Les Cahiers du GERAD ISSN: 0711–2440

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G–2008–62

September 2008

La publication de ces rapports de recherche bénéficie d'une subvention du Fonds québécois de la recherche sur la nature et les technologies.

Edge Realizability of Connected Simple Graphs

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September 2008

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Abstract

Necessary and sufficient conditions are provided for existence of a simple graph G, and for a simple and connected graph G' with given numbers m_{ij} of edges with end-degrees i, j for $i \leq j \in \{1, 2, \ldots, \Delta\}$ where Δ denotes the maximum degree of G or G'.

Résumé

On présente des conditions nécessaires et suffisantes pour l'existence d'un graphe simple G et d'un graphe simple et connexe G' avec des nombres donnés m_{ij} d'arêtes dont les degrés des sommets sont i et j pour $i \leq j \in 1, 2, \ldots, \Delta$ où Δ désigne le degré maximum de G ou de G'.

1 Introduction

Realizability problems in graph theory consist in finding necessary and/or sufficient conditions for graphs with prescribed values of some invariants to exist, and to provide algorithms to obtain such graphs. Since, the pioneering work of S. L. Hakimi [1, 2] they are mostly focused on conditions related to the degrees of the graph under study. More recently conditions involving the pairs of degrees of edges have been studied in mathematical chemistry. On the one hand, such conditions have been used by Caporossi et al. [3] to determine trees with minimum Randić index [4] using mixed integer programming. This approach was extended by several authors [5, 6, 7]. On the other hand, such conditions have also been investigated by Vukičević and Graovac [8, 9, 10] and Vukičević and Trinajstić [11, 12] to analyze discriminative properties of molecular descriptors such as the Zagreb index [13], modified Zagreb index [14] and Randic index. Several classes of graphs have been considered: chemical trees, i.e. trees with maximal degree 4 [15], unicyclic chemical graphs [9], and general chemical graphs [12].

Given a class Γ of graphs G, the edge realizability problem can be defined as follows: find necessary and sufficient conditions on the numbers m_{ij} of edges with vertex degrees i and j for a graph G in that class Γ to exist.

In this note, we consider the edge realizability problem for the classes of simple graphs and of connected simple graphs for which the maximum degree Δ is given. Results obtained generalize those of [9, 12, 15] for chemical graphs.

2 Edge Realizability of Simple Graphs

Let us introduce some notation. Let $G = (V(G), E(G))$ denote an arbitrary graph with vertex set $V(G)$ and edge set $E(G)$. Its order $n(G) = |V(G)|$ and size $m(G) = |E(G)|$. Moreover, let $n_i(G)$ denote the number of vertices of degree i in G and $m_{ij}(G)$ the number of edges with end-vertex degrees i and j in G (multiple edges contribute by their multiplicity to both of their end-degrees and loops contribute by 2 to the degree of their unique end-vertex).

We next characterize the vectors of numbers m_{ij} for which exists a simple graph G, i.e. a graph without loops or multiple edges.

Theorem 1 *Let Δ be an arbitrary integer and $M = [m_{ij}]$ a symmetric matrix of non-negative integers of order Δ. Then, there is a simple graph G with exactly m_{ij} edges connecting vertices of degrees i and j if and only if the following conditions hold:*

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

2) $m_{ii} \leq \binom{n_i}{2}$, *for all* $i = 1, \ldots, \Delta$;

3) $m_{ij} \leq n_i \cdot n_j$, *for all* $i \neq j \in \{1, \ldots, \Delta\}$.

Proof. Necessity: let G be a graph that corresponds to matrix M. The number of vertices of degree i in graph G is equal to $\frac{\sum_{j=1}^{\Delta} m_{ij} + m_{ii}}{i}$, hence it is a non-negative integer. Since G is a simple graph, there are at most $\binom{n_i}{2}$ edges that connect vertices of degree i, therefore $m_{ii} \leq \binom{n_i}{2}$, for all i. Similarly, $m_{ij} \leq n_i \cdot n_j$ for all $i \neq j$.

Sufficiency: first let us prove that there is a graph G_1 (not necessarily simple or connected) such that $m_{ij} = m_{ij}(G)$ for all i and j. Let Γ_1 be the family of graphs G'_1 that satisfy the following conditions:

1) $N(G'_1) = \bigcup_{i\in\{1,\dots,\Delta\}} X_i$, $|X_i| = n_i$ where the sets X_i are pairwise disjoint;
2) for each $v_i \in X_i$, the degree $d(v_i) \leq i$.

Note that Γ_1 is a non-empty set as it contains an empty graph. Let G''_1 be a graph with the maximal number of edges in Γ_1. If $d(v_i) = i$ for each $v_i \in X_i$ and $i \in \{1, \dots, \Delta\}$, then it is sufficient to take $G_1 = G''_1$. Assume the contrary. From, the hand-shaking Lemma, it follows that there are two cases:

CASE A1: There are vertices $v_i \in X_i$ and $v_j \in X_j$ such that $d(v_i) < i$ and $d(v_j) < j$. Then, the graph $G'' + v_iv_j$ is also in Γ_1, which is in contradiction with maximality of G''_1.

CASE A2: There is a vertex $v_i \in X_i$ such that $d(v_i) < i - 2$. Then, the graph $G'' + v_iv_i$ (with a loop at vertex v_i) is also in Γ_1, which contradicts again the maximality of G''_1.

Let Γ_2 be the set of graphs G'_2 such that exactly m_{ij} edges connect vertices of degrees i and j in G'_2. Note that Γ_2 is non-empty, because at least $G_1 \in \Gamma_2$. Let us prove that there is a loopless graph G_2 in Γ_2. Let G''_2 be a graph in Γ_2 with the smallest number of loops. If G''_2 has no loops, it is sufficient to take $G_2 = G''_2$. Assume the contrary. Let v_i be a vertex of degree i with a loop. Since $1 \leq m_{ii} \leq \binom{n_1}{2}$, it follows that $n_i \geq 2$, hence there is a vertex $w_i \neq v_i$ of degree i. Distinguish two cases:

CASE B1: w_i is incident to a loop w_iw_i. In this case graph $G''_2 - v_iv_i - w_iw_i + 2 \cdot v_iw_i \in \Gamma_2$ and has a smaller number of loops than G''_2, which contradicts the minimality of G''_2.

CASE B2: w_i is not incident with any loop. Then w_i has a neighbor $p \neq v_i$ and the graph $G''_2 - v_iv_i - w_ip + v_ip + v_iw_i \in \Gamma_2$ and has a smaller number of loops than G''_2, which contradicts the minimality of G''_2.

Let Γ_3 be the set of all loopless graphs G'_3 such that exactly m_{ij} edges connect vertices of degrees i and j in G'_3. Note that Γ_3 is non-empty, because at least $G_2 \in \Gamma_3$. Let us prove that there is a simple graph $G_3 \in \Gamma_3$. Let G''_3 be a graph in Γ_3 with the smallest number of repetition of edges where double edge are counted for one repetition, triple edge for two, quadruple for three and so forth. If G''_3 has no multiple edges, it is sufficient to take $G = G''_3$. Assume the contrary, i.e. that there is pair of vertices v_i and v_j that are connected by a multiple edge. Then, at least one vertex w_i (w_i is not necessarily different from v_i) of degree i is not connected to the vertex w_j (w_j is not necessarily different from v_j) of degree j. We distinguish three case:

CASE C1: $w_i = v_i$ and $w_j \neq v_j$.

If there is a vertex q connected with w_j by a multiple edge, then the graph $G''_3 - v_iv_j - w_jq + v_iw_j + v_jq \in \Gamma_3$ has at least one repetition of edge less then G''_3 (because v_iw_j is not a multiple edge) which is a contradiction. Hence, suppose that all edges incident to w_j are single. It follows that w_j has more neighbors than v_j, because they are of the same degree and w_j has multiple edges. Let $w_jp \in E(G''_3)$ and $v_jp \notin E(G''_3)$. Note that graph $G''_3 - v_iv_j - pw_j + v_iw_j + v_jp \in \Gamma_3$ has at least one repetition of edges less then G''_3 (because v_iw_j and v_jp are not multiple edges) which is a contradiction.

CASE C2: $w_i \neq v_i$ and $w_j = v_j$.

By symmetry, a proof similar to that of CASE C1 holds.

CASE C3: $w_i \neq v_i$ and $w_j \neq v_j$.

We may assume that $v_i w_j, w_i v_j \in E(G_3'')$, because otherwise we have the situation analyzed in previous cases. Distinguish two subcases:

SUBCASE C3.1 At least one of the vertices w_i and w_j is incident to a multiple edge. Without loss of generality (because of the symmetry) we may assume that w_i is connected with vertex p by a multiple edge. Than, graph $G_3''' = G_3'' - v_i v_j - w_i p + w_i v_j + v_i p$ has at most as many repetitions of edges as G_3'', but vertices w_i, v_j and w_j in G_3''' (with relabeling $w_i \leftrightarrow v_i$) satisfy the conditions of Case C1, which is a contradiction.

SUBCASE C3.2 Vertices w_i and w_j are incident only to single edges. Since v_i and w_i are of the same degree, but w_i is incident only to single edges, it follows that there is a vertex z_i such that $w_i z_i \in E(G_3'')$ and $v_i z_i \notin E(G_3'')$. Similarly, there is a vertex z_j such that $w_j z_j \in E(G_3'')$ and $v_j z_j \notin E(G_3'')$ (vertices z_i and z_j are not necessarily distinct). Graph $G_3'' - v_i v_j - w_i z_i - w_j z_j + v_i z_i + v_j z_j + w_i w_j \in \Gamma_3$ has a smaller number of multiple edges than G_3, which is a contradiction. □

3 Edge Realizability of Connected Simple Graphs

A supplementary family of constraints must be added to those of Theorem 1 in order to ensure existence of a connected graph G associated with matrix M.

Theorem 2 *Let Δ be an arbitrary integer and $M = [m_{ij}]$ a symmetric matrix of non-negative integers of order Δ. Then, there is a simple connected graph G with exactly m_{ij} edges connecting vertices of degrees i and j if and only if the following conditions hold:*

1) $n_i = \frac{\sum_{j=1}^{\Delta} m_{ij} + m_{ii}}{i}$ *is non-negative integer for each* $i = 1, \ldots, \Delta$

2) $m_{ii} \leq \binom{n_i}{2}$, *for all* $i = 1, \ldots, \Delta$

3) $m_{ij} \leq n_i \cdot n_j$, *for all i and j,* $i \neq j \in \{1, \ldots, \Delta\}$

4) $\sum_{1 \leq p < q \leq k} \sum_{\substack{i \in A_p \\ j \in A_q}} m_{ij} + \sum_{1 \leq p \leq k} \sum_{\substack{i \in A_p \\ j \in B}} m_{ij} + \sum_{i,j \in B} m_{ij} \geq \sum_{i \in B} n_i + k - 1$, *where $A_1, \ldots, A_k, B$ is any partition of the set* $S_\Delta = \{i \in \{1, \ldots, \Delta\} : n_i \geq 1\}$ *such that B contains 1 if* $1 \in S_\Delta$.

Proof. Necessity: let G_0 be a graph that corresponds to matrix M. From the proof of Theorem 1, it follows that conditions 1)-3) hold and that n_i is the number of vertices of degree i. Let $A_1, \ldots, A_k, B$ be any partition of S_Δ such that B contains 1 if $1 \in S_\Delta$. Let G_0' be a (multi)-graph obtained by contraction of all vertices with index in A_i to the single vertex v_i for all $i = 1, \ldots, k$. Let G_0'' be the (multi)-graph obtained from G_0' by deletion of all loops.

Note that.

$$\begin{aligned} n\left(G_0''\right) &= \sum_{i\in B} n_i + k; \\ m\left(G_0''\right) &= \sum_{1\le p<q\le k}\sum_{\substack{i\in A_p\\ j\in A_q}} m_{ij} + \sum_{1\le p\le k}\sum_{\substack{i\in A_p\\ j\in B}} m_{ij} + \sum_{i,j\in B} m_{ij}. \end{aligned}$$

Since, G_0'' is connected, it follows that $m\left(G_0''\right) \geq n\left(G_0''\right) - 1$, hence 4) holds.

Sufficiency: Let Γ be the set of all simple graphs G' such that exactly m_{ij} edges connect vertices of degrees i and j in G'. Theorem 1 implies that Γ is nonempty. Let us prove that there is a connected graph G in Γ. Let G'' be a graph with the smallest number of components in Γ. If G'' is connected, then it is sufficient to take $G = G''$. Assume the contrary. First, let us prove the following Claim:

Claim 1. Let C be a cycle in G'' passing through some vertices of degrees $i_1, i_2, \ldots, i_t$. Then all vertices of degrees $i_1, i_2, \ldots, i_t$ are in the same component.

Proof (of Claim 1): Denote the component containing cycle C by K. Suppose to the contrary that there is a vertex w_j of degree $j \in \{i_1, \ldots, i_t\}$, that is not in K. Denote by v_j the vertex of degree j that is in C and by p one of its neighbors in C. Let q be any neighbor of w_j. Since w_j is not in K, it follows that $v_jq, w_jp \notin E\left(G''\right)$, but then the graph $G'' - v_jp - w_jq + v_jq + w_jp \in \Gamma$ and has a smaller number of components than G'' which is a contradiction. □

Let us introduce the relation $\simeq$ on S_Δ by

$$\begin{aligned} i \;\simeq\; & j \Leftrightarrow \text{ there is a cycle } C' \text{ in } G' \text{ that contains at least} \\ & \text{one vertex of degree } i \text{ and one vertex of degree } j. \end{aligned}$$

Now, let $\sim$ be the relation on S_Δ defined by

$$\begin{aligned} i &\sim j \Leftrightarrow \text{ there are numbers } i_1, \ldots, i_r \text{ such that} \\ i &\simeq i_1, i_1 \simeq i_2, \ldots, i_r \simeq j. \end{aligned}$$

From Claim 1, it easily follows that

Claim 2. If $i \sim j$, then all vertices of degrees i and j are in the same component in G'. □

Let

$$\begin{aligned} S_\Delta^+ &= \left\{ i \in S_\Delta : \text{there is a vertex of degree } i \text{ contained in some cycle of } G'' \right\}; \\ B' &= \left\{ i \in S_\Delta : \text{no vertex of degree } i \text{ is contained in any cycle in } G'' \right\}. \end{aligned}$$

It can easily be seen that $\sim$ is an equivalence relation on S_Δ^+. Denote the classes of equivalence on that set by $A_1, \ldots, A_l$ and by $A_i', \ldots, A_l'$ the corresponding set of vertices. Note that:

1) $A'_1, \ldots, A'_l, B'$ is a partition of the vertices of G'';
2) There is no cycle in G' that contains vertices in more than one class of this partition;
3) Claim 2 implies that the subgraph $G''[A'_i]$ of G'' induced by A'_i is connected for all $i = 1, \ldots, l$;
4) There is no cycle in $G''[B']$.

Let G'_1 be obtained by contraction of all vertices in A'_i to a single vertex v_i and G''_1 be the (multi)-graph obtained from G'_1 by elimination of all loops. Since all $G''[A_i]$ are connected and G'' is not connected, it follows that G''_1 is also not connected. Note that

$$\begin{aligned} n\left(G''_1\right) &= \sum_{i\in B} n_i + k; \\ m\left(G''_1\right) &= \sum_{1\le p<q\le k} \sum_{\substack{i\in A_p \\ j\in A_q}} m_{ij} + \sum_{1\le p\le k} \sum_{\substack{i\in A_p \\ j\in B}} m_{ij} + \sum_{i,j\in B} m_{ij}. \end{aligned}$$

Since G''_1 is not connected and

$$\sum_{1\le p<q\le k} \sum_{\substack{i\in A_p \\ j\in A_q}} m_{ij} + \sum_{1\le p\le k} \sum_{\substack{i\in A_p \\ j\in B}} m_{ij} + \sum_{i,j\in B} m_{ij} \ge \sum_{i\in B} n_i + k - 1,$$

it follows that G''_1 contains a cycle C' or multiple edge(s). Distinguish three cases:

CASE 1: Vertices $b \in B$ and v_i are connected by a multiple edge. It follows that b has (in G'') two neighbors $v_{i,1}$ and $v_{i,2}$ in A'_i. Since A'_i is connected there is a path $v_{i,1}w_1w_2\ldots w_sv_{i,2}$ in $G''[A_1]$,but then there is a cycle $bv_{i,1}w_1w_2\ldots w_sv_{i,2}b$ in G'', which is a contradiction.

CASE 2: Vertices v_i and v_j are connected by a multiple edge. It follows that there are (not necessarily distinct) vertices $v_{i,1}$ and $v_{i,2}$ in A'_i; and (not necessarily distinct, unless $v_{i,1} = v_{i,2}$) vertices $v_{j,1}$ and $v_{j,2}$ in A'_j such that $v_{i,1}v_{j,1}, v_{i,2}v_{j,2} \in E\left(G''\right)$. Since A'_i is connected there is a path $v_{i,1}w_1w_2\ldots w_sv_{i,2}$ in $G''[A'_1]$ and since A'_j is connected there is a path $v_{j,1}u_1u_2\ldots u_{s'}v_{j,2}$ in $G''[A_2]$, but then there is a cycle

$$v_{i,1}w_1w_2\ldots w_sv_{i,2}v_{j,2}u_{s'}\ldots u_2u_2v_1v_{j,1}v_{i,1},$$

which is a contradiction.

CASE 3: G''_1 contains a cycle $C' = w_1w_2\ldots w_sw_1$. Note that vertices in C' can be associated with ordered pairs of vertices in G'' $(w_{11}w_{12})(w_{21}w_{22})\ldots(w_{s1}w_{s2})$ in such way that:

1) If the original vertex w was in B then w is replaced by (w, w) ;
2) if the original vertex is some v_j then it is replaced by a pair of, not necessarily adjacent or distinct, vertices $(w'w'')$ both from A'_j;
3) the second vertex of each pair is adjacent to the first vertex of the next pair.

Now, replace all pairs of vertices that are in A'_i by the shortest path that connects them and all pairs of vertices from B by a single vertex. In this way a cycle is obtained. From the definition it can be seen that this cycle either contains a vertex from B or contains vertices from two different classes A'_i and A'_j. In both cases, a contradiction is obtained, and the theorem is proved. □

While conditions (4) of Theorem 2 are numerous, particularly for large Δ, they may prove to be useful when Δ is moderate, which is the case for chemical graphs.

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