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ON THE EDGE DEGREES OF TREES

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Abstract. Let $m_{ij}(G)$ be the number of edges of graph G, connecting vertices of degrees i and j. Necessary and sufficient conditions are established on a symmetric matrix M of type $\Delta \times \Delta$ such that there is a tree T for which $M_{ij} = m_{ij}(T)$ holds for all i, j.

1. Introduction

In this paper we are concerned with simple graphs. Let G be such a graph, let $v_1, v_2, \ldots, v_n$ be its vertices, and let $d(v) = d_G(v)$ be the degree (=number of first neighbors) of its vertex v. Let $n_i(G)$ be the number of vertices of G having degree equal to i, $i = 0, 1, 2, \ldots$

A sequence of numbers $k_0, k_1, k_2, \ldots$ is said to be "graphic" if there exists a graph G such that $k_i = n_i(G)$ holds for all $i \geq 0$. Necessary and sufficient conditions for graphic sequences were established long time ago [1] and belong nowadays among standard textbook facts of graph theory [4,8]. In this paper, we consider an analogous problem, pertaining to the degrees of the edges.

An edge e of a graph G is said to have degree (i, j) or (j, i) if e connects vertices of u and v, and $d(u) = i$, $d(v) = j$. The number of edges of G having degree equal to (i, j) will be denoted by $m_{ij} = m_{ij}(G)$. Of course, $m_{ij} = m_{ji}$. Note that for a given graph the numbers m_{ij} are defined for all $i, j \in \mathbb{N}$. The greatest value of j for which $m_{ij}(G)$ differs from 0 will be denoted by Δ. Evidently, Δ is equal to the maximal degree of a vertex of G.

Let M be a symmetric $\Delta \times \Delta$ matrix, we say that graph G of maximal degree Δ realizes M if and only if $M_{ij} = m_{ij}(G)$ for every $i, j \in 1, \ldots, \Delta$. In this case, we say that matrix is edge-graphic. In what follows we establish conditions needed that a matrix M is edge-graphic and to pertain to a tree.

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Let us note that these numbers m_{ij} have important applications in chemistry. Namely, several molecular descriptors can be expressed in the terms of m_{ij}'s. The most famous ones are:

- Randić index [7]

$$\chi(G) = \sum_{1 \le i \le j \le \Delta} \frac{m_{ij}(G)}{\sqrt{i \cdot j}};$$

- Zagreb index [2]

$$M_2(G) = \sum_{1 \le i \le j \le \Delta} i \cdot j \cdot m_{ij}(G);$$

- modified Zagreb index [6]

$$^{m}M_2(G) = \sum_{1 \le i \le j \le \Delta} \frac{m_{ij}(G)}{i \cdot j}.$$

- variable Zagreb index [5] (generalization of these concepts)

$$^{\lambda}M_2(G) = \sum_{1 \le i \le j \le \Delta} (i \cdot j)^{\lambda} \cdot m_{ij}(G), \qquad \lambda \in R.$$

The exhaustive search of mathematical properties of these Randić-type molecular structure descriptors can be found in [3]. All these imply that study of valence-connectivities is interesting and applicable in chemistry. This paper furthers the results already achieved in study of these numbers. First, in paper [10], they have been studied for the graphs with maximal degree at most 4. Then in papers [9, 11] for acyclic graphs with maximal degree at most 4 (these graphs cover the family of kenographs of acyclic hydrocarbons), in paper [12] monocyclic graphs have been studied and finally in [13] thorny monocyclic graphs with prescribed number of thorns have been studied. Here, this research is extended to acyclic graphs of arbitrary degree.

2. Basic definitions and main results

Let G be an arbitrary graph. By $N(G)$ we denote set of vertices in G, by $N_i(G)$ set of vertices of degree i and by $E(G)$ set of edges of G. Cardinalities of $N(G)$, $N_i(G)$ and $E(G)$ are denoted by $n(G)$, $n_i(G)$ and $e(G)$. If G is unconnected graph, then we say that some component of G is cyclic if it contains at least one cycle.

Our main result is given by:

Theorem 2.1. *Let $\Delta \in \mathbb{N}$ and let M be a symmetric $\Delta \times \Delta$ matrix with entries in $\mathbb{N}_0$ and at least one non-zero entry in the last row. Then, there exists a tree G that corresponds to M if and only if:*

1) $n_i = \frac{1}{i} \cdot \left(M_{ii} + \sum_{j=1}^{\Delta} M_{ij} \right)$ *is a non-negative integer for each* $i = 1, \ldots, \Delta$;

2) $\sum_{\substack{i,j \in S \\ i \le j}} M_{ij} \le \max \left\{ 0, \sum_{i \in S} n_i - 1 \right\}$ *for each* $S \subseteq \{1, \ldots \Delta\}$;

3) $\sum_{\substack{i,j \in \{1,\ldots,\Delta\} \\ i \le j}} M_{ij} = \sum_{i \in \{1,\ldots,\Delta\}} n_i - 1.$

Proof. We first prove necessity. Note that n_i is the number of vertices of degree i in G, hence indeed it is a non-negative integer and 1) holds. Statement 3) just states that the number of edges is one less then number of vertices, so it is true. Let S be any subset of $\{1, \ldots, \Delta\}$ and let G' be a subgraph of G induced by vertices that have degree (in G) contained in set S. It can be easily seen that $e(G') = \sum_{\substack{i,j \in S \\ i \le j}} M_{ij}(G)$ and that $n(G') = \sum_{i \in S} n_i$, hence 2) holds.

Now, let us prove sufficiency. First, let us prove that there is a graph (not necessarily acyclic, simple or connected) G_1 with $m_{ij}(G_1) = M_{ij}$ for each $1 \le i \le j \le \Delta$. Let Γ_1 be a class of graphs H_1 with its vertices partitioned in classes $S_1, \ldots, S_\Delta$ such that:

1) $|S_i| = n_i$ for each $i = 1, \ldots, \Delta$;
2) $d_{H_1}(v) \le i$ for each $v \in S_i$;
3) number of edges connecting vertices in S_i and S_j is at most M_{ij} for each $1 \le i \le j \le \Delta$.

Denote by $s_{ij}(H_1)$ number of edges that have one end-vertex in S_i and other in S_j (edges connecting vertices in the same set are counted twice). Note that Γ_1 is non-empty, because at least graph with no edges is in Γ_1. Let G_1' be a graph in Γ_1 with maximal number of edges. Distinguish three cases:

Case 1: $s_{ij}(G_1') = M_{ij}$ for each $1 \le i \le j \le \Delta$.

In this case, vertices in S_i are incident to

$$s_{ii}(G_1') + \sum_{k=1}^{\Delta} s_{ik}(G_1') = M_{ii} + \sum_{k=1}^{\Delta} M_{ik} = i \cdot n_i$$

edges. Since, each vertex is incident to at most i edges, it follows that every vertex is in fact incident to exactly i edges. Hence, each vertex in S_i is of degree i. Therefore, $m_{ij}(G_1') = s_{ij}(G_1') = M_{ij}$ and it is sufficient to take $G_1 = G_1'$.

Case 2: $s_{ij}(G_1') < M_{ij}$ for some $1 \le i < j \le \Delta$.

In this case vertices in S_i are incident to

$$s_{ij}(G_1') + s_{ii}(G_1') + \sum_{\substack{1\le k\le\Delta \\ k\ne j}} s_{ik}(G_1') \le$$

$$\le M_{ij} - 1 + M_{ii} + \sum_{\substack{1\le k\le\Delta \\ k\ne j}} M_{ik} = M_{ii} + \sum_{1\le k\le\Delta} M_{ik} - 1$$

edges. Hence, there is some vertex u in S_i such that $d_{G_1'}(u) \le i-1$. It can be analogously shown that there is some vertex v in S_j such that $d_{G_1'}(v) \le j-1$, but then $G_1' + uv \in \Gamma_1$ which is in contradiction with maximality of G_1'.

Case 3: $s_{ii}(G_1') < M_{ii}$ for some $1 \le i \le \Delta$.

In this case vertices in S_i are incident to

$$2s_{ii}(G_1') + \sum_{\substack{1\le k\le\Delta \\ k\ne i}} s_{ik}(G_1') \le 2(M_{ii} - 1) + \sum_{\substack{1\le k\le\Delta \\ k\ne i}} M_{ik} = M_{ii} + \sum_{1\le k\le\Delta} M_{ik} - 2$$

edges. Hence, there are two possible subcases: there are vertices $u, v \in S_i$ such that $d_{G_1'}(u), d_{G_1'}(v) \le i-1$ or there is a vertex $u \in S_i$ such that $d_{G_1'}(u) \le i-2$. In the first subcase graph $G_1' + uv$ is in Γ_1 and in the second subcase graph $G_1' + uu$ is in Γ_1. In both subcases contradiction on maximality of Γ_1 is obtained, hence case 3 can not occur.

Now, let us prove that there is a loopless graph G_2 such that $m_{ij}(G) = M_{ij}$. Let Γ_2 be a class of graphs H_2 such that $m_{ij}(H_2) = M_{ij}$. Note that Γ_2 is non-empty, because $G_1 \in \Gamma_2$. Let G_2' be a graph with the smallest number of loops in Γ_2. If there is no loop in G_2', then it is sufficient to take $G_2 = G_2'$ and the claim is proved, hence we should suppose that G_2' contains at least one loop. Let vertex $v \in N_i$ be incident to that loop l_v. Since $M_{ii} \le n_i - 1$, there is at least one more vertex w of degree i in G_2'. If there is a loop l_w at w then graph $G_2' - l_v - l_w + 2vw \in \Gamma_2$ has less loops than G_2' which is contradiction. Hence, suppose that w has no loop. Since w and v are of the same degree and v has a loop, it follows that there is a vertex $z \ne v$ such that $wz \in E(G_2')$, but then $G_2' - l_v - wz + vw + vz$ has smaller number of loops then G_2' which is contradiction.

Now, let us prove that there is a simple graph G_3 such that $m_{ij}(G_3) = M_{ij}$. Let Γ_3 be a class of loopless graphs H_3 such that $m_{ij}(H_3) = M_{ij}$. Note that Γ_3 is non-empty, because $G_2 \in \Gamma_3$. Let G_3' be a graph with the smallest number of multiple edge (double edge is counted as 1, triple as 2,…) in Γ_3. If there are no multiple edges in G_3', then it is sufficient to take $G_3 = G_3'$ and the claim is proved, hence it is sufficient to show that the assumption that G_3' contains at least one multiple edge leads to contradiction. Distinguish two cases:

Case 1: G_3' contains a multiple edge connecting vertices of the same degree.

Let vertices $u, v \in N_i$ be connected by two parallel edges. Since, $m_{ii} \leq n_i(G_3') - 1$, it follows that there is a vertex w in N_i not adjacent to any of vertices u and v. Distinguish two subcases:

Subcase 1.1: Vertex w is incident to a double edge.

Let w' be another end-vertex of this double edge. Let us observe graph $G_3' - 1 \cdot uv - 1 \cdot ww' + uw + vw' \in \Gamma_3$. We have deleted two multiple edges (uv and vw) and added at most one. This is in contradiction with the fact that G_3' has minimal number of multiple edges.

Subcase 1.2: Vertex w is not incident to any double edge.

It follows that w has more neighbors then v, hence there is a vertex w' that is adjacent to w, but not to v. Then graph $G_3 - ww' - 1 \cdot uv + vw' + uw \in \Gamma_3$ contradicts the fact that G_3' has minimal number of multiple edges.

Hence, case 1 is not possible.

Case 2: G_3' contains a multiple edge connecting vertices of different degrees.

Let vertices $u \in N_i$ and $v \in N_j$ be connected by two parallel edges. Since $m_{ij}(G_3) \leq n_i + n_j - 1$, it follows that there is a vertex $w \in N_j$ not adjacent to u or vertex $w' \in N_i$ not adjacent to v. Without loss of generality, we may assume that there is a vertex $w \in N_j$ not adjacent to u. Similarly as in previous case, we distinguish two subcases:

Subcase 2.1: Vertex w is incident to a double edge.

This case is proved by the complete analogy with the Subcase 1.1.

Subcase 2.1: Vertex w is not incident to any double edge.

This case is proved by the complete analogy with the Subcase 1.2.

This proves that both cases are impossible, hence indeed there is a simple graph $G_3 \in \Gamma_3$.

Now, let us prove that there is a tree G such that $m_{ij}(G) = M_{ij}$. Let Γ be a class of simple graphs H such that $m_{ij}(H) = M_{ij}$. Note that Γ is non-empty, because $G_3 \in \Gamma$. If there is a graph H in Γ with only one component. Then, $G = H$ is tree with the required properties. Hence, assume that all graphs H in Γ are cyclic.

Denote components of H by $K_1, \ldots, K_a$. We say that these are the components on the first level. Let K_{i_1} be one of these components. If K_{i_1} is not cyclic, stop with its analysis. Otherwise, denote by $NC(K_{i_1})$ the set of all vertices contained in at least one cycle of K_{i_1}; by $ND(K_{i_1})$ set of vertices which degree exclusively appears in K_{i_1}, i.e., set of vertices u such that $d(u) = d(v) \Rightarrow v \in K_{i_1}$; and denote $NN(K_{i_1}) = N(K_{i_1}) \setminus ND(K_{i_1})$. Note that we have always one of the following two possibilities:

1) $NC(K_{i_1}) \setminus ND(K_{i_1}) \neq \emptyset$;
2) $NC(K_{i_1}) \subseteq ND(K_{i_1})$ and $NN(K_{i_1}) \neq \emptyset$.

Suppose to the contrary that $NC(K_{i_1}) \setminus ND(K_{i_1}) = \emptyset$ and $NN(K_{i_1}) = \emptyset$. Denote by $SD(K_{i_1})$ set of all vertex degrees appearing in K_{i_1}. Note that K_{i_1}

is connected graph that contains at least one cycle. Hence,

$$\sum_{i\in SD\left(K_{i_1}\right)} n_i = n\left(K_{i_1}\right) \leq e\left(K_{i_1}\right) = \sum_{\substack{i,j\in SD\left(K_{i_1}\right)\\ i\leq j}} M_{ij}$$

$$\leq \max\left\{0, \sum_{i\in SD\left(K_{i_1}\right)} n_i - 1\right\} = \sum_{i\in SD\left(K_{i_1}\right)} n_i - 1,$$

which is a contradiction. If 1) is true, stop with the analysis of K_{i_1}. If 2) is true note that each vertex in $NN\left(K_{i_1}\right)$ is cut vertex (in K_{i_1}). Observe the graph $K_{i_1} \setminus NN\left(K_{i_1}\right)$. Note that it has at least one cyclic component. Denote by $K_{i_1,1}, K_{i_1,2}, \ldots, K_{i_1,b}$ all its components. We say that these components are components on the second level having K_{i_1} as a father (we say that these components are its sons). Let K_{i_1,i_2} be one of these components. Note that, from construction, it follows that vertex degrees (in G) that appear in K_{i_1,i_2} do not appear in any of the components $K_1, \ldots, K_a$ except K_{i_1}. If K_{i_1,i_2} is not cyclic, stop with its analysis. Otherwise, denote $NC\left(K_{i_1,i_2}\right)$, $ND\left(K_{i_1,i_2}\right)$ and $NN\left(K_{i_1,i_2}\right)$ analogously as above. Similar analysis as above shows that we have one of the following two possibilities:

1) $NC\left(K_{i_1,i_2}\right) \setminus ND\left(K_{i_1,i_2}\right) \neq \emptyset$;
2) $NC\left(K_{i_1,i_2}\right) \subseteq ND\left(K_{i_1,i_2}\right)$ and $NN\left(K_{i_1,i_2}\right) \neq \emptyset$.

Again, if 1) is true stop; and if 2) is true observe the graph $K_{i_1} \setminus NN\left(K_{i_1}\right)$. It has at least one cyclic component. Denote by $K_{i_1,i_2,1}, K_{i_1,i_2,2}, \ldots, K_{i_1,i_2,c}$ all its components. These are components on the third level having K_{i_1,i_2} as a father (of course there may be more components on the third level having different fathers and different grandfathers). We proceed with the analysis of all these components. Since each component on the lower level has smaller number of vertices than its parenting component, the number of components constructed in this way is finite.

Denote by $\alpha_i\left(H\right)$ the number of components on the i-th level and denote $\alpha\left(H\right) = \left(\alpha_1\left(H\right), \alpha_2\left(H\right), \ldots\right)$. Let G' be a graph with the smallest value of $\alpha\left(H\right)$ according to the lexicographical order. Let $K_{j_1\ldots,j_t}$ be a component such that $NC\left(K_{j_1,\ldots,j_t}\right) \setminus ND\left(K_{j_1,\ldots,j_t}\right) \neq \emptyset$. Then, there is a vertex u_1 contained in some cycle C of $K_{j_1,\ldots,j_t}$ and there is vertex $u_2 \in N\left(K_{j_1,\ldots,j_{t-1}}\right) \setminus N\left(K_{j_1,\ldots,j_t}\right)$ (if $t=1$, then $K_{j_1,\ldots,j_{t-1}}$ is in fact G') such that $d_{G'}\left(u_1\right) = d_{G'}\left(u_2\right)$. Let us show that there is a vertex u_2' such that $u_2u_2' \in E\left(G'\right)$ and $u_1u_2' \notin E\left(G'\right)$. If $t=1$, the claim is obvious, since u_1 and u_2 are in different components. If $t>1$, let $u_1v_1v_2\ldots v_ku_2$ be a path from u_1 to u_2 in $K_{j_1,\ldots,j_{t-1}}$. Then, there is a vertex $v_i \in NN\left(K_{j_1,\ldots,j_{t-1}}\right)$ on this path. Since, $NC\left(K_{j_1,\ldots,j_{t-1}}\right) \subseteq ND\left(K_{j_1,\ldots,j_{t-1}}\right)$, it follows that vertex v_i is not contained in any cycle in $K_{j_1,\ldots,j_{t-1}}$ (and therefore, it is not contained in any cycle in G', because in each step only cut-vertices have been removed). Hence, there is a neighbor u_2'

of u_2 in G' such that $u_1u_2' \notin G'$. Denote by u_1' neighbor of u_1 that is on the cycle in $K_{j_1,\ldots,j_t}$. Obviously, $u_1'u_2 \notin G'$. Hence, graph $G'' = G' - u_1u_1' - u_2u_2' + u_1u_2' + u_2u_1'$ is element of Γ. Let us compare the components of G'' and G'. Either they induce the same partition of vertices or G'' has one component less. In the second case $\alpha(G'') < \alpha(G')$, which is a contradiction. In the first case all components of G' and G'' are the same, but K_{j_1} and its counterpart in G'' (let us denote it $K_{j_1}^*$). If $K_{j_1}^*$ is not cyclic in G'', then $\alpha(G'') < \alpha(G')$, which is a contradiction. Hence, assume that $K_{j_1}^*$ is cyclic.

Let us observe the decompositions of $K_{j_1} \setminus NN(K_{j_1})$ and $K_{j_1} \setminus NN\left(K_{j_1}^*\right)$. Note that $NN(K_{j_1}) = NN\left(K_{j_1}^*\right)$, hence either they induce the same components or $K_{j_1}^*$ has one component less. In the second case $\alpha(G'') < \alpha(G')$, which is a contradiction. In the first case all components of are the same, but K_{j_1,j_2} and its counterpart in G'' (let us denote it K_{j_1,j_2}^*). Proceeding in the same way we obtain the contradiction in all cases, but in the case in which all components on levels from 1 to t coincide, but $K_{j_1}, K_{j_1,j_2}, \ldots, K_{j_1,j_2,\ldots,j_{t-1}}$ whose decomposition coincide with the decomposition of its counterparts. Let us observe $K_{j_1,\ldots,j_{t-1}}$ and its counterpart $K_{j_1,\ldots,j_{t-1}}^*$. Note that $NN(K_{j_1,\ldots,j_t}) = NN\left(K_{j_1,\ldots,j_t}^*\right)$ and that

$$K_{j_1,\ldots,j_{t-1}}^* \setminus NN(K_{j_1,\ldots,j_t})$$

has one component less than

$$K_{j_1,\ldots,j_{t-1}} \setminus NN(K_{j_1,\ldots,j_t}).$$

Therefore, $\alpha(G'') < \alpha(G')$, which is a contradiction. Thus, assumption that all graphs in Γ are cyclic is not true, i.e., there is a tree G in Γ. □

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