

Proof of a Conjecture on Distance Energy of Complete Multipartite Graphs

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Abstract

Caporossi, Chasser and Furtula in [Les Cahiers du GERAD (2009), G-2009-64] derived certain spectral properties of the distance matrix of complete multipartite graphs, and conjectured that the distance energy of a complete multipartite graph on n vertices having γ parts, each of size at least two, is equal to $4(n - \gamma)$. We prove this conjecture.

1 Introduction

Let $G = (V, E)$ be a simple, connected graph with $n = |V|$ vertices. The distance matrix of G is the $n \times n$ matrix D , indexed by V , such that $D_{u,v}$ is the distance between the vertices u and v . One of the earliest uses of the distance matrix in chemistry was by Clark and Kettle [1] in 1975, who used it for studying the permutational isomers of stereochemically

nonrigid molecules, while a review of other early uses of the distance matrix in chemistry was given by Mihalić et al [2].

Topological indices based on the spectrum of the distance matrix, in particular its largest eigenvalue and its energy, play a significant role in research. Balaban et al [3] proposed the use of the largest eigenvalue of distance matrix as a molecular descriptor, while Gutman and Medeleanu [4] successfully used it to infer the extent of branching and model boiling points of alkanes. Consonni and Todeschini [5] further showed that the energy of distance matrix is also a useful molecular descriptor as it appears among the best univariate models for the motor octane number of the octane isomers and for the water solubility of polychlorobiphenyls. An extensive review of the spectral properties of the distance matrix was given recently by Stevanović and Ilić [6].

The distance energy E_D is defined as

$$E_D = \sum_{i=1}^n |\rho_i|,$$

where ρ_1, \dots, ρ_n are the eigenvalues of the distance matrix D . This expression stems from the general definition of energy of a general matrix, stated as the total absolute deviation of matrix eigenvalues from their average. This definition was put forward by Consonni and Todeschini [5] and further elaborated in a recent book by Li et al [7, Chapter 11].

The complete multipartite graph K_{p_1, \dots, p_r} , $p_1, \dots, p_r \geq 1$, is obtained from the union of empty graphs $\overline{K}_{p_1} \cup \dots \cup \overline{K}_{p_r}$ by adding edges between any two vertices from different empty graphs. The distance energy $E_D(K_{p_1, p_2}) = 4(p_1 + p_2 - 2)$ of the complete bipartite graph K_{p_1, p_2} with $p_1, p_2 \geq 2$, was obtained by Stevanović and Indulal in [8], and also as a corollary of the results of Caporossi et al [9] on spectral properties of the distance matrix of complete multipartite graphs. For the complete multipartite graphs, Caporossi et al [9] proposed the following

Conjecture 1 ([9]) *If $p_1, \dots, p_r \geq 2$ then*

$$E_D(K_{p_1, \dots, p_r}) = 4(p_1 + \dots + p_r - r).$$

Our goal here is to prove this conjecture.

2 Proof of Conjecture 1

Without loss of generality, suppose that $2 \leq p_1 \leq \dots \leq p_r$. Label the vertices of the complete multipartite graph K_{p_1, \dots, p_r} in such a way that the vertices belonging to the same empty graph \overline{K}_{p_i} are consecutive. The distance matrix of K_{p_1, \dots, p_r} then has the form

$$D = \begin{pmatrix} 2J_{p_1, p_1} - 2I_{p_1} & J_{p_1, p_2} & \cdots & J_{p_1, p_{r-1}} & J_{p_1, p_r} \\ J_{p_2, p_1} & 2J_{p_2, p_2} - 2I_{p_2} & \cdots & J_{p_2, p_{r-1}} & J_{p_2, p_r} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ J_{p_{r-1}, p_1} & J_{p_{r-1}, p_2} & \cdots & 2J_{p_{r-1}, p_{r-1}} - 2I_{p_{r-1}} & J_{p_{r-1}, p_r} \\ J_{p_r, p_1} & J_{p_r, p_2} & \cdots & J_{p_r, p_{r-1}} & 2J_{p_r, p_r} - 2I_{p_r} \end{pmatrix},$$

where J_{p_i, p_j} is the $p_i \times p_j$ all-ones matrix and I_{p_i} is the $p_i \times p_i$ unit matrix.

It has been observed by Caporossi et al [9, Lemma 2] that, for $p_1, \dots, p_r \geq 2$, the matrix D has eigenvalue -2 with multiplicity at least $\sum_{i=1}^r (p_i - 1)$.

In order to estimate the remaining eigenvalues of D , we have to resort to the concept of equitable matrix partition, an analog of the concept of equitable partition of a graph. A partition $V = \bigcup_{i=1}^r V_i$ of the index set of matrix A is called an *equitable matrix partition* if there exists an $r \times r$ matrix B such that for every $i, j \in \{1, \dots, r\}$ and for every $u \in V_i$ holds

$$\sum_{v \in V_j} A_{u,v} = B_{i,j}.$$

Apparently, the vertex sets of the empty graphs \overline{K}_{p_i} , $i = 1, \dots, r$, form an equitable matrix partition of D , with the matrix B being equal to

$$B = \begin{pmatrix} 2(p_1 - 1) & p_2 & \cdots & p_{r-1} & p_r \\ p_1 & 2(p_2 - 1) & \cdots & p_{r-1} & p_r \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p_1 & p_2 & \cdots & 2(p_{r-1} - 1) & p_r \\ p_1 & p_2 & \cdots & p_{r-1} & 2(p_r - 1) \end{pmatrix}. \tag{1}$$

We have the following fundamental

Lemma 1 *Let matrix D has an equitable matrix partition $V = \bigcup_{i=1}^r V_i$ with the corresponding matrix B . Each eigenvalue of B is then also an eigenvalue of D .*

Proof Let ρ be an eigenvalue of B with an eigenvector x such that $Bx = \rho x$. Form a vector y , indexed by V , given by

$$y_u = x_i \quad \text{if } u \in V_i.$$

Then for $u \in V_i$ holds

$$(Dy)_u = \sum_{v \in V} D_{u,v} y_v = \sum_{j=1}^r \sum_{v \in V_j} D_{u,v} x_j = \sum_{j=1}^r B_{i,j} x_j = (Bx)_i = \rho x_i = \rho y_u.$$

Since this holds for arbitrary u , we have $Dy = \rho y$ and ρ is an eigenvalue of D . ■

If ρ has multiplicity k as an eigenvalue of B , then there is a set of k mutually independent eigenvectors of B corresponding to ρ . Clearly, linear independence is preserved by the construction in the proof of previous lemma, so we obtain a set of k mutually independent eigenvectors of D corresponding to ρ . This implies that ρ , as an eigenvalue of D , has multiplicity at least k . Hence, the spectrum of B is fully contained in the spectrum of D .

The characteristic polynomial of the matrix B given by (1), after subtracting the last row from each of the previous rows, becomes

$$\begin{aligned} \det(\rho I - B) &= \begin{vmatrix} \rho - p_1 + 2 & 0 & \dots & 0 & -\rho + p_r - 2 \\ 0 & \rho - p_2 + 2 & \dots & 0 & -\rho + p_r - 2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \rho - p_{r-1} + 2 & -\rho + p_r - 2 \\ -p_1 & -p_2 & \dots & -p_{r-1} & \rho - 2p_r + 2 \end{vmatrix} \\ &= (\rho - 2p_r + 2) \prod_{i=1}^{r-1} (\rho - p_i + 2) - \sum_{i=1}^{r-1} p_i \prod_{j=1, j \neq i}^r (\rho - p_j + 2) \\ &= \prod_{i=1}^r (\rho - p_i + 2) - \sum_{i=1}^r p_i \prod_{j=1, j \neq i}^r (\rho - p_j + 2) \tag{2} \\ &= \prod_{i=1}^r (\rho - p_i + 2) \left(1 - \sum_{i=1}^r \frac{p_i}{\rho - p_i + 2} \right). \end{aligned}$$

Let $q_1 < \dots < q_k$ be the distinct values among $p_1 \leq \dots \leq p_r$, and let $m_i \geq 1$ be the multiplicity of q_i in p_1, \dots, p_r for $i = 1, \dots, k$. Then

$$\det(\rho I - B) = \prod_{i=1}^k (\rho - q_i + 2)^{m_i} \left(1 - \sum_{i=1}^k \frac{m_i q_i}{\rho - q_i + 2} \right).$$

Clearly, $q_i - 2$ is the root of $\det(\rho I - B)$ with multiplicity at least $m_i - 1$.

Let $F(\rho) = 1 - \sum_{i=1}^k \frac{m_i q_i}{\rho - q_i + 2}$. We have

$$\begin{aligned} \lim_{\rho \rightarrow -\infty} F(\rho) &= 1, \\ \lim_{\rho \rightarrow (q_i - 2)_-} F(\rho) &= +\infty, \quad i = 1, \dots, k, \\ \lim_{\rho \rightarrow (q_i - 2)_+} F(\rho) &= -\infty, \quad i = 1, \dots, k, \\ \lim_{\rho \rightarrow +\infty} F(\rho) &= 1. \end{aligned}$$

Since $F(\rho)$ is continuous on each of the intervals $(q_1 - 2, q_2 - 2), \dots, (q_{k-1} - 2, q_k - 2), (q_k - 2, +\infty)$, we conclude that each of them contains a root of the function $F(\rho)$.

Suppose now that $\rho_1 \leq \rho_2 \leq \dots \leq \rho_r$ are the eigenvalues of the matrix B . Taking into account that $q_i - 2$ is an eigenvalue of B with multiplicity at least $m_i - 1$, $i = 1, \dots, k$, and that B also has an eigenvalue in each of the above mentioned intervals, we conclude, by replacing q_1, \dots, q_k back with p_1, \dots, p_r , that the following chain of inequalities hold

$$0 \leq p_1 - 2 \leq \rho_1 \leq p_2 - 2 \leq \rho_2 \leq \dots \leq p_r - 2 \leq \rho_r.$$

Therefore, the eigenvalues of B are nonnegative and so

$$\sum_{i=1}^r |\rho_i| = \sum_{i=1}^r \rho_i.$$

From the Vieta's formula for the characteristic polynomial of B (see (2)) we further have

$$\sum_{i=1}^r \rho_i = 2 \sum_{i=1}^r (p_i - 1).$$

Since all r nonnegative eigenvalues of B are also eigenvalues of the distance matrix D , we get that the multiplicity of eigenvalue -2 of D has to be indeed equal to $\sum_{i=1}^r (p_i - 1)$.

The distance energy of K_{p_1, \dots, p_r} is, therefore, equal to

$$E_D(K_{p_1, p_2, \dots, p_r}) = |-2| \sum_{i=1}^r (p_i - 1) + \sum_{i=1}^r |\rho_i| = 4(p_1 + \dots + p_r - r).$$

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References

- [1] M. J. Clark, S. F. A. Kettle, Incidence and distance matrices, *Inorg. Chim. Acta* **14** (1975) 201–205.
- [2] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić, The distance matrix in chemistry, *J. Math. Chem.* **11** (1992) 223–258.
- [3] A. T. Balaban, D. Ciubotariu, M. Medeleanu, Topological indices and real number vertex invariants based on graph eigenvalues or eigenvectors, *J. Chem. Inf. Comput. Sci.* **31** (1991) 517–523.

- [4] I. Gutman, M. Medeleanu, On the structure–dependence of the largest eigenvalue of the distance matrix of an alkane, *Indian J. Chem.* **A37** (1998) 569–573.
- [5] V. Consonni, R. Todeschini, New spectral indices for molecule description, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 3–14.
- [6] D. Stevanović, A. Ilić, Spectral properties of distance matrix of graphs, in: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs — Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 139–176.
- [7] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [8] D. Stevanović, G. Indulal, The distance spectrum and energy of the compositions of regular graphs, *Appl. Math. Lett.* **22** (2009) 1136–1140.
- [9] G. Caporossi, E. Chasset, B. Furtula, Some conjectures and properties on distance energy, *Les Cahiers GERAD* (2009) G-2009-64, available at <http://www.gerad.ca/fichiers/cahiers/G-2009-64.pdf> .