JOURNAL OF MATHEMATICAL NANOSCIENCE

JMNS

Vol. 2, No. 1, 2012, 37-41

A note on eccentric distance sum

MAHIN SONGHORI

Department of Mathematics, Faculty of Science, Shahid Rajaee

Teacher Training University, Tehran, 16785 – 136, I R. Iran

ABSTRACT. The eccentric distance sum is a graph invariant defined as $\sum_{v\in V(G)}\varepsilon_G(v)D_G(v)$, where $\varepsilon_G(v)$ is the eccentricity of a vertex v in G and $D_G(v)$ is the sum of distances of all vertices in G from v. In this paper, we compute the eccentric distance sum of Volkmann tree and then we obtain some results for vertex–transitive graphs

Keywords: eccentricity, eccentric distance sum, Volkmann tree.

1. INTRODUCTION

A **graph** is a collection of points and lines connecting a subset of them. The points and lines of a graph are also called vertices and edges of the graph, respectively. The vertex and edge sets of the graph G are denoted by $V(G)$ and $E(G)$, respectively.

A **molecular graph** is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. **Chemical graph theory** is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences.

In this paper, in the next section we give necessary definitions and some preliminary results. Section 3 contains the main results, i.e., the explicit formulas for the eccentric distance sum of Volkmann tree.

Journal of Mathematical NanoScience

2. PRELIMINARY NOTES

If $x, y \in V(G)$ then the **distance** $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y. For a vertex u of $V(G)$ its **eccentricity** $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G, $\varepsilon_G(u) = \max_{v\in V(G)} d_G(u,v)$. The maximum and minimum eccentricity over all vertices of G are called the **diameter** and **radius** of G and denoted by $d(G)$, $r(G)$ respectively, see [9]. The **total eccentricity** of the graph G, can be defined as $\zeta(G) = \sum_{u\in V(G)} \varepsilon_G(u)$, see [2]. The **eccentric distance sum** $\xi^d(G)$ of a graph G is defined as [7]:

$$\xi^d(G) = \sum_{u\in V(G)} \varepsilon_G(u) D_G(u),$$

where $D_G(u)$ denotes the sum of distances of all vertices in G from v. The eccentric distance sum was a novel distance-based molecular structure descriptor which can be used to predict biological and physical properties. It has a vast potential in structure activity/property relationships, se for more details [1,3-8] Here our notation is standard and mainly taken from [9].

3. MAIN RESULTS

The aim of this section is to compute $\xi^d(G)$ of Volkmann tree. In continuing we compute this index for vertex–transitive graphs and non - vertex transitive graphs that their automorphism group has exactly two orbits. In the following examples, we present the eccentric distance sum of two well-known graphs.

Example 1. Let K_n be the complete graph on n vertices. Then for every $v \in V(K_n)$, $D(v) = n-1$ and $ecc_G(v) = 1$. This implies that $\xi^d(K_n) = n(n-1)$.

Example 2. Let C_n denote the cycle of length n. Then if n is an odd number, $D(v) = (n^2-1)/4$, else $D(v) = n^2/4$ and $ecc_G(v) = \lfloor n/2 \rfloor$ for all vertices v. Hence,

$$\xi^d(C_n) = \begin{cases} n(n^2-1)\lfloor n/2 \rfloor / 4 & 2 \nmid n \\ n^3 \lfloor n/2 \rfloor / 4 & 2 \mid n \end{cases}.$$

3.1 Vertex–transitive graphs

An automorphism of the graph $G = (V,E)$ is a bijection σ on V which preserves the edge set E, i.e., if $e=uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Here the image of vertex u is denoted by $\sigma(u)$. The set of all automorphisms of G under the

Journal of Mathematical NanoScience

composition of mappings forms a group which is denoted by $Aut(G)$. We say $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ such that $\alpha(u)=v$.

Theorem 1. If $Aut(G)$ acts transitively on V, then we have the following Theorem:

$$\xi^d(G)=2d(G)W(G).$$

Proof. Since this action is transitive, there exist an automorphism such as $\alpha \in Aut(G)$ such that $\alpha(u)=v$ and so

$$\varepsilon_G(v)=\max_{x\in V(G)} d_G(v,x)=\max_{y\in V(G)} d_G(\alpha(u),\alpha(y))=\varepsilon_G(u).$$

This completes the proof.

3.2 Actions with two orbits

In all over of this section by Γ and $\gamma(G)$ mean the automorphism graph $\Gamma=Aut(G)$ and $\gamma(G)=d(G)-r(G)$, respectively. Also the action of group Γ on the set Ω is denoted by $(\Gamma|\Omega)$. Suppose Γ is a group which acts on the set Ω. If $x\in\Omega$, let $O(x)=\{g.x \mid g\in\Gamma\}$. The set $O(x)$ is called the orbit of x. The stabilizer of x is the subset $\Gamma_x=\{g\in\Gamma \mid g.x=x\}$. In other words, when group Γ acts on set Ω, then $\Omega=\Omega_1\cup\Omega_2\cup\ldots\cup\Omega_n$ where $\Omega_i\,(1\le i\le n)$ are orbits of Γ. In the following lemma, we can deduce a generally formula for eccentric distance sum of G.

Lemma 2. Let $G=(V,E)$ be a graph and it's action $(\Gamma|V)$ has orbits $V_i, 1\le i\le s$. Then

$$\xi^d(G)=\sum_{i=1}^{s}|V_i|\,\varepsilon(u_i)\sum_{v\in V_i} D_G(v).$$

Proof. It is well-known fact that the action of a group on its orbits is transitive. Hence by using Theorem 1, the proof is straightforward.

In continuing we consider graph G such that it's action $(\Gamma|V)$ has exactly two orbits. We denote this graph by *TO*-graphs. The vertex set V under this action divides to subsets V_1 and V_2, where $n_1=V_1$, $n_2=V_2$ and $n=n_1+n_2=|V|$. Further, It is easy to see that degrees of vertices of V_i are the same and we denote them by $k_i, (i=1,2)$. Hence, by above notations, we have the following theorem.

Theorem 3. Let G be a *TO*-graph with m edges, $V = V_1\cup V_2$ and $v_i\in V_i\,(i=1,2)$. Then,

$$\xi^d(G)=k_1n_1\gamma(G)D(v_1)+2W(G)(\zeta(G)-r(G)).$$

Proof. It is not difficult to see that

$$\xi^d(G) = \sum_{v_1 \in V} D(v_1)\varepsilon(v_1) + \sum_{v_2 \in V} D(v_2)\varepsilon(v_2)$$

$$= k_1 n_1 \varepsilon(v_1) D(v_1) + k_2 n_2 \varepsilon(v_2) D(v_2) = k_1 n_1 \varepsilon(v_1) D(v_1) + (2m - k_1 n_1)\varepsilon(v_2) D(v_2).$$

Since $k_1 n_1 D(v_1) + k_2 n_2 D(v_2) = 2W(G)$ thus

$$\xi^d(G) = k_1 n_1 \varepsilon(v_1) D(v_1) + (2W(G) - k_1 n_1 D(v_1))\varepsilon(v_2) = k_1 n_1 \gamma(G) D(v_1) + 2W(G).r(G).$$

3.3 Eccentric distance sum of Volkmann tree

The Volkmann tree $V_{n,\Delta}$ is a tree on n vertices and maximum vertex degree Δ defined as follows:

Start with the root having Δ neighbors. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ neighbors. In the last level, while not all vertices need to exist, the vertices that do exist fill the level consecutively. Thus, at most one vertex on the level second to last has its degree different from Δ and 1, see Figure 1.

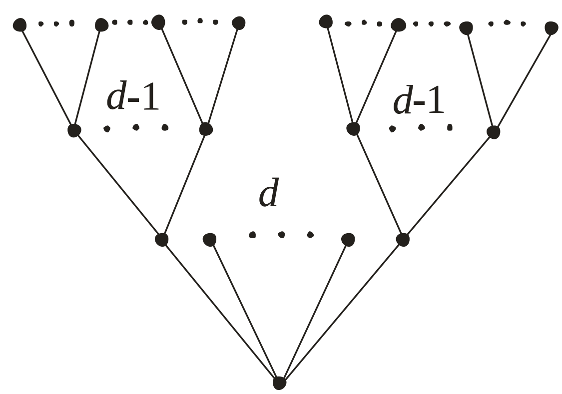

Figure 1. The Volkmann tree $V_{n,\Delta}$.

Theorem 4. The eccentric distance sum of Volkmann tree is as follows

$$\xi^d\left(V_{n,\Delta}\right) = \sum_{m=1}^{[(k+1)/2]} (A+B+C)d(d-1)^{m-1}(k-m+2) + \sum_{m=[(k+1)/2]}^{k} (A+B+C)d(d+1)^{m-1}m$$

$$+ k\sum_{i=1}^{k} id(d-1)^{i-1},$$

where,

$$S = \sum_{n=2}^{m-1}[(m-n)+(m+n)(d-1)^n + \sum_{i=1}^{n-1}(m-n+2i)(d-2)(d-1)^{i-1}],$$

$$A = 2m-1+(m+1)(d-1)+S, \quad B = (\sum_{i=1}^{m-1} 2i(d-2)(d-1)^{i-1}) + 2m(d-1)^m$$

$$R = \sum_{i=0}^{m-2}(n-m+2(i+1)(d-2)(d-1)^{n-m+i},$$

$$C=\sum_{n=m+1}^{k}((n-m)(d-1)^{n-m}+(n+m)(d-1)^{n}+R).$$

Proof. The proof is straightforward.

REFERENCES

[1]. A. R. Ashra i, M. Saheli and M. Ghorbani, The eccentric connectivity index of nanotubes and nanotori, *Journal of Computational and Applied Mathematics*, 235 (2011), 4561 – 4566.

[2] T. Doslić, M. Ghorbani and M. Hosseinzadeh, Eccentric connectivity polynomial of some graph operations, *Utilitas Mathematica*, 84 (2011), 297-309.

[3] M. Ghorbani, Connective eccentric index of fullerenes, *J. Math. NanoSci*., 1 (2011), 43–52.

[4] M. Songhori, ccentric connectivity index of fullerene graphs, *J. Math. NanoSci*., 2 (2011), 21–27.

[4] V. Sharma, R. Goswami and A. K. Madan, Eccentric connectivity index: Anovel highly discriminating topological descriptor for structure-property andstructure-activity studies, *J. Chem. Inf. Model*., 37 (1997), 273 – 282.

[5] S. Gupta, M. Singh and A.K. Madan, Eccentric distance sum: a novel graph invariant for predicting biological and physical properties, *J. Math. Anal. Appl*., 275 (2002), 386 – 401.

[6] A. Ilić, G. Yu and L. Feng, On the eccentric distance sum of graphs, *J. Math. Anal. Appl*., 381 (2011), 590 – 600.

[7] V. Lather and A. K. Madan, Application of graph theory: Topological models for prediction of CDK-1 inhibitory activity of aloisines, *Croat. Chem. Acta*, 78 (2005), 55 – 61.

[8] B. E. Sagan, Y.-N. Yeh and P. Zhang, The Wiener polynomial of a graph, *Int. J. Quantum. Chem*., 60 (1996), 959 – 969.

[9] D. B. West, Introduction to Graph Theory, Prentice Hall, Upper Saddle River, 1996.

Journal of Mathematical NanoScience