On the Wiener index and the eccentric distance sum of hypergraphs

J. A. Rodríguez∗
Departamento de Matemáticas
Universidad Carlos III de Madrid
Avda. de la Universidad 30, 28911 Leganés (Madrid), Spain

(Received May 6, 2004)

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 \( \Gamma \) 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

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

∗e-mail: juanalberto.rodriguez@uc3m.es
The distance of a vertex \( v \) in a connected hypergraph \( H \) is defined by
\[
S(v) := \sum_{u \in V(H)} \partial(u, v).
\]

The Wiener index \( W(\Gamma) \) of a graph \( \Gamma \) with vertex set \( \{v_1, v_2, ..., v_n\} \) defined as the sum of distances between all pairs of vertices of \( \Gamma \),
\[
W(\Gamma) := \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \partial(v_i, v_j) = \frac{1}{2} \sum_{v \in V(\Gamma)} S(v),
\]

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 \( \xi_{DS} \), 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 dihydroselens 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 a 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 \( H \), between the vertices \( u \) and \( v \) or \( u - v \) walk, to be a
finite sequence \( u = \nu_0 e_1 v_1 \cdots v_{t-1} e_{t-1} v_t = v \) of vertices \( v_i \) and edges \( e_i \) of \( H \) such that \( v_i \in e_{i+1} \) for \( i = 0, \ldots k - 1 \), and \( v_k \in v_t \) for \( i = 1, \ldots, k \). A \( u-v \) walk is called a cycle in which no vertex is repeated. A path is a walk in which no edge is repeated.

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

Note that a path in a hypertree is not necessarily a shortest path. For instance, the path \( 3e_12e_1e_25 \) 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 \( e_2 = \{1, 4, 5\} \).

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

\[
\text{Lemma 2. There is a unique shortest path between two vertices of a hypertree.}
\]

\textbf{Proof.} Let \( u \) and \( v \) be two vertices of a hypertree \( T \) such that \( \partial(u,v) = k \). Suppose that \( u = \nu_0 e_1 v_1 \cdots v_0 e_{t-1} v_t = v \) and \( u = \nu_0 e_1' v_1' \cdots v_{t-1}' e_{t-1}' v_t' = v \) 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 \( v_i = v_{i+1}' \), then \( T = r_i \). That is, if \( v_i = v_{i+1}' \) and \( r < r' \), then the path \( u = \nu_0 e_1 v_1 \cdots v_{t-1} e_{t-1} v_t = v \) has length less than \( k \), thus contradicting that \( \partial(u,v) = k \). Similarly we can see that the case \( e_i = e_i' \), with \( r \neq r' \), is not possible.

If \( v_i = v_{i+1} \) for \( i = 0, \ldots, k \), then \( e_{i+1} \neq e_{i+1}' \) for some \( j, 0 \leq j \leq k - 1 \). Thus, \( T \) has a cycle \( e_{i+1} v_{i+2} e_{j+1}' v_{j+1} \), in contradiction to \( T \) being a hypertree.

If there are two integers \( j \) and \( r \) such that \( 0 \leq j < r \leq k \) and \( j + r = 2 \), then the path \( u = v_i v_{i+1} v_{i+2} v_{i+3} \) for every \( i \) such that \( j < i < r \) and \( v_j = v_{j+1}' \), then we consider the following cases:

\begin{itemize}
  \item If \( e_{i+1} \neq e_{i+1}' \) for every \( t \) such that \( j \leq t < r \), then \( T \) has a cycle \( v_j e_{i+1} v_{j+1} \cdots v_{r-1}' e_{i+1}' v_r \), thus contradicting that \( T \) is a hypertree.
  \item If \( e_i = e_i' \) and \( e_{i+1} = e_{i+1}' \) for some \( t \) such that \( j < t < r \), then \( T \) is a hypertree.
  \item If \( e_i = e_i' \) and \( e_{i+1} = e_{i+1}' \) for some \( t \) such that \( j < t < r \), then \( T \) is a hypertree.
  \item The case \( e_{i+1} \neq e_{i+1}' \) for every \( t \) such that \( t' < t < r \), where \( j \leq t' \) and \( e_{i+1} = e_{i+1}' \), is analogous to the previous one.
  \item If \( e_i = e_i' \) and \( e_{i+1} = e_{i+1}' \) for some \( t \) such that \( j < t' < t' < r \) and \( e_{i+1} \neq e_{i+1}' \) for every \( t \) with \( j < t < r' \), then \( T \) has a cycle \( v_j e_{j+1} v_{j+1} \cdots v_{r-1}' e_{r-1}' v_r \), thus contradicting that \( T \) is a hypertree.
\end{itemize}

Therefore, the result follows.
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 \(u \in V(T)\) 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 \(\Gamma_T\) considering that \(V(T) = V(\Gamma_T)\) where two vertices of \(\Gamma_T\) are adjacent if they are adjacent in \(T\). In such case, each edge of \(T\) induces a complete subgraph in \(\Gamma_T\), two complete subgraphs of \(\Gamma_T\) only can share one vertex and \(\Gamma_T\) has no cycles of complete subgraphs. See, for instance, Figure 2.

Figure 2: The graph \(\Gamma_T\) 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 \(c_j\) \((1 \leq j \leq D)\);
The eccentric distance sum: each vertex of \( H \) obtained directly from the intersection array.

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

\[
\begin{align*}
\{0,1,2\}, \quad \{0,2,3\}, \quad \{0,3,4\}, \quad \{0,4,5\}, \quad \{0,1,5\}, \\
\{1,2,8\}, \quad \{1,5,7\}, \quad \{1,7,8\}, \quad \{2,3,9\}, \quad \{2,8,9\}, \\
\{3,4,10\}, \quad \{3,9,10\}, \quad \{4,5,11\}, \quad \{4,10,11\}, \quad \{5,7,11\}, \\
\{6,7,8\}, \quad \{6,7,11\}, \quad \{6,8,9\}, \quad \{6,9,10\}, \quad \{6,10,11\},
\end{align*}
\]

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

**Theorem 4.** Let \( H \) 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

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

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

\[
|H_{i-1}(v)| \cdot b_{i-1} = |H_i(v)| \cdot c_i.
\]

Therefore, it follows from (1) that the number of vertices at distance \( i \) of a vertex \( v \), \( |H_i(v)| \), is obtained directly from the intersection array

\[
|H_i(v)| = \frac{\prod_{j=2}^{i-1} b_j}{\prod_{j=2}^{i-1} c_j} \quad (2 \leq i \leq D) \quad \text{and} \quad |H_1(v)| = b_0.
\]

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, \( H_k \) \((k \geq 2)\), 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

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

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

\[
\xi^{DS}(H) \leq 2D(H)W(H).
\]

If all vertices of \( H \) 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 \( H \) 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

\[
\xi^{DS}(H) = nD(H)b_0 \left( 1 + \sum_{i=2}^{d} \frac{\prod_{j=2}^{i-1} b_j}{\prod_{j=2}^{i-1} c_j} \right).
\]
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 $A = A(H)$ the adjacency matrix of $H$. Given two distinct vertices $v_i, v_j \in V(H)$, the entry $a_{ij}$ of $A$ is the number of edges in $H$ containing both $v_i$ and $v_j$; the diagonal entries of $A$ are zero.

If $v_i, v_j \in V(H)$, then the number of walks of length $k$ in $H$, from $v_i$ to $v_j$, is the entry in position $(i,j)$ of the matrix $A^k$ (see [15]).

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 $A^k$ has its diagonal entries all equal to $Tr\{A^k\}/n$. 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 $v_i \in V(H)$ as $\delta_i(v_i) := \sum_{j=1}^n a_{ij}$. We say that the hypergraph $H$ is Laplacian regular of degree $\delta_i$ if any vertex $v_i \in V(H)$ has Laplacian degree $\delta_i(v_i) = \delta$. Obviously, every walk-regular hypergraph is Laplacian regular.

A simple count shows that the Laplacian degree of an $(n,r,\delta)$-design satisfies

$$\delta_i = (r-1)\delta = \frac{mr(r-1)}{n}. \quad (4)$$

Moreover, if $H$ is a graph then $\delta_i(v_i) = \delta(v_i)$.

The Laplacian matrix of a hypergraph $H$, denoted by $L = L(H)$, is defined as $L := D - A$ where $D = diag(\delta_1(v_1), \delta_2(v_2), \ldots, \delta_n(v_n))$. This version of Laplacian matrix was introduced by the 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 $L$ is symmetric and positive semidefinite, the smallest eigenvalue of $L$ is $\mu = 0$ and a corresponding eigenvector is $j = (1, 1, \ldots, 1)$. Moreover, the multiplicity of $\mu = 0$ is equal to the number of connected components of $H$.

The eigenvalues of $L$ are denoted by $\mu_0 = 0 < \mu_1 < \cdots < \mu_k$ and their multiplicities are denoted by $m_0 = 1, m_1, \ldots, m_k$. Hence, the Laplacian spectrum of $H$ is denoted by $Spec(L) = \{\mu_1^m, \mu_2^m, \ldots, \mu_k^m\}$.

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

$$A = \sum_{i=1}^n m_i \mu_i = \sum_{i=1}^n \delta_i(v_i). \quad (5)$$

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

We denote by $\lambda_0 > \lambda_1 > \cdots > \lambda_k$ the adjacency eigenvalues of a Laplacian regular hypergraph $H$ of degree $\delta_i$. Then, since $L = \delta_i I - A$, the eigenvalues of both matrices, $A$ and $L$, are related by

$$\mu_l = \delta_i - \lambda_l, \quad l = 0, \ldots, b = d. \quad (6)$$

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

---

1 An $r$-uniform, $\delta$-regular hypergraph, of order $n$, is called $(n,r,\delta)$-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 \( v \) we can consider the spectral decomposition of the corresponding unit vector \( e \):

\[
e_i = \sum_{l=0}^{k} z_{il}, \quad \text{where} \quad z_{il} \in \text{Ker}(L(H) - \mu_l I).
\]

(7)

The \( v \)-local multiplicity of the Laplacian eigenvalue \( \mu_l \) is defined as

\[
m_i(\mu_l) := \|z_{il}\|_2.
\]

Thus, the \( v \)-local eigenvalues of \( L \) are denoted by \( 0 < \psi_1 < \cdots < \psi_b \) and they are defined as the Laplacian eigenvalues with nonnull \( v \)-local multiplicities. The \( v \)-local spectrum of \( L \) is defined as

\[
\text{Spec}_i(L) = \{0^2, \psi_1^{m_1(\psi_1)}, \ldots, \psi_b^{m_b(\psi_b)}\}.
\]

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 \( v \)-local spectrum of \( L \), we define the \( v \)-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 \( \psi_0 = 0 < \psi_1 < \cdots < \psi_b \) be the \( v \)-local eigenvalues of \( L \). For each \( k = 0, \ldots, b \), the mapping \( \| \cdot \| : \mathbb{R}_k[x] \to \mathbb{R} \) defined by \( \|P\| = \|P(L)e_i\| \) is a norm of the space \( \mathbb{R}_k[x] \). In this normed space, we consider the closed unit ball \( B_k = \{P \in \mathbb{R}_k[x] : \|P\|_1 \leq 1\} \). On this compact set, the linear continuous function \( P \mapsto P(0) \) attains its maximum at a point \( q_i \), which we call \( v \)-local \( k \)-Laplacian polynomial. Notice that, such a point must be on the border of \( B_k \), that is, \( \|q_i\|_1 = 1 \).

Between the main properties of the \( v \)-local \( k \)-Laplacian polynomials we emphasize the following:

- Each \( v \)-local \( k \)-Laplacian polynomial has degree \( k \).
- \( 1 = q_0(0) < q_1(0) < \cdots < q_b(0) = \sqrt{n} \).

As we are going to see in the following sections, in practice, we only need the independent term \( q_0(0) \) of \( q_i \).

In the case of walk-regular hypergraphs, the polynomials \( q_i \) do not depend on \( v \) (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]:

\[
\text{maximize} \quad \alpha_0, \quad \text{subject to} \quad \alpha_0^2 + \sum_{l=1}^{k} m_l(\alpha_0 + \alpha_1 \mu_l + \cdots + \alpha_k \mu_l^k)^2 = n.
\]

(8)

Now we collect some results that we will use in the following sections.
We define for any \( k = 0, 1, \ldots, D(H) \), the \( k \)-excess of a vertex \( u \in V(H) \), denoted by \( e_k(u) \), as the number of vertices which are at distance greater than \( k \) from \( u \). That is, 
\[
e_k(u) := |\{ v \in V : d(u, v) > k \}|.
\]
Then, trivially, \( e_0(u) = n - 1 \), \( e_2(u) = 0 \) if and only if \( e(u) \leq k \). 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 \( q_k \) be its \( k \)-local \( k \)-Laplacian polynomial. Then,
\[
q_k(0) > \sqrt{n - 1} \Rightarrow e(v_i) \leq k.  \tag{9}
\]
\[
e_k(v_i) \leq \left| n - (q_k(0))^2 \right|.  \tag{10}
\]

The \( k \)-excess of \( H \), denoted by \( e_k \), is defined as 
\[
e_k := \max_{v \in V(H)} \{ e_k(v) \}.
\]

**Lemma 7.** \[16\] Let \( H \) be a walk-regular hypergraph and let \( q_k \) be its \( k \)-Laplacian polynomial. Then,
\[
q_k(0) > \sqrt{n - 1} \Rightarrow D(H) \leq k.  \tag{11}
\]
\[
e_k \leq \left| n - (q_k(0))^2 \right|.  \tag{12}
\]

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 \( M = \{ \mu_1 < \cdots < \mu_b \} \) be a mesh of real numbers. For any \( k = 0, 1, \ldots, b - 1 \) let \( Q_k \) be the \( k \)-alternating polynomial associated with \( M \). That is, the polynomial of \( \mathbb{R}[x] \) with norm \( \|Q_k\|_\infty = \max_{\mu \in \mathbb{R}}|Q_k(\mu)| \leq 1 \), such that 
\[
Q_k(\mu) = \sup \{ P(\mu) : P \in \mathbb{R}[x], \|P\|_\infty \leq 1 \}
\]
where \( \mu \) is any real number smaller than \( \mu_1 \). In \[3\] it was shown that, for any \( k = 0, 1, \ldots, b - 1 \),
- 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 \( \pm 1 \) 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 \( H \) of order \( n \). Then,
\[
Q_k(0) > n - 1 \Rightarrow D(H) \leq k.  \tag{13}
\]
\[
e_k \leq \left| n(n - 1) \right| \frac{1}{Q_k(0) + n - 1}.  \tag{14}
\]
4.3 Bounds

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

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

where \( m \) denotes the size of \( \Gamma \) and \( \overline{m} \) denotes the size of the complement of \( \Gamma \). 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 \( \Gamma \), 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 \( \Gamma \). 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

\[ W(\mathcal{H}) = \frac{1}{2} \sum_{v \in V(\mathcal{H})} D(\mathcal{H})_{-1} \sum_{k=0}^{D(\mathcal{H})-1} e_k(v) \]

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

\[ S(v) = \sum_{u \in V(\mathcal{H})} d(u, v) \]

Satisfies

\[ S(v) = \sum_{k=0}^{D(\mathcal{H})} k(e_k(v) - e_{k-1}(v)). \]

Moreover, by a simple calculation we have

\[ S(v) = \sum_{k=0}^{D(\mathcal{H})-1} e_k(v). \tag{17} \]

Hence, by (17) we have

\[ W(\mathcal{H}) = \frac{1}{2} \sum_{v \in V(\mathcal{H})} S(v) = \frac{1}{2} \sum_{v \in V(\mathcal{H})} \sum_{k=0}^{D(\mathcal{H})-1} e_k(v) \]

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 \( H \) of order \( n \). If \( Q_k(0) > n - 1 \) then,

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

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

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

Proof. By (14) and Lemma 9 we have

\[
W(H) \leq \frac{n}{2} \sum_{l=0}^{\ell(n)-1} \left\lfloor \frac{n(n-1)}{Q_l(0) + n - 1} \right\rfloor
\]

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

For instance, let \( H \) 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 \( W(H) = 18 \) and Laplacian eigenvalues \( \mu_0 = 0, \mu_1 = 4 \) and \( \mu_2 = 6 \). Then, Theorem 10 leads to \( W(H) \leq 18 \).

Theorem 11. Let \( H \) be a connected hypergraph of order \( n \) and let \( q_k \) be its \( v_i \)-local \( k \)-Laplacian polynomials. Then,

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

where

\[ k(H)_i = \min\{k \in \{0, \ldots, b_i\} : q_k(0) > \sqrt{n - 1} \}. \]

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

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

\[
W(H) \leq \frac{n}{2} \sum_{l=0}^{k-1} \left| n - (q_l(0))^2 \right| ; \tag{20}
\]

\[
\xi^{DS}(H) \leq nk \sum_{l=0}^{k-1} \left| n - (q_l(0))^2 \right|. \tag{21}
\]

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

Let \( H \) be the \((5,3,3)\)-design whose blocks are

\[
b_1 = \{1, 2, 3\} \quad b_2 = \{2, 3, 4\} \quad b_3 = \{3, 4, 5\} \quad b_4 = \{4, 5, 1\} \quad b_5 = \{5, 1, 2\}.
\]
The hypergraph $\mathcal{H}$ is walk-regular, that is,
\[
\delta_5 = \frac{\text{Tr}(L)}{5} = 6, \quad \frac{\text{Tr}(L^2)}{5} = 46, \quad \frac{\text{Tr}(L^3)}{5} = 360, \ldots
\]
The Laplacian spectrum of $\mathcal{H}$ is
\[
\text{Spec}(\mathcal{H}) = \left\{0, \left(15 - \sqrt{5}\right)^2, \left(15 + \sqrt{5}\right)^2\right\}
\]
Thus, by solving the constrained optimization problem (8), we calculated the independent terms of $q_k$, $k = 0, \ldots, 2$: $q_0(0) = 1$, $q_1(0) = \frac{23}{\sqrt{115}}$, $q_2(0) = \sqrt{5}$. 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
\[
k(\mathcal{H})_i := \min\{k \in \{0, \ldots, b_i\} : q_k(0) > \sqrt{n - 1}\}
\]
and
\[
es(\mathcal{H})_i := \sum_{l=0}^{k(b_i)-1} \left[n - (q_l(0))^2\right].
\]
Then we obtain the following result on $\xi_{DS}$.

**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
\[
\epsilon(v_i) \cdot S(v_i) \leq k(\mathcal{H})_i \cdot es(\mathcal{H})_i, \quad i = 1, \ldots, n. \quad (22)
\]
Thus, (22) leads to the result. \(\square\)

**References**


