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On the Wiener index and the eccentric distance sum of hypergraphs

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Abstract

The Wiener index of an n-vertex tree T can be calculated by means of the expression

$$W(T) = \sum_e [n_1(e)n_2(e)],$$

where $n_1(e)$ and $n_2(e) = n - n_1(e)$ are the number of vertices on the two sides of the edge e, and the summation goes over all edges of T. Here we generalize this result to the case of hypertrees and we propose formulas for the Wiener index and the eccentric distance sum of distance-regular hypergraphs in terms of its intersection array. Moreover, using the alternating polynomials and the Laplacian polynomials, we obtain upper bounds on the eccentric distance sum and Wiener index of hypergraphs.

1 Introduction

Throughout this paper $\mathcal{H} = (V, E)$ denotes a connected, simple and finite hypergraph with vertex set $V = V(\mathcal{H})$, $|V| = n$, and edge set $E = E(\mathcal{H})$, $|E| = m$. A hypergraph in which all edges have the same cardinality r is called *r-uniform*. The class of r-uniform hypergraphs contains, for instance, the class of graphs ($r = 2$) and the class of block designs. In the particular case of graphs we will use de notation Γ instead $\mathcal{H}$.

The *distance* $\partial(u, v)$ between two vertices u and v is the minimum of the lengths of paths between u and v. The *eccentricity* of a vertex v is defined as

$$\epsilon(v) := \max_{u \in V(\mathcal{H})} \partial(u, v)$$

and the *diameter* $D(\mathcal{H})$ of a hypergraph $\mathcal{H}$ is defined as

$$D(\mathcal{H}) := \max_{v \in V(\mathcal{H})} \epsilon(v).$$

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The distance of a vertex v in a connected hypergraph $\mathcal{H}$ is defined by

$$S(v) := \sum_{u \in V(\mathcal{H})} \partial(u, v).$$

The *Wiener index* $W(\Gamma)$ of a graph Γ with vertex set $\{v_1, v_2, ..., v_n\}$ defined as the sum of distances between all pairs of vertices of Γ,

$$W(\Gamma) := \frac{1}{2} \sum_{i=1,j=1}^{n} \partial(v_i, v_j) = \frac{1}{2} \sum_{v \in V(\Gamma)} S(v),$$

is the first mathematical invariant reflecting the topological structure of a molecular graph.

This topological index has been extensively studied, for instance, a comprehensive survey on the direct calculation, applications and the relation of the Wiener index of trees with other parameters of graphs can be found in [2]. Moreover, a list of 120 references of the main works on the Wiener index of graphs can be found in the referred survey.

The *eccentric distance sum,* denoted by ξ^{DS}, is a novel graph invariant introduced in [9]. It can be defined as the summation of product of eccentricity and distance of each vertex in the graph,

$$\xi^{DS}(\Gamma) := \sum_{i=1}^{n} [\epsilon(v_i) \cdot S(v_i)].$$

In [9] the relationship of eccentric distance sum and the Wiener index with anti-human immunodeficiency virus (HIV) activity of dihydroseselins has been investigated to facilitate the development of potent and safe anti-HIV agents. The relationship of eccentric distance sum and the Wiener index with physical properties in data sets of diverse nature was also investigated in the referred article.

The hypergraphs as mathematical model for representation of nonclassical molecular structures with polycentric delocalized bonds have been investigated in [11].

The purpose of this work is to find closed formulas or bounds for the Wiener index of hypergraphs. As consequence of the study we derive similar results on the eccentric distance sum. The plan of the paper is the following: in Section 2 we propose a closed formula for the Wiener index of hypertrees that generalizes the previous one on trees. In Section 3 we present closed formulas for the Wiener index and the eccentric distance sum of distance-regular hypergraphs in terms of its intersection array. Section 4 is devoted to obtain spectral-like bounds on the studied parameters.

2 The Wiener index of hypertrees

The following result is well known [2, 10].

Theorem 1. (Harold Wiener, 1947) *Let T be a tree on n vertices. Then*

$$W(T) = \sum_{e} [n_1(e) n_2(e)],$$

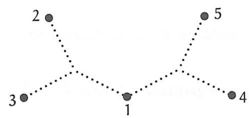
where $n_1(e)$ and $n_2(e) = n - n_1(e)$ are the number of vertices on the two sides of the edge e, and the summation goes over all edges of T.

Here we propose the generalization, to the case of hypertrees, of Theorem 1. We recall that a *walk* of length k in an hypergraph $\mathcal{H}$, between the vertices u and v or $u - v$ walk, to be a finite sequence $u = v_0e_1v_1 \cdots v_{k-1}e_kv_k = v$ of vertices v_i and edges e_i of $\mathcal{H}$ such that $v_i \in e_{i+1}$ for $i = 0, \dots k-1$, and $v_i \in e_i$ for $i = 1, \dots, k$. A $u-v$ walk is *closed* if $u = v$. A *path* is a walk in which no vertex is repeated. A *cycle* is a closed walk in which the first and last vertex coincide, but, apart from that, neither vertices nor edges repeat.

We say that a hypergraph $\mathcal{H}$ is a *hypertree* if it is connected, has no cycles and $|a \cap b| \leq 1$, $\forall a, b \in E(\mathcal{H})$.

Note that a path in a hypertree is not necessarily a shortest path. For instance, the path $3e_12e_11e_25$ in the hypertree of Figure 1 is not the shortest path between 3 and 5.

Figure 1: Example of hypertree. It has two edges, $e_1 = \{1, 2, 3\}$ and $e_2 = \{1, 4, 5\}$



Lemma 2. *There is a unique shortest path between two vertices of a hypertree.*

Proof. Let u and v be two vertices of a hypertree T such that $\partial(u, v) = k$. Suppose that $u = v_0e_1v_1 \cdots v_{k-1}e_kv_k = v$ and $u = v_0e'_1v'_1 \cdots v'_{k-1}e'_kv_k = v$ are two shortest paths between u and v such that they are different from each other. We shall show that in fact they are equal.

We claim that if $v_r = v'_{r'}$, then $r = r'$. That is, if $v_r = v'_{r'}$ and $r < r'$, then the path $u = v_0e_1v_1 \cdots v_re'_{r+1}v'_{r+1} \cdots v'_{k-1}e'_kv_k = v$ has length less than k, thus contradicting that $\partial(u, v) = k$. Similarly we can see that the case $e_r = e'_{r'}$, with $r \neq r'$, is not possible.

If $v_i = v'_i$, $i = 0, \dots, k$, then $e_{j+1} \neq e'_{j+1}$ for some j, $0 \leq j \leq k-1$. Thus, T has a cycle $v_je_{j+1}v_{j+1}e'_{j+1}v_j$, in contradiction to T being a hypertree.

If there are two integers j and r such that, $0 \leq j < r \leq k$, $r - j \geq 2$, $v_i \neq v'_i$ for every i such that $j < i < r$, $v_j = v'_j$ and $v_r = v'_r$, then we consider the following cases:

- If $e_{t+1} \neq e'_{t+1}$ for every t such that $j \leq t < r$, then T has a cycle

$$v_je_{j+1}v_{j+1} \cdots v_re'_rv'_{r-1} \cdots v'_{j+1}e'_{j+1}v_j,$$

  thus contradicting that T is a hypertree.

- If $e_t = e'_t$ and $e_{t+1} = e'_{t+1}$ for some t such that $j < t < r$, then $|e_t \cap e_{t+1}| \geq 2$. This fact contradicts the hypothesis that T is a hypertree.

- If $e_{t+1} \neq e'_{t+1}$ for every t such that $j \leq t < t'$, where $t' < r$ and $e_{t'+1} = e'_{t'+1}$, then T has a cycle $v_je_{j+1}v_{j+1} \cdots v_{t'}e_{t'+1}v'_{t'} \cdots v'_{j+1}e'_{j+1}v_j$, thus contradicting that T is a hypertree.

- The case $e_{t+1} \neq e'_{t+1}$ for every t such that $t' < t < r$, where $j \leq t'$ and $e_{t'+1} = e'_{t'+1}$, is analogous to the previous one.

- If $e_{j'} = e'_{j'}$ and $e_{t'+1} = e'_{t'+1}$ for some j' and t' such that $j < j' < t' < r$ and $e_{t+1} \neq e'_{t+1}$ for every t with $j' \leq t < t'$, then T has a cycle $v'_{j'}e_{j'}v_{j'} \cdots v_{t'}e_{t'+1}v'_{t'} \cdots v'_{j'+1}e'_{j'+1}v'_{j'}$. This cycle contradicts the hypothesis that T is a hypertree.

Therefore, the result follows. $\square$

After a labelling $(v_1(e), v_2(e), ..., v_{|e|}(e))$ of the endpoints of an edge $e \in E(T)$, we say that a vertex $u \in V(T)\backslash\{e\}$ is on the side $v_i(e)$ of the edge e if there is a path, that does not contain the edge e, from $v_i(e)$ to u. We denote by $V_i(e)$ the set of vertices of $T\backslash\{e\}$ on the side $v_i(e)$ of the edge e. Let $n_i(e) = 1 + |V_i(e)|$, $i = 1, 2, ..., |e|$.

Theorem 3. *With the notation above, the Wiener index of a hypertree T is*

$$W(T) = \sum_{e\in E(T)} \sum_{i\neq j} [n_i(e)n_j(e)].$$

Proof. As there is a unique shortest path between any two vertices of T (Lemma 2), and the number of edges traversed in the shortest path joining two vertices is the distance between them, we only need to count the number of shortest paths containing each edge of T.

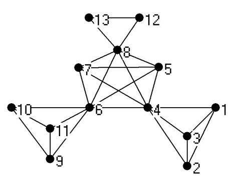
The number of shortest path containing the edge e in T can be calculated by

$$\sum_{i,j\in\{1,2,...,|e|\}, i\neq j} [n_i(e)n_j(e)].$$

Thus, the result follows. $\square$

The above result can be regarded as a generalization of Theorem 1 to a more general class of graphs. That is, a hypertree T can be seen as a block graph Γ_T considering that $V(T) = V(\Gamma_T)$ where two vertices of Γ_T are adjacent if they are adjacent in T. In such case, each edge of T induces a complete subgraph in Γ_T, two complete subgraphs of Γ_T only can share one vertex and Γ_T has no cycles of complete subgraphs. See, for instance, Figure 2.

Figure 2: The graph Γ_T associated to the hypertree T whose edges are $e_1 = \{1, 2, 3, 4\}$, $e_2 = \{4, 5, 6, 7, 8\}$, $e_3 = \{6, 9, 10, 11\}$ and $e_4 = \{8, 12, 13\}$.



3 The Wiener index of distance-regular hypergraphs

We can obtain an explicit formula for the Wiener index in the case of distance-regular hypergraphs in terms of its intersection array

$$\{b_0, b_1, ..., b_{D-1}; c_1 = 1, c_2, ..., c_D\}.$$

We say that a distance-regular hypergraph is a connected hypergraph with diameter D, for which following holds. There are natural numbers $b_0, b_1, ..., b_{D-1}$, $c_1 = 1$, $c_2, ..., c_D$ such that for each pair (u, v) of vertices satisfying $\partial(u, v) = j$ we have

(1) the number of vertices in $\mathcal{H}_{j-1}(v)$ adjacent to u is c_j $(1 \leq j \leq D)$;

(2) the number of vertices in $\mathcal{H}_{j+1}(v)$ adjacent to u is b_j $(0 \le j \le D-1)$,

where $\mathcal{H}_i(v) = \{u \in V(\mathcal{H}) : \partial(u,v) = i\}$.

For example, the (12,3,5)-design whose blocks are

$$\{0,1,2\}, \quad \{0,2,3\}, \quad \{0,3,4\}, \quad \{0,4,5\}, \quad \{0,1,5\},$$
$$\{1,2,8\}, \quad \{1,5,7\}, \quad \{1,7,8\}, \quad \{2,3,9\}, \quad \{2,8,9\},$$
$$\{3,4,10\}, \quad \{3,9,10\}, \quad \{4,5,11\}, \quad \{4,10,11\}, \quad \{5,7,11\},$$
$$\{6,7,8\}, \quad \{6,7,11\}, \quad \{6,8,9\}, \quad \{6,9,10\}, \quad \{6,10,11\},$$

is a distance-regular hypergraph whose intersection array is (5,2,1;1,2,5).

Theorem 4. *Let $\mathcal{H}$ be a distance-regular hypergraph whose intersection array is*

$$\{b_0, b_1, ..., b_{D-1}; c_1 = 1, c_2, ..., c_D\}.$$

Then we have

$$W(\mathcal{H}) = \frac{nb_0}{2}\left(1 + \sum_{i=2}^{D} i\frac{\prod_{j=1}^{i-1} b_j}{\prod_{j=2}^{i} c_j}\right).$$

Proof. For any vertex $v \in V(\mathcal{H})$, each vertex of $\mathcal{H}_{i-1}(v)$ is joined to b_{i-1} vertices in $\mathcal{H}_i(v)$ and each vertex of $\mathcal{H}_i(v)$ is joined to c_i vertices in $\mathcal{H}_{i-1}(v)$. Thus

$$\mid \mathcal{H}_{i-1}(v) \mid b_{i-1} = \mid \mathcal{H}_i(v) \mid c_i. \tag{1}$$

Therefore, it follows from (1) that the number of vertices at distance i of a vertex v, $|\mathcal{H}_i(v)|$, is obtained directly from the intersection array

$$|\mathcal{H}_i(v)| = \frac{\prod_{j=0}^{i-1} b_j}{\prod_{j=2}^{i} c_j} \quad (2 \le i \le D) \quad \text{and} \quad |\mathcal{H}_1(v)| = b_0. \tag{2}$$

The result is a direct consequence of the definition of the Wiener index. □

We remark that, in the case of graphs, (2) is a well-known result (see, for instance [1]).

Another example of distance-regular hypergraphs (graphs) is the family of the hypercubes, H_k $(k \ge 2)$, whose intersection array is $\{k, k-1, ..., 1; 1, 2, ..., k\}$. Thus, from Theorem 4 we obtain that the Wiener index of the hypercube H_k is

$$W(H_k) = 2^{k-1}k\sum_{l=0}^{k-1}\binom{k-1}{l} = k2^{2(k-1)}.$$

From $\epsilon(v) \le D(\mathcal{H})$, $\forall v \in V(\mathcal{H})$, we have the following relation between the Wiener index and the eccentric distance sum:

$$\xi^{DS}(\mathcal{H}) \le 2D(\mathcal{H})W(\mathcal{H}). \tag{3}$$

If all vertices of $\mathcal{H}$ are diametral, the equality holds. In the case of a distance-regular hypergraphs, Theorem 4 and (3) lead to the following result.

Corollary 5. *Let $\mathcal{H}$ be a distance-regular hypergraph whose intersection array is*

$$\{b_0, b_1, ..., b_{D-1}; c_1 = 1, c_2, ..., c_D\}.$$

Then we have

$$\xi^{DS}(\mathcal{H}) = nD(\mathcal{H})b_0\left(1 + \sum_{i=2}^{D(\mathcal{H})} i\frac{\prod_{j=1}^{i-1} b_j}{\prod_{j=2}^{i} c_j}\right).$$

4 Bounding the Wiener index and the eccentric distance sum

In this section we derive several spectral type tight upper bounds on the studied parameters. To begin with, we present some additional terminology and the main tools: the alternating polynomials and the Laplacian polynomials.

4.1 Laplacian Matrix

We denote by $\mathbf{A} = \mathbf{A}(\mathcal{H})$ the adjacency matrix of $\mathcal{H}$. Given two distinct vertices $v_i, v_j \in V(\mathcal{H})$ the entry a_{ij} of $\mathbf{A}$ is the number of edges in $\mathcal{H}$ containing both v_i and v_j; the diagonal entries of $\mathbf{A}$ are zero.

If $v_i, v_j \in V(\mathcal{H})$, then the number of walks of length k in $\mathcal{H}$, from v_i to v_j, is the entry in position (i, j) of the matrix $\mathbf{A}^k$ (see [16]).

A hypergraph is *walk-regular* if for every k the number of walks of length k with both endpoints at v does not depend on the vertex v. In other words, any power $\mathbf{A}^k$ has its diagonal entries all equal to $Tr\left(\mathbf{A}^k\right)/n$. The class of walk-regular graphs contains the class of vertex transitive graphs and the class of distance-regular graphs.

We define the *Laplacian degree of a vertex* $v_i \in V(\mathcal{H})$ as $\delta_\ell(v_i) := \sum_{j=1}^n a_{ij}$. We say that the hypergraph $\mathcal{H}$ is *Laplacian regular* of degree δ_ℓ if any vertex $v \in V(\mathcal{H})$ has Laplacian degree $\delta_\ell(v) = \delta_\ell$. Obviously, every walk-regular hypergraph is Laplacian regular.

A simple count shows that the Laplacian degree of an (n, r, δ)-design[1] satisfies

$$\delta_\ell = (r-1)\delta = \frac{mr(r-1)}{n}. \tag{4}$$

Moreover, if $\mathcal{H}$ is a graph then $\delta_\ell(v_i) = \delta(v_i)$.

The *Laplacian matrix of a hypergraph* $\mathcal{H}$, denoted by $\mathbf{L} = \mathbf{L}(\mathcal{H})$, is defined as $\mathbf{L} := \mathbf{D} - \mathbf{A}$ where $\mathbf{D} = diag(\delta_\ell(v_1), \delta_\ell(v_2), \ldots, \delta_\ell(v_n))$. This version of Laplacian matrix was introduced by author of this paper in [14] to extend, to the case of hypergraphs, results related with several metric parameters of graphs.

We recall that the matrix $\mathbf{L}$ is symmetric and positive semidefinite, the smallest eigenvalue of $\mathbf{L}$ is $\mu = 0$ and a corresponding eigenvector is $\mathbf{j} = (1, 1, \ldots, 1)$. Moreover, the multiplicity of $\mu = 0$ is equal to the number of connected components of $\mathcal{H}$.

The eigenvalues of $\mathbf{L}$ are denoted by $\mu_0 = 0 < \mu_1 < \cdots < \mu_b$ and their multiplicities are denoted by $m_0 = 1, m_1, \ldots, m_b$. Hence, the *Laplacian spectrum* of $\mathcal{H}$ is denoted by $Spec(\mathcal{H}) = \{\mu_0^1, \mu_1^{m_1}, ..., \mu_b^{m_b}\}$.

Thus, the *total adjacency index* [18], defined as $\mathcal{A} := \sum_{i,j=1}^n a_{ij}$, can be calculated by

$$\mathcal{A} = \sum_{l=1}^{b} m_l \mu_l = \sum_{i=1}^{n} \delta_\ell(v_i). \tag{5}$$

Moreover, in the case of an (n, r, δ)-design, by (4) and (5), we have $\mathcal{A} = n(r-1)\delta = mr(r-1)$.

We denote by $\lambda_0 > \lambda_1 > \cdots > \lambda_d$ the adjacency eigenvalues of a Laplacian regular hypergraph $\mathcal{H}$ of degree δ_ℓ. Then, since $\mathbf{L} = \delta_\ell \mathbf{I} - \mathbf{A}$, the eigenvalues of both matrices, $\mathbf{A}$ and $\mathbf{L}$, are related by

$$\mu_l = \delta_\ell - \lambda_l, \quad l = 0, \ldots, b = d. \tag{6}$$

Notice also that δ_ℓ is the trivial eigenvalue of $\mathbf{A}$ with $\mathbf{j}$ as eigenvector. Hence, in this case, the matrices $\mathbf{A}$ and $\mathbf{L}$ lead to equivalent spectral results.

[1] An r-uniform, δ-regular hypergraph, of order n, is called (n, r, δ)-design

As principal tools we will use the so-called alternating polynomials and the Laplacian polynomials.

4.2 Laplacian and Alternating Polynomials

In [7] Fiol, Garriga and Yebra defined and studied the properties of the local spectrum of a graph. In [16] we extend this concept to the case of the Laplacian matrix of a hypergraph as follows. For a given vertex v_i we can consider the spectral decomposition of the corresponding unit vector e_i

$$e_i = \sum_{l=0}^{b} z_{il}, \quad \text{where} \quad z_{il} \in \mathrm{Ker}(\mathbf{L}(\mathcal{H}) - \mu_l \mathbf{I}). \tag{7}$$

The v_i-*local multiplicity* of the Laplacian eigenvalue μ_l is defined as $m_i(\mu_l) := \|z_{il}\|^2$. Thus, the v_i-local multiplicity of $\mu_0 = 0$ is $m_i(0) = \frac{1}{n}$. The v_i-*local eigenvalues* of $\mathbf{L}$ are denoted by $0 < \psi_1 < \cdots < \psi_{b_i}$ and they are defined as the Laplacian eigenvalues with nonnull v_i-local multiplicities. The v_i-*local spectrum* of $\mathbf{L}$ is defined as $Spec_i(\mathbf{L}) = \left\{0^{\frac{1}{n}}, \psi_1^{m_i(\psi_1)}, \ldots, \psi_{b_i}^{m_i(\psi_{b_i})}\right\}$. When we "see" the hypergraph from a given vertex, its local spectrum plays a similar role as the global spectrum, thus justifying the terminology used.

By using the v_i-local spectrum of $\mathbf{L}$, we define the v_i-local k-Laplacian polynomials that we will use as tool in the following sections. The study of these polynomials is completely analogous to the study of the local adjacency polynomials defined and studied by Fiol and Garriga in [8], therefore, we collect here some of its main properties, referring the reader to [8] for a more detailed study.

Let $\psi_0 = 0 < \psi_1 < \cdots < \psi_{b_i}$ be the v_i-local eigenvalues of $\mathbf{L}$. For each $k = 0, ..., b_i$, the mapping $\| \ \|_i$: $\mathbb{R}_k[x] \mapsto \mathbb{R}$ defined by $\|P\|_i = \|P(\mathbf{L})e_i\|$ is a norm of the space $\mathbb{R}_k[x]$. In this normed space, we consider the closed unit ball $B_k = \{P \in \mathbb{R}_k[x] : \|P\|_i \leq 1\}$. On this compact set, the linear continuous function $P \mapsto P(0)$ attains its maximum at a point q_k^i, which we call v_i-*local* k-*Laplacian polynomial*. Notice that, such a point must be on the border of B_k; that is, $\|q_k^i\|_i = 1$.

Between the main properties of the v_i-local k-Laplacian polynomials we emphasize the following.

- Each v_i-local k-Laplacian polynomial has degree k.
- $1 = q_0^i(0) < q_1^i(0) < \cdots < q_{b_i}^i(0) = \sqrt{n}$.

As we are going to see in the following sections, in practice, we only need the independent term $q_k^i(0)$ of q_k^i.

In the case of walk-regular hypergraphs, the polynomials q_k^i do not depend on v_i (see [16]). Hence we call these polynomials k-Laplacian polynomials and they will be denoted as q_k. The independent term of q_k can be calculated by the following constrained optimization problem [16]:

$$\text{maximize } \alpha_0, \text{ subject to}$$

$$\alpha_0^2 + \sum_{l=1}^{b} m_l(\alpha_0 + \alpha_1\mu_l + \cdots + \alpha_k\mu_l^k)^2 = n. \tag{8}$$

Now we collect some results that we will use in the following sections.

We define for any $k = 0, 1, \ldots, D(\mathcal{H})$, the *k-excess* of a vertex $u \in V(\mathcal{H})$, denoted by $\mathbf{e}_k(u)$, as the number of vertices which are at distance greater than k from u. That is,

$$\mathbf{e}_k(u) := |\{v \in V : \partial(u, v) > k\}|.$$

Then, trivially, $\mathbf{e}_0(u) = n - 1$, $\mathbf{e}_{D(\mathcal{H})}(u) = \mathbf{e}_{\epsilon(u)}(u) = 0$ and $\mathbf{e}_k(u) = 0$ if and only if $\epsilon(u) \leq k$. The excess of a vertex of a graph was studied by Fiol and Garriga [8] using the adjacency eigenvalues and by Yebra and the author of this paper [17] using the Laplacian eigenvalues.

Lemma 6. ([16], and see [8] for the previous result on graphs) *Let v_i be a vertex of a hypergraph of order n, and let q_k^i be its v_i-local k-Laplacian polynomial. Then,*

$$q_k^i(0) > \sqrt{n-1} \Rightarrow \epsilon(v_i) \leq k. \tag{9}$$

$$\mathbf{e}_k(v_i) \leq \left\lfloor n - \left(q_k^i(0)\right)^2 \right\rfloor. \tag{10}$$

The *k-excess* of $\mathcal{H}$ denoted by $\mathbf{e}_k$, is defined as

$$\mathbf{e}_k := \max_{v_i \in V(\mathcal{H})} \{\mathbf{e}_k(v_i)\}.$$

Lemma 7. [16] *Let $\mathcal{H}$ be a walk-regular hypergraph and let q_k be its k-Laplacian polynomial. Then,*

$$q_k(0) > \sqrt{n-1} \Rightarrow D(\mathcal{H}) \leq k. \tag{11}$$

$$\mathbf{e}_k \leq \left\lfloor n - (q_k(0))^2 \right\rfloor \tag{12}$$

In this work, we also use the k-alternating polynomials studied by Fiol, Garriga and Yebra in [3]. These polynomials can be defined as follows: let $\mathcal{M} = \{\mu_1 < \cdots < \mu_b\}$ be a mesh of real numbers. For any $k = 0, 1, ..., b - 1$ let Q_k be the *k-alternating polynomial* associated with $\mathcal{M}$. That is, the polynomial of $\mathbb{R}_k[x]$ with norm $\|Q_k\|_\infty = \max_{1 \leq i \leq b}\{|Q_k(\mu_i)|\} \leq 1$, such that

$$Q_k(\mu) = \sup\{P(\mu) : P \in \mathbb{R}_k[x], \quad \|P\|_\infty \leq 1\}$$

where μ is any real number smaller than μ_1. In [3] it was shown that, for any $k = 0, 1, ..., b - 1$,

- There is a unique Q_k which, moreover, is independent of the value of $\mu(< \mu_1)$;
- Q_k has degree k;
- $Q_0(\mu) = 1 < Q_1(\mu) < \cdots < Q_{b-1}(\mu)$;
- Q_k takes $k + 1$ alternating values ± 1 at the mesh points;
- There are explicit formulae for $Q_0(= 1)$, Q_1, Q_2, and Q_{b-1}, while the other polynomials can be computed by solving a linear programming problem (for instance by the simplex method).

The alternating polynomials have been applied extensively to the study of metric properties of graphs and hypergraph [3–6, 12–15]. For instance, here we collect some results that we will use in the following sections.

Lemma 8. ([14], and see [3] for the previous result on graphs) *Let Q_k be the k-alternating polynomial associated to the mesh of the Laplacian eigenvalues of a hypergraph $\mathcal{H}$ of order n. Then,*

$$Q_k(0) > n - 1 \Rightarrow D(\mathcal{H}) \leq k. \tag{13}$$

$$\mathbf{e}_k \leq \left\lfloor \frac{n(n-1)}{Q_k^2(0) + n - 1} \right\rfloor. \tag{14}$$

4.3 Bounds

In the case of graphs, we obtain the following upper bound on the Wiener index

$$W(\Gamma) \leq \frac{1}{2}\sum_{i=1}^{n}\left[\delta(v_i) + D(\Gamma)\left(n - \delta(v_i) - 1\right)\right] = m + D(\Gamma)\overline{m},$$

where m denotes the size of Γ and $\overline{m}$ denotes the size of the complement of Γ. The equality holds if and only if $\Gamma = K_n$ or $D(\Gamma) = 2$. Moreover, it is well-known that if $b+1$ denotes the number of Laplacian eigenvalues of Γ, then $D(\Gamma) \leq b$. Therefore,

$$W(\Gamma) \leq m + b\overline{m} \tag{15}$$

An analogous result for the adjacency matrix is obtained by replacing in (15) the number $b+1$, of different Laplacian eigenvalues, by the number $d+1$ of different adjacency eigenvalues. We recall that in the non-regular case b and d may be different. Obviously, the best bound is obtained with the matrix that has the smallest number of eigenvalues.

If $D(\Gamma) \leq k < b$, we can improve the above bounds. Let Q_k be the k alternating polynomial defined over the Laplacian eigenvalues of a graph Γ. Then,

$$Q_k(0) > n - 1 \Rightarrow W(\Gamma) \leq k\overline{m} + m \tag{16}$$

The above result immediately follows from (13) and (15).

However we can improve the above bounds from bounds on the k-excess.

Lemma 9. *Let $W(\mathcal{H})$ be the Wiener index of a hypergraph $\mathcal{H}$. Then*

$$W(\mathcal{H}) = \frac{1}{2}\sum_{v\in V(\mathcal{H})}\sum_{k=0}^{D(\mathcal{H})-1}\mathbf{e}_k(v)$$

Proof. The distance of a vertex v in a connected hypergraph $\mathcal{H}$

$$S(v) = \sum_{u\in V(\mathcal{H})}\partial(u,v)$$

Satisfies

$$S(v) = \sum_{k=1}^{D(\mathcal{H})} k(\mathbf{e}_{k-1}(v) - \mathbf{e}_k(v)).$$

Moreover, by a simple calculation we have

$$S(v) = \sum_{k=0}^{D(\mathcal{H})-1}\mathbf{e}_k(v). \tag{17}$$

Hence, by (17) we have

$$W(\mathcal{H}) = \frac{1}{2}\sum_{v\in V(\mathcal{H})}S(v) = \frac{1}{2}\sum_{v\in V(\mathcal{H})}\sum_{k=0}^{D(\mathcal{H})-1}\mathbf{e}_k(v)$$

□

Therefore, it follows from Lemma 9 that bounds on the k-excess of $\mathcal{H}$ lead to bounds on its Wiener index.

Theorem 10. *Let Q_k be the k-alternating polynomial defined over the Laplacian eigenvalues of a hypergraph $\mathcal{H}$ of order n. If $Q_k(0) > n-1$ then,*

$$W(\mathcal{H}) \leq \frac{n}{2}\sum_{l=0}^{k-1}\left\lfloor \frac{n(n-1)}{Q_l^2(0)+n-1}\right\rfloor; \tag{18}$$

$$\xi^{DS}(\mathcal{H}) \leq nk\sum_{l=0}^{k-1}\left\lfloor \frac{n(n-1)}{Q_l^2(0)+n-1}\right\rfloor. \tag{19}$$

Theorem 10 can be obtained from the previous bound on the mean distance obtained in [14].

Proof. By (14) and Lemma 9 we have

$$W(\mathcal{H}) \leq \frac{n}{2}\sum_{k=0}^{D(\mathcal{H})-1}\left\lfloor \frac{n(n-1)}{Q_k^2(0)+n-1}\right\rfloor$$

and by (13) we conclude the proof of (18). It follows from (3) that bounds on the Wiener index of $\mathcal{H}$ lead to bounds on its eccentric distance sum. Thus, from (18) we derive (19). □

For instance, let $\mathcal{H}$ be the dual hypergraph of the affine plane of rank $r=2$. That is, the hypergraph dual of a sub-hypergraph obtained from the Fano plane (finite projective plane of rank 3) by suppressing the point of a given line. This hypergraph of order $n=6$ has Wiener index $W(\mathcal{H}) = 18$ and Laplacian eigenvalues $\mu_0 = 0$, $\mu_1 = 4$ and $\mu_2 = 6$. Then, Theorem 10 leads to $W(\mathcal{H}) \leq 18$.

Theorem 11. *Let $\mathcal{H}$ be a connected hypergraph of order n and let q_k^i be its v_i-local k-Laplacian polynomials. Then,*

$$W(\mathcal{H}) \leq \frac{1}{2}\sum_{i=1}^{n}\sum_{l=1}^{k(\mathcal{H})_i-1}\left\lfloor n-\left(q_l^i(0)\right)^2\right\rfloor,$$

where

$$k(\mathcal{H})_i = \min\{k\in\{0,\ldots,b_i\} : q_k^i(0) > \sqrt{n-1}\}.$$

Proof. The result is a direct consequence of Lemma 6 and Lemma 9. □

Corollary 12. *Let $\mathcal{H}$ be a walk-regular hypergraph and let q_k be its k-Laplacian polynomial. If $q_k(0) > \sqrt{n-1}$, then*

$$W(\mathcal{H}) \leq \frac{n}{2}\sum_{l=0}^{k-1}\left\lfloor n-\left(q_l(0)\right)^2\right\rfloor; \tag{20}$$

$$\xi^{DS}(\mathcal{H}) \leq nk\sum_{l=0}^{k-1}\left\lfloor n-\left(q_l(0)\right)^2\right\rfloor. \tag{21}$$

Corollary 12 can be obtained from the previous bound on the mean distance obtained in [16].

Let $\mathcal{H}$ be the $(5,3,3)$-design whose blocks are

$$b_1=\{1,2,3\}\quad b_2=\{2,3,4\}\quad b_3=\{3,4,5\}\quad b_4=\{4,5,1\}\quad b_4=\{5,1,2\}.$$

The hypergraph $\mathcal{H}$ is walk-regular, that is,

$$\delta_\ell = \frac{Tr(\mathbf{L})}{5} = 6, \quad \frac{Tr(\mathbf{L}^2)}{5} = 46, \quad \frac{Tr(\mathbf{L}^3)}{5} = 360, \dots$$

The Laplacian spectrum of $\mathcal{H}$ is

$$Spec(\mathcal{H}) = \left\{ 0^1, \left(\frac{15-\sqrt{5}}{2}\right)^2, \left(\frac{15+\sqrt{5}}{2}\right)^2 \right\}.$$

Thus, by solving the constrained optimization problem (8), we calculated the independent terms of q_k, $k = 0, \dots, 2$: $q_0(0) = 1$, $q_1(0) = \frac{23\sqrt{115}}{115}$, $q_2(0) = \sqrt{5}$. Corollary 12 gives $W(\mathcal{H}) \leq 10$ and the bound is attained.

Now let $k(\mathcal{H})$ and $es(\mathcal{H})$ be vectors of $\mathbb{R}^n$ defined by

$$k(\mathcal{H})_i := \min\{k \in \{0, ..., b_i\} : q^i_k(0) > \sqrt{n-1}\}$$

and

$$es(\mathcal{H})_i := \sum_{l=0}^{k(\mathcal{H})_i - 1} \left\lfloor n - \left(q^i_l(0)\right)^2 \right\rfloor.$$

Then we obtain the following result on ξ^{DS}.

Theorem 13. *With notation as above,*

$$\xi^{DS}(\mathcal{H}) \leq \langle k(\mathcal{H}), es(\mathcal{H}) \rangle.$$

Proof. By Lemma 6 and (17) we have

$$\epsilon(v_i) \cdot S(v_i) \leq k(\mathcal{H})_i \cdot es(\mathcal{H})_i \qquad i = 1, ..., n. \tag{22}$$

Thus, (22) leads to the result. □

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