_i(\mu_l)\mu_l^2$; in particular, $C_i(2) = \delta_i$. Furthermore, analogous to the relation of the diameter and the number of different eigenvalues, the eccentricity of

a vertex i of a connected graph is bounded above by the number of eigenvalues different from λ_0 in its local spectrum,

$$\text{ecc}(i) \leq d_i = |\text{ev}_i\, G| - 1.$$

Let us define the characteristic polynomial corresponding to the i-local spectrum, defined in (24), as

$$\phi_i(x) = \prod_{l=0}^{d_i} (x - \mu_l)^{m_i(\mu_l)}.$$

A graph G is said to be *spectrally regular* if all the vertices have the same local spectrum. The following proposition gives several characterizations of such a graph (see [10, 6]).

Proposition 3.3 *The following statements are equivalent:*

(a) *G is spectrally regular.*

(b) *$\phi_i = \phi_j$ for any $i, j \in V$.*

(c) *The i-local multiplicities only depend on λ_l, so that, $m_i(\lambda_l) = m(\lambda_l)/n$ for any $\lambda_l \in \text{ev}\, G$.*

(d) *G is walk regular, i.e. $\mathcal{C}_i(k)$ only depends on k.*

(e) *$\text{sp}\, G \setminus i = \text{sp}\, G \setminus j$ for any $i, j \in V$, where $G \setminus v$ is the graph obtained by deleting the vertex v from G.*

Moreover, we have

$$\frac{\phi_{G \setminus i}(x)}{\phi_G(x)} = \frac{\phi_i'(x)}{\phi_i(x)}.$$

3.3 Local distance-regularity and the local predistance polynomials

Let $i \in V$ be a vertex with eccentricity $\text{ecc}(i) = \varepsilon$ of a regular graph G. Let $V_k := \Gamma_k(i)$ and consider the numbers $c_k(j) := |\Gamma(j) \cap V_{k-1}|$, $a_k(j) := |\Gamma(j) \cap V_k|$, $b_k(j) := |\Gamma(j) \cap V_{k+1}|$, defined for any $j \in V_k$ and $0 \leq k \leq \varepsilon$ (where, by convention, $c_0(i) = 0$ and $b_\varepsilon(j) = 0$ for any $j \in V_\varepsilon$). We say that G is *distance-regular around i* whenever $c_k(j)$, $a_k(j)$, $b_k(j)$ do not depend on the considered vertex $j \in V_k$ but only on the value of k. In such a case, we simply denote them by c_k, a_k and b_k, respectively, and we call them the *intersection numbers*. The matrix

$$\mathcal{I}(i) := \begin{pmatrix} 0 & c_1 & \cdots & c_{\varepsilon-1} & c_\varepsilon \\ a_0 & a_1 & \cdots & a_{\varepsilon-1} & a_\varepsilon \\ b_0 & b_1 & \cdots & b_{\varepsilon-1} & 0 \end{pmatrix}$$
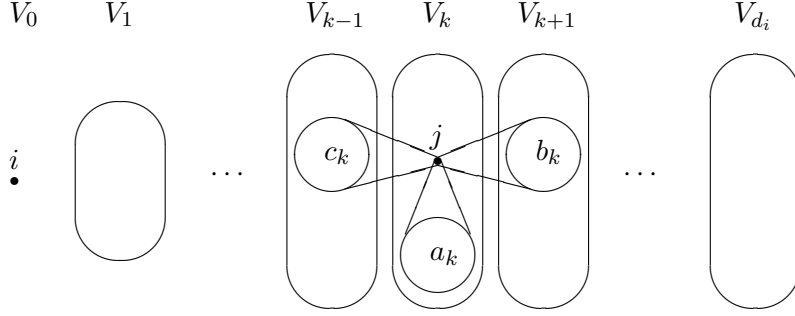
Figure 3: Intersection numbers.

is called the *intersection array around vertex i.*

A graph G is *distance-regular* when it is distance-regular around each of its vertices and with the same intersection array. In other words, if we consider the partition $\Pi(i)$ of $V(G)$ defined by the sets $\Gamma_k(i)$, $k = 0, 1, \ldots, \mathrm{ecc}(i)$, the corresponding quotient $G/\Pi(i)$ is a weighted path with structure independent of the chosen vertex i.

Let G be distance-regular around vertex $i \in V$. Note that, for a given vertex $u \in V$, $(\boldsymbol{A}\boldsymbol{\rho}V_k)_u = |\Gamma(u) \cap V_k|$. Thus,

$$\boldsymbol{A}\boldsymbol{\rho}V_k = b_{k-1}\boldsymbol{\rho}V_{k-1} + a_k\boldsymbol{\rho}V_k + c_{k+1}\boldsymbol{\rho}V_{k+1}.$$

Let $\boldsymbol{A}_r$, $1 \le r \le d$, be the adjacency matrix of G^r, that is, $(\boldsymbol{A}_r)_{ij} = 1$ if $\mathrm{dist}(i,j) = r$ and $(\boldsymbol{A}_r)_{ij} = 0$ otherwise. Since G is regular, $\boldsymbol{\rho}V_r = \boldsymbol{A}_r\boldsymbol{e}_i$, $1 \le r \le d$, and the previous recurrence reads

$$\boldsymbol{A}\boldsymbol{A}_k\boldsymbol{e}_i = b_{k-1}\boldsymbol{A}_{k-1}\boldsymbol{e}_i + a_k\boldsymbol{A}_k\boldsymbol{e}_i + c_{k+1}\boldsymbol{A}_{k+1}\boldsymbol{e}_i.$$

Thus, the polynomials obtained from the recurrence

$$x r_k = b_{k-1}r_{k-1} + a_k r_k + c_{k+1}r_{k+1}, \quad \text{with} \quad r_0 = 1, \quad r_1 = x, \tag{25}$$

satisfy $r_k(\boldsymbol{A})\boldsymbol{e}_i = \boldsymbol{\rho}V_k$. Note that, if G is distance-regular, the intersection numbers are the same for all the vertices and we also have $r_k(\boldsymbol{A}) = \boldsymbol{A}_k$, but this is not true in general.

In what follows, we consider the *i-local scalar product* defined as the scalar product associated to the mesh $\mathcal{M} = \mathrm{sp}_i G$ and normalized weight function $g_l = m_i(\mu_l)$, $0 \le l \le d_i$:

$$\langle f, g \rangle_i := \sum_{l=0}^{d_i} m_i(\mu_l) f(\mu_l) g(\mu_l) = (f(\boldsymbol{A})g(\boldsymbol{A}))_{ii},$$

Lemma 3.4 *If G is distance-regular around a vertex i, the polynomials r_k, $1 \le k \le d$, obtained from the recurrence (25) coincide with the canonical orthogonal system associated to the mesh $\mathcal{M} = \mathrm{sp}_i G$ and normalized weight function $g_l = m_i(\mu_l)$, $0 \le l \le d_i$.*

20

Proof. Let us show, first, that the polynomials r_k, $1 \le k \le d$ are mutually orthogonal. Notice that the vectors $\boldsymbol{\rho}V_s$ and $\boldsymbol{\rho}V_t$, $s \ne t$, are orthogonal. Then,

$$\langle r_s, r_t \rangle_i = (r_s(\boldsymbol{A})r_t(\boldsymbol{A}))_{ii} = \langle r_s(\boldsymbol{A})\boldsymbol{e}_i, r_t(\boldsymbol{A})\boldsymbol{e}_i \rangle = \langle \boldsymbol{\rho}V_s, \boldsymbol{\rho}V_t \rangle = 0.$$

Finally, by applying Proposition 2.6, since $\mathrm{dgr}(r_k) = k$, we conclude the proof. □

Given any connected graph G and a vertex of it i, in [13] the authors defined the *i-local predistance polynomials*, p_k^i, $0 \le k \le d_i$, as the canonical orthogonal system associated to the mesh $\mathcal{M} = \mathrm{sp}_i\, G$ and normalized weight function $g_l = m_i(\mu_l)$, $0 \le l \le d_i$. As the previous result suggests, these polynomials can be a useful tool to determine whether a graph is distance-regular around a vertex i. In this direction, in [18] is proved that G is distance-regular around vertex i, $\mathrm{ecc}(i) = \varepsilon$, if and only if

$$p_k^i(\boldsymbol{A})\boldsymbol{e}_i = \boldsymbol{\rho}V_k = \sum_{j \in V_k} \boldsymbol{e}_j \qquad (0 \le k \le \varepsilon), \tag{26}$$

generalizing the result in [11] for the so-called predistance polynomials.

Since $m_i(\lambda_0) = 1/\|\boldsymbol{v}\|^2 = 1/n$, we can deduce from (12) that the i-local multiplicities of G are given by

$$m_i(\mu_l) = \frac{\pi_0 p_{d_i}^i(\lambda_0)}{n\pi_l p_{d_i}^i(\mu_l)} \qquad (0 \le l \le d_i),$$

where $\pi_l = \prod_{h=0(h \ne l)}^{d_i} |\mu_l - \mu_h|$, and Corollary 2.7 gives us the value at λ_0 of the highest degree polynomial:

$$p_{d_i}^i(\lambda_0) = \left(\sum_{l=0}^{d_i} \frac{m_i^2(\lambda_0)\pi_0^2}{m_i(\mu_l)\pi_l^2} \right)^{-1}.$$

Given $i \in V$, we say that a vertex $j \in V$ is *i-extremal* if it is at spectrally maximum distance from it, $\mathrm{dist}(i,j) = d_i = |\mathrm{ev}_i\, G| - 1$. The number of i-extremal vertices is bounded by

$$|V_{d_i}| \le p_{d_i}^i(\lambda_0) = \left(\sum_{l=0}^{d_i} \frac{m_i^2(\lambda_0)\pi_0^2}{m_i(\mu_l)\pi_l^2} \right)^{-1}, \tag{27}$$

and, as it is shown in [13], the equality holds if and only if G is distance-regular around vertex i.

21

3.4   Characterizing distance-regularity

Let G be a regular graph on n vertices, with spectrum $\operatorname{sp} G = \{\lambda = \lambda_0, \lambda_1^{m_1}, \ldots, \lambda_d^{m_d}\}$, $\lambda_0 > \lambda_1 > \cdots \lambda_d$, and canonical orthogonal system $p_0, p_1, \ldots, p_d$ satisfying Proposition 2.6. In [13], the authors obtainded a characterization of distance-regularity through the following results.

Proposition 3.5 *Let G be a graph as above. Let $q_k = \sum_{l=0}^{k} p_l$, $0 \leq k \leq d$ and let $exc_i(d-1)$ denote the number of vertices at distance greater than $d-1$ from i. Then, G is spectrally regular if*
$$exc_i(d-1) = n - q_{d-1}(\lambda) = p_d(\lambda)$$
for every vertex i.

Theorem 3.6 *Let G be a spectrally-regular graph. Then the following statements are equivalent:*

(a) G is distance-regular around each of its vertices.

(b) G is distance-regular.

As mentioned, in [13], from this two results, jointly with (27), a quasi-spectral characterization of distance-regular graphs is obtained:

Theorem 3.7 *Let G be a regular graph on n vertices with spectrum $\operatorname{sp} G = \{\lambda_0, \lambda_1^{m_1}, \ldots, \lambda_d^{m_d}\}$, and let $p_0, p_1, \ldots, p_d$ be the associated canonical orthogonal system. Then G is distance-regular if and only if, for every vertex i,*

$$|\Gamma_d(i)| = p_d(\lambda_0) = n \left(\sum_{l=0}^{d} \frac{\pi_0^2}{m_l \pi_l^2} \right)^{-1}.$$

Using some results from [13, 18], the third author proved in [11] the following result, which gives a bound satisfied by every polynomial, attainable only if the involved graph is distance-regular. It is not unusual that distance-regularity appears when a bound is attained, other example of such a case is the bound given in (27).

Theorem 3.8 *Let G be a regular graph with n vertices and $d+1$ distinct eigenvalues. For every vertex $i \in V$, let $s_{d-1}(i) := |N_{d-1}(i)|$. Then, any polynomial $r \in \mathbb{R}_{d-1}[x]$ satisfies the bound*

$$\frac{r(\lambda_0)^2}{\|r\|_G^2} \leq \frac{n}{\sum_{i \in V} \frac{1}{s_{d-1}(i)}}, \tag{28}$$

and equality is attained if and only if G is a distance-regular graph. Moreover, in this case, we have

$$\frac{r(\lambda_0)}{\|r\|_G^2} r = q_{d-1} = \sum_{k=0}^{d-1} p_k,$$

where p_k, $0 \leq k \leq d$, are the distance polynomials of G.

Note that the above upper bound is, in fact, the harmonic mean of the numbers $s_{d-1}(i)$, $i \in V$. Moreover, in case of equality, $q_{d-1}(\boldsymbol{A}) = \sum_{k=0}^{d-1} \boldsymbol{A}_k = \boldsymbol{J} - \boldsymbol{A}_d$, and the distance-$d$ polynomial of G is just

$$p_d = q_d - q_{d-1} = q_d - \frac{r(\lambda_0)}{\|r\|_G^2} r, \tag{29}$$

where q_d represents the *Hoffman polynomial*; that is, $q_d = H_0 = \frac{n}{\pi_0} \prod_{l=1}^{d} (x - \lambda_l)$ (see [23]).

3.5 Bounding special vertex sets

Let $i \in V$ be a vertex with eccentricity $\mathrm{ecc}(i) = \varepsilon$. Given the integers k, μ such that $0 \leq k \leq \varepsilon$ and $\mu > 0$, let $\Gamma_k^\mu(i)$ denote the set of vertices which are at distance k from $i \in V$ and there exist exactly μ (shortest) k-paths from i to each of such vertices; so we have the partition $\Gamma_k(i) = \cup_{\mu \geq 1} \Gamma_k^\mu(i)$.

As shown in the following theorem of [9], the i-local predistance polynomials can be used to derive some bounds on the cardinality of the set $\Gamma_k^\mu(i)$, giving also a characterization of the extremal cases. Moreover, when the results are particularized to spectrally regular graphs, we get a proof of a conjecture of Van Dam (see Corollary 3.10 below).

Theorem 3.9 *Let i be a vertex of a regular graph G, with local spectrum $\mathrm{sp}_i G$, and let $(p_k^i)_{0 \leq k \leq d_i}$ be the i-local predistance polynomials. Let a_k denote the leading coefficient of p_k^i, and consider the sum polynomials $q_k^i = \sum_{l=0}^{k} p_l^i$. For any given integers $\mu > 0$ and $0 \leq k < d_i$, consider the spectral k-excess $e_k = n - q_k^i(\lambda_0)$, and define $\sigma_k(\mu) := a_k \mu - 1$. Then,*

$$|\Gamma_k^\mu(i)| \leq \frac{p_k^i(\lambda_0) e_k}{p_k^i(\lambda_0) \sigma_k(\mu)^2 + a_k^2 \mu^2 e_k}, \tag{30}$$

and equality is attained if and only if either

(a) *When $k = \varepsilon$:*

$$P^* \boldsymbol{e}_i = \beta_\varepsilon^* \boldsymbol{j} + \gamma_\varepsilon^* \boldsymbol{\rho} \Gamma_\varepsilon^\mu(i), \tag{31}$$

with the polynomial

$$P^* := a_\varepsilon \mu e_\varepsilon p_\varepsilon^i + p_\varepsilon^i(\lambda_0) \sigma_\varepsilon(\mu) q_\varepsilon^i \tag{32}$$

and constants

$$\beta_\varepsilon^* := p_\varepsilon^i(\lambda_0) \sigma_\varepsilon(\mu), \quad \gamma_\varepsilon^* := p_\varepsilon^i(\lambda_0) \sigma_\varepsilon(\mu)^2 + a_\varepsilon^2 \mu^2 e_\varepsilon; \tag{33}$$

(b) *When $k < \varepsilon$:*

$$p_k^i \boldsymbol{e}_i = \boldsymbol{\rho} V_k \,, \tag{34}$$

in which case

$$n_k^\mu = n_k = p_k^i(\lambda_0). \tag{35}$$

In the case of spectrally regular graphs (which implies that $p_k^i = p_k$ for every vertex i) and $k = d - 1$, we have

$$e_{d-1} = n - q_{d-1}(\lambda_0) = q_d(\lambda_0) - q_{d-1}(\lambda_0) = p_d(\lambda_0)$$

and we get

$$n_{d-1}^\mu \leq \frac{p_{d-1}(\lambda_0)p_d(\lambda_0)}{p_{d-1}(\lambda_0)\sigma_{d-1}(\mu)^2 + a_{d-1}^2\mu^2 p_d(\lambda_0)}. \tag{36}$$

When $d = 3$ the above result proves the following the following result conjectured by Van Dam in [7].

Corollary 3.10 *Let G be a regular graph with four distinct eigenvalues, and predistance polynomials p_k with leading coefficients a_k. Then, for any vertex $i \in V$, the number n_2^μ of vertices non-adjacent to i, which have μ common neighbours with i, is upper-bounded by*

$$n_2^\mu \leq \frac{p_2(\lambda_0)p_3(\lambda_0)}{p_2(\lambda_0)(a_2\mu - 1)^2 + a_2^2\mu^2 p_3(\lambda_0)}. \tag{37}$$

Example. Let G be a regular graph with spectrum

$$\operatorname{sp} G = \{4^1, 2^3, 0^3, -2^5\}.$$

Then $n = 12$, and its proper polynomials and their values at $\lambda_0 = 4$ are:

- $p_0 = 1, \quad 1$;

- $p_1 = x, \quad 4$;

- $p_2 = \frac{2}{3}(x^2 - x - 4), \quad \frac{16}{3}$;

- $p_3 = \frac{1}{12}(3x^3 - 8x^2 - 16x + 20), \quad \frac{5}{3}$;

Then, (37) gives

$$n_2^\mu \leq \left\lfloor \frac{20}{7\mu^2 - 16\mu + 12} \right\rfloor$$

and hence

- $\mu = 0, 1, 2, 3, 4, \ldots \quad \Rightarrow \quad n_2^\mu \leq 1, 6, 2, 0, 0, \ldots$

An example of a graph with such a spectrum is the one given by Godsil [22] (as an example of walk-regular graph which is neither vertex-transitive nor distance-regular, see Fig. 4) This graph can be constructed as follows: take two copies of the 8-cycle with vertex set $\mathbb{Z}_8$ and chords $\{1,5\}$, $\{3,7\}$; joint them by identifying vertices with the same even number and, finally, add edges between vertices labelled with equal odd number. The automorphism group of this graph has two orbits, formed by "even" and "odd" vertices, respectively. For such vertices we have (see again Fig. 4):

- $n_2^\mu = 0, 6, 1, 0, 0, \ldots$ (for an even vertex);

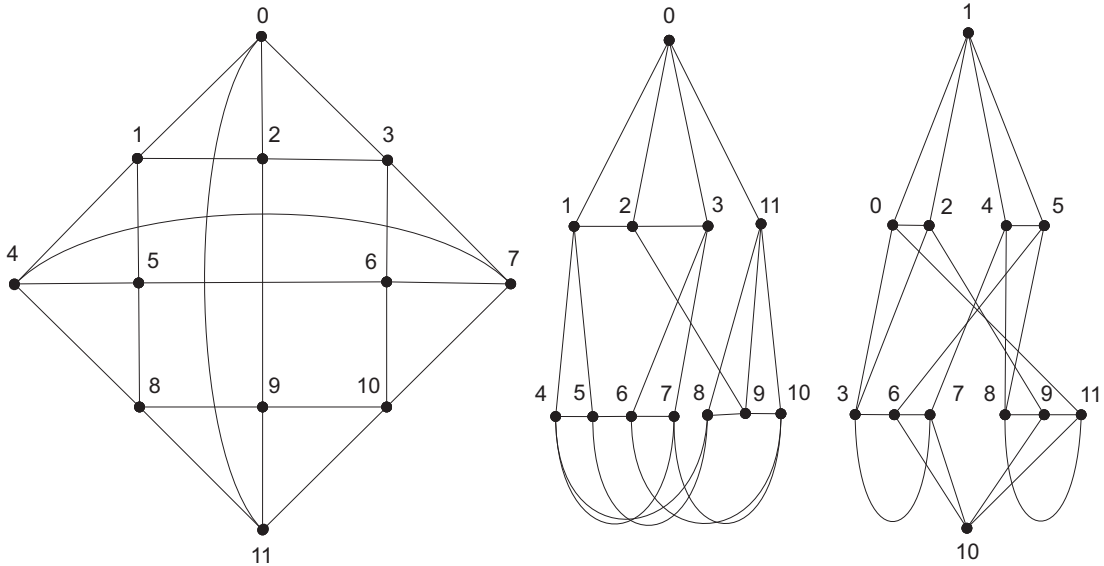- $n_2^\mu = 1, 4, 2, 0, 0, \ldots$ (for an odd vertex).

Figure 4: Three drawings of a walk regular graph which is not distance-regular.

3.6   Representation theory

Given a graph G and $\lambda_l \in \mathrm{ev}\, G$, we define, for every pair of vertices i, j the ij-cosine respect to λ_l to be

$$w_{ij}(\lambda_l) = \frac{\langle \boldsymbol{E}_l \boldsymbol{e}_i, \boldsymbol{E}_l \boldsymbol{e}_j \rangle}{\|\boldsymbol{E}_l \boldsymbol{e}_i\| \|\boldsymbol{E}_l \boldsymbol{e}_j\|} = \frac{m_{ij}(\lambda_l)}{\sqrt{m_i(\lambda_l) m_j(\lambda_l)}},$$

where $m_{ij}(\lambda_l) := m_{ij}(\lambda_l)$ is called the *crossed (ij-)local multiplicity* of λ_l (see [20]). The name given to this parameter emphasizes the fact that it coincides with the cosine of the angle formed by the projection of the vectors $\boldsymbol{e}_i$ and $\boldsymbol{e}_j$ onto the eigenspace associated with λ_l. When G is a distance-regular graph, $w_{ij}(\lambda_l)$ only depends on the distance $r = \mathrm{dist}(i, j)$

(see for instance [22]), and it is referred to as the *r-th cosine* $w_r(\lambda_l)$. In this case the following recurrence holds

$$\lambda_l w_r = c_r w_{r-1} + a_r w_r + b_r w_{r+1} \quad (0 \le r \le d),$$

where c_r, a_r, and b_r are the intersection parameters of G; w_{-1} and w_{d+1} are irrelevant (since $c_0 = b_d = 0$); and $w_0 = 1$.

If G is distance-regular around a vertex i and $\text{dist}(i, j) = r$ the crossed ij-local multiplicity of $\mu_l \in \text{sp}_i G$ can be obtained from the i-local predistance polynomials,

$$m_{ij}(\mu_l) = \frac{p_r^i(\mu_l)}{p_r^i(\mu_0)} m_i(\mu_l) \quad (0 \le l \le d_i),$$

and hence

$$w_{ij}(\mu_l) = \frac{p_r^i(\mu_l)}{p_r^i(\mu_0)} \sqrt{\frac{m_i(\mu_l)}{m_j(\mu_l)}}.$$

So we can infer that in a distance-regular graph the r-th cosine is

$$w_r(\lambda_l) = \frac{p_r(\lambda_l)}{p_r(\lambda_0)} \quad (0 \le l \le d).$$

3.7 Distance-regularity around a vertex set

Given a vertex subset $C \subset V$ of a (regular) graph G, its normalized vector is defined by

$$\boldsymbol{e}_C := \frac{1}{\sqrt{|C|}} \boldsymbol{\rho} C = \frac{1}{\sqrt{|C|}} \sum_{i \in C} \boldsymbol{e}_i.$$

Consider the spectral decomposition of the vector $\boldsymbol{e}_C = \boldsymbol{z}_0 + \boldsymbol{z}_1 + \cdots + \boldsymbol{z}_d$, where $\boldsymbol{z}_i \in \text{Ker}(\boldsymbol{A} - \lambda_l \boldsymbol{I})$. Similar to the case of the local spectrum, we define the *C-multiplicity* of the eigenvalue λ_l to be

$$
\begin{aligned}
m_C(\lambda_l) \quad &:= \quad \|\boldsymbol{z}_l\|^2 = \|\boldsymbol{E}_l \boldsymbol{e}_C\|^2 = \langle \boldsymbol{E}_l \boldsymbol{e}_C, \boldsymbol{e}_C \rangle = \frac{1}{|C|} \sum_{i,j \in C} \langle \boldsymbol{E}_l \boldsymbol{e}_i, \boldsymbol{e}_j \rangle \\
&= \quad \frac{1}{|C|} \sum_{i,j \in C} m_{ij}(\lambda_l) \quad (0 \le l \le d). \quad (38)
\end{aligned}
$$

The sequence of C-multiplicities $(m_C(\lambda_0), \ldots, m_C(\lambda_d))$ corresponds in fact to the so-called *"McWilliams transform"* of the vector $\boldsymbol{e}_C$ (see [22]). Since $\boldsymbol{e}_C$ is unitary, we have $\sum_{l=0}^d m_C(\lambda_l) = 1$. If $\mu_0 (= \lambda_0), \mu_1, \ldots, \mu_{d_C}$ represent the eigenvalues λ_i of G with non-zero C-multiplicities, then the (local) *C-spectrum* of G is

$$\text{sp}_C G := \{\lambda_0^{m_C(\lambda_0)}, \mu_1^{m_C(\mu_1)}, \ldots, \mu_{d_C}^{m_C(\mu_{d_C})}\}$$

26

where $d_C(\leq d)$ is called the *dual degree* of C (see again [22]).

Notice that we have similar results to the presented in Proposition 3.2 and its direct consequence for the spectrum of a vertex set. For any polynomial $p \in \mathbb{R}[x]$, we have

$$
\begin{aligned}
\langle p(\boldsymbol{A})\boldsymbol{e}_C, \boldsymbol{e}_C \rangle &= \left\langle \sum_{l=0}^{d} p(\lambda_l)\boldsymbol{E}_l\boldsymbol{e}_C, \boldsymbol{e}_C \right\rangle = \sum_{l=0}^{d} p(\lambda_l)\langle \boldsymbol{E}_l\boldsymbol{e}_C, \boldsymbol{e}_C \rangle \\
&= \sum_{l=0}^{d} m_C(\lambda_l)p(\lambda_l),
\end{aligned}
$$

and the number of walks of length k from the vertices of C to itself is

$$
\mathcal{C}_C(k) := \sum_{u,v \in C} (\boldsymbol{A}^k)_{uv} = |C|\langle \boldsymbol{A}^k\boldsymbol{e}_C, \boldsymbol{e}_C \rangle = |C|\sum_{l=0}^{d} m_C(\lambda_l)\lambda_l^k \qquad (k \geq 0).
$$

Proceeding as we did for the local spectrum, the *C-local predistance polynomials* $(p_k^C)_{0 \leq k \leq d_C}$ are the canonical orthogonal system with respect to the scalar product

$$
\langle f, g \rangle_C := \sum_{l=0}^{d_C} m_C(\mu_l)f(\mu_l)g(\mu_l)
$$

with normalized weight function $g_l = m_C(\mu_l)$, satifying $\|p_k^C\|_C^2 = p_k^C(\lambda_0)$. The sum polynomials will be also of our interest, they are defined by $q_k^C := \sum_{h=0}^{k} p_h^C$, $0 \leq k \leq d_C$. In this context, Theorem 4.2 of [15] reads as follows:

Theorem 3.11 *Let C be a vertex subset of a regular graph G, with C-local predistance polynomials $(p_k^C)_{0 \leq k \leq d}$. Then, for any polynomial $q \in \mathbb{R}_k[x]$,*

$$
\frac{q(\lambda_0)^2}{\|q\|_C^2} \leq \frac{|N_k(C)|}{|C|}, \tag{39}
$$

and equality is attained if and only if

$$
\frac{1}{\|q\|_C}q(\boldsymbol{A})\boldsymbol{e}_C = \boldsymbol{e}_{N_k}, \tag{40}
$$

where $\boldsymbol{e}_{N_k}$ represents the unitary characteristic vector of $N_k(C)$. Moreover, if this is the case, q is any multiple of q_k^C, whence (39) and (40) become

$$
\begin{aligned}
q_k^C(\lambda_0) &= \frac{|N_k(C)|}{|C|}, \tag{41} \\
q_k^C(\boldsymbol{A})\boldsymbol{\rho}C &= \boldsymbol{\rho}N_k(C). \tag{42}
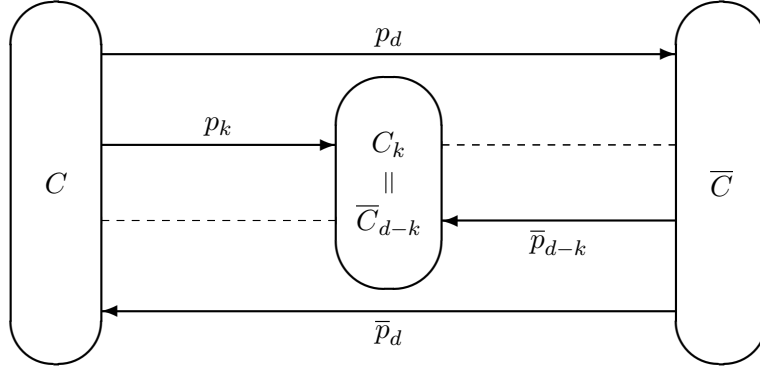\end{aligned}
$$

Figure 5: Antipodal tight sets and their distance partition

The above result motivated the following definition. A subset C of the vertices of a graph G is *tight* if $q_k^C(\boldsymbol{A})\boldsymbol{\rho}C = \boldsymbol{\rho}N_k(C)$ for any $0 \leq k \leq d_C$. For every vertex subset C, we consider also its antipodal set $\overline{C}$. As the following proposition states, the tight character of a set C —or, equivalently, the existence of the C-local predistance polynomial p_d^C— leads to the existence of all the C-local predistance polynomials with respect to both sets C and $\overline{C}$, and that they are just the members of their associated orthogonal system (see [15]).

Proposition 3.12 *Let C be a tight set of vertices with predistance orthogonal system $(p_k)_{0 \leq k \leq d_C}$, and let $(\overline{p}_k)_{0 \leq k \leq d_C}$ be the predistance orthogonal system associated to its antipodal set $\overline{C}$. Then,*

(a) The polynomials $(\overline{p}_k)_{0 \leq k \leq d_C}$ are just the conjugate polynomials of $(p_k)_{0 \leq k \leq d_C}$:

$$\overline{p}_k = p_d^{-1} p_{d-k}, \qquad p_k = p_d \overline{p}_{d-k} \quad (0 \leq k \leq d_C). \tag{43}$$

(b) $\overline{C}$ is also tight. (If the family $\mathcal{T}$ of tight vertex sets of a graph G is not empty, then the application which maps every set to its antipodal fixes $\mathcal{T}$ and it is involutive).

What is more, for every $0 \leq k \leq d$, the action of the polynomial p_k on $\boldsymbol{\rho}C$ coincides with the action of $\overline{p}_{d-k}$ on $\boldsymbol{\rho}\overline{C}$, so revealing the symmetry between the roles of C and $\overline{C}$ (See Fig. 5).

Proposition 3.13 *If C is a tight set with antipodal set $\overline{C}$, and $(p_k)_{0 \leq k \leq d}$, $(\overline{p}_k)_{0 \leq k \leq d}$ are the corresponding predistance orthogonal systems. Then,*

$$p_k \boldsymbol{\rho}C = \boldsymbol{\rho}C_k = \boldsymbol{\rho}\overline{C}_{d-k} = \overline{p}_{d-k}\boldsymbol{\rho}\overline{C} \quad (0 \leq k \leq d).$$

28

3.8 Completely regular codes in distance-regular graphs

Let $C \subset V$ be a vertex set. The distance from C to a given vertex j of V is given by $\operatorname{dist}(C,j) = \min_{i \in C}\{\operatorname{dist}(i,j)\}$. This definition gives us a distance partition of V where each part C_k is the set of vertices at distance k from C. It is natural to say that the eccentricity of C is given by $\operatorname{ecc}(C) = \max_{j \in V}\{\operatorname{dist}(C,j)\}$.

We say that G is *distance-regular around* C, with eccentricity $\varepsilon = \operatorname{ecc}(C)$, if the distance partition $V = C_0 \cup C_1 \cup \cdots \cup C_\varepsilon$ is regular, that is the numbers

$$c_k(i) := |\Gamma(i) \cap C_{k-1}|, \quad a_k(i) := |\Gamma(i) \cap C_k|, \quad b_k(i) := |\Gamma(i) \cap C_{k+1}|,$$

where $i \in C_k$, $0 \le k \le \varepsilon$, depend only on the value of k, but not on the chosen vertex i. The set C is also referred to as a *completely regular set* or *completely regular code* (see [22]).

There are similar characterizations of distance-regularity around a vertex set to those given for local distance-regularity in previous sections. Analogously to (26), a graph G is distance-regular around a set $C \subset V$, with eccentricity ε, if and only if the C-local predistance polynomials $p_0^C, p_1^C, \ldots, p_\varepsilon^C$ satisfy

$$\boldsymbol{\rho}C_k = p_k^C(\boldsymbol{A})\boldsymbol{\rho}C \qquad (0 \le k \le \varepsilon). \tag{44}$$

In [16] the authors gave the following characterization of completely regular codes in terms of the number of vertices at spectrally maximum distance from C. From this point of view it can be seen as the analogue of Theorem 3.7.

Theorem 3.14 *Let $G = (V,E)$ be a regular graph. A vertex subset $C \subset V$, with r vertices and local spectrum $\operatorname{sp}_C G = \{\lambda_0^{m_C(\lambda_0)}, \mu_1^{m_C(\mu_1)}, \ldots, \mu_{d_C}^{m_C(\mu_{d_C})}\}$, is a completely regular code if and only if the number of vertices at distance d_C from C; that is, $n_{d_C}(C) := |C_{d_C}|$ satisfies*

$$
\begin{aligned}
n_{d_C}(C) = p_{d_C}^C(\lambda_0) &= r\left(\sum_{l=0}^{d_C} \frac{m_C(\lambda_0)^2 \pi_0^2}{m_C(\mu_l)\pi_l^2}\right)^{-1} \\
&= \frac{n^2}{r}\left(\sum_{l=0}^{d_C} \frac{\pi_0^2}{m_C(\mu_l)\pi_l^2}\right)^{-1}.
\end{aligned}
$$

The number of ordered pairs (i,j) of vertices from C which are k apart in a distance-regular graph G is given by

$$\sum_{i,j \in C} (\boldsymbol{A}_k)_{ij} = \langle \boldsymbol{A}_k \boldsymbol{e}_C, \boldsymbol{e}_C \rangle = |C|\langle p_k(\boldsymbol{A})\boldsymbol{e}_C, \boldsymbol{e}_C \rangle = |C|\sum_{l=0}^{d} m_C(\lambda_l)p_k(\lambda_l).$$

From this we see that, within C, the *mean number* of vertices at distance k (from a vertex) in G is

$$\overline{n}_k := \frac{1}{|C|} \sum_{i \in C} |\Gamma_k(i) \cap C| = \sum_{l=0}^{d} m_C(\lambda_l) p_k(\lambda_l) \qquad (0 \le k \le d). \tag{45}$$

The numbers $\overline{n}_k$, $0 \le k \le d$, are called the *inner distribution* of C and, as commented by Godsil [22], they represent the probability, through the ratio $\overline{n}_k/|C|$, that a randomly chosen pair of vertices from C are at distance k. Notice that always $\overline{n}_0 = 1$ and $\sum_{k=0}^{d} \overline{n}_k = |C|$.

These last two observations lead us to conclude that, in a distance regular graph, the local multiplicities of a vertex subset C can be easily computed from the distance polynomials of G, its spectrum, and the inner distribution of C (see [16]).

Proposition 3.15 *Let G be a distance-regular graph with a given subset C of r vertices. Then there exist nonnegative numbers $r_0(= 1), r_1, \ldots, r_k$, such that $\overline{n}_k = r_k$ for every $0 \le k \le d$, if and only if the C-multiplicities satisfy*

$$m_C(\lambda_l) = \frac{m(\lambda_l)}{n} \sum_{k=0}^{d} r_k \frac{p_k(\lambda_l)}{p_k(\lambda_0)} \qquad (0 \le l \le d). \tag{46}$$

In particular $m_C(\lambda_0) = \frac{r}{n}$ and if C is a single vertex, $C = \{i\}$, we have $r_0 = 1, r_1 = \cdots = r_d = 0$, so $m_i(\lambda_l) = \frac{m(\lambda_l)}{n} \frac{p_0(\lambda_l)}{p_0(\lambda_0)} = \frac{m(\lambda_l)}{n}$, as expected.

In the case when all vertices in C are at distance k from each other, (46) gives:

$$m_C(\lambda_l) = \frac{m(\lambda_l)}{n} \left(1 + (r - 1) \frac{p_k(\lambda_l)}{p_k(\lambda_0)} \right) \qquad (0 \le l \le d).$$

But, when $k = d$, we know from Corollary 2.7 that $p_d(\lambda_l) < 0$ for every odd l. This fact, together with $m_C(\lambda_l) \ge 0$, yields the following upper bound for the maximum number of vertices mutually at maximum distance d:

$$r \le 1 + \min_{l=1,3,\ldots} \frac{p_d(\lambda_0)}{|p_d(\lambda_l)|}.$$

A similar upper bound is given in [6] for the more general case of spectrally regular graphs.

References

[1] E. Bannai and T. Ito, *Algebraic Combinatorics I: Association Schemes.* Benjamin/Cummings, Menlo Park, CA, 1984.

[2] N. Biggs, *Algebraic Graph Theory.* Cambridge University Press, Cambridge, 1974; second edition: 1993.

[3] A.E. Brouwer, A.M. Cohen and A. Neumaier, *Distance-Regular Graphs.* Springer-Verlag, Berlin, 1989.

[4] T.S. Chihara, *An Introduction to Orthogonal Polynomials*, Gordon and Breach, New York, 1978.

[5] F.R.K. Chung, V. Faber, and T.A. Manteuffel, An upper bound on the diameter of a graph from eigenvalues associated with its Laplacian, *SIAM J. Discrete Math.* **7** (1994), 443–457.

[6] C. Dalfó, M.A. Fiol and E. Garriga, On k-walk-regular graphs, *European J. Combin.*, submitted.

[7] E. R. van Dam, Graphs with few eigenvalues, *Ph.D. Thesis, Tilburg University*, 1996.

[8] E.R. van Dam and W.H. Haemers, Eigenvalues and the diameter of graphs, *Linear Multilinear Algebra* **39** (1995), 33–44.

[9] M.A. Fiol, Some applications of the proper and adjacency polynomials in the theory of graph spectra, *Electron. J. Combin.* **4** (1997), no. 1, Research Paper 21, 24 pp. (electronic).

[10] M.A. Fiol, On pseudo-distance-regularity, *Linear Algebra Appl.* **323** (2001), 145–165.

[11] M.A. Fiol, Algebraic characterizations of distance-regular graphs, *Discrete Math.* **246** (2002), 111–129.

[12] M.A. Fiol, Spectral bounds and distance-regularity, *Linear Algebra Appl.* **397** (2005), 17–33.

[13] M.A. Fiol and E. Garriga, From local adjacency polynomials to locally pseudo-distance-regular graphs, *J. Combin. Theory Ser. B* **71** (1997), no. 2, 162–183.

[14] M.A. Fiol and E. Garriga, The alternating and adjacency polynomials, and their relation with the spectra and diameters of graphs, *Discrete Appl. Math.* **87** (1998), no. 1-3, 77–97.

[15] M.A. Fiol and E. Garriga, On the algebraic theory of pseudo-distance-regularitiy around a set, *Linear Algebra and its Applications* **298** (1999), 115–141.

[16] M.A. Fiol and E. Garriga, An algebraic characterization of completely regular codes in distance-regular graphs, *SIAM J. Discrete Math.* **15** (2002), no. 1, 1–13.

[17] M.A. Fiol, E. Garriga, and J.L.A. Yebra, On a class of polynomials and its relation with the spectra and diameters of graphs, *J. Combin. Theory Ser. B* **67** (1996), 48–61.

[18] M.A. Fiol, E. Garriga, and J.L.A. Yebra, Locally pseudo-distance-regular graphs, *J. Combin. Theory Ser. B* **68** (1996), 179–205.

[19] M.A. Fiol, E. Garriga and J.L.A. Yebra, From regular boundary graphs to antipodal distance-regular graphs, *J. Graph Theory* **27** (1998), no. 3, 123–140.

[20] M.A. Fiol, E. Garriga, and J.L.A. Yebra, Boundary graphs: The limit case of a spectral property, *Discrete Math.* **226** (2001), no. 1-3, 155–173.

[21] E. Garriga, Contribució a la Teoria Espectral de Grafs: Problemes Mètrics i Distancia-Regularitat. (Catalan) *Ph.D. Thesis, Universitat Politècnica de Catalunya* (1997).

[22] C.D. Godsil, *Algebraic Combinatorics.* Chapman and Hall, New York, 1993.

[23] A.J. Hoffman, On the polynomial of a graph, *Amer. Math. Monthly* **70** (1963), 30–36.

[24] P. Rowlinson, Linear algebra, *in: Graph Connections* (ed. L.W. Beineke and R.J. Wilson), Oxford Lecture Ser. Math. Appl., Vol. 5, 86–99, Oxford Univ. Press, New York, 1997.

[25] G. Szegö, *Orthogonal Polynomials*, Fourth edition, Amer. Math. Soc., Providence, R.I., 1975.