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Abstract: Necessary and sufficient conditions are provided for the existence of a simple graph, or a simple connected graph with given numbers m_{ij} of edges with end-degrees i, j for $i \leq j \in \{1, 2, \ldots, \Delta\}$, where Δ is the maximum degree. Moreover this allows to determine the k^{th} minimum or maximum value of all Adriatic indices together with the corresponding graphs.

Résumé : Nous donnons des conditions nécessaires et suffisantes pour l'existence d'un graphe simple, ou d'un graphe connexe simple, ayant des nombres donnés m_{ij} d'arêtes avec extrémités de degré i et j, pour $i \leq j \in \{1, 2, \ldots, \Delta\}$, où Δ est le degré maximum. De plus, ceci nous permet de déterminer la k^{me} valeur minimale ou maximale de tous les indices Adriatiques, ainsi que les graphes atteignant ces valeurs.

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 [8, 9] they are mostly focused on conditions related to the degrees of the graph under study. More recently conditions involving the pairs of degrees of the end-vertices of the edges have been studied in mathematical chemistry. Such conditions have been used by Caporossi et al. [1] to determine trees with minimum Randić index [14] using mixed integer programming. This approach was extended by several authors [2, 5, 13]. Similar conditions have also been investigated by Vukičević and Graovac [18, 19, 20] and Vukičević and Trinajstić [17, 21] to analyze discriminative properties of molecular descriptors such as the Zagreb index [7], the modified Zagreb index [12], and the Randić index. Several classes of graphs have been considered: chemical trees, i.e. trees with maximum degree at most 4 [16], unicyclic chemical graphs [19], and general chemical graphs [21].

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 end-degrees i and j for a graph G in that class Γ to exist. Deng, Huang, and Jiang [4] present a unified linear-programming model of some topological indices : Randic, Zagreb, sum-connectivity, GA, ABC, and harmonic indices. This model does not imply that the graphs obtained are connected.

Simple graphs are graphs without loops or multiple edges. In this paper, we consider the edge realizability problem for the classes of simple graphs and of simple connected graphs for which the maximum degree Δ is given. Results obtained generalize those of [16, 19, 21] for chemical graphs. Hence, the main contibution of the present paper is to provide concise necessary and sufficient conditions on the numbers m_{ij} of edges with end-degrees i and j for the existence of a simple graph or a simple connected with fixed maximum degree.

The paper is organised as follows. Edge realizability of simple graphs is studied in the next section, while the edge realizability of simple connected graphs is studied in Section 3. An integer programming model implementing the conditions of the previous sections is given in Section 4. Algorithms to construct simple graphs or simple connected graphs with given numbers m_{ij} of edges with end-degrees i and j are given in Section 5. The use of the integer programming model and of the proposed constructive algorithms is illustrated in Section 6 by a study of extremal graphs for the Randić index and the second Zagreb index.

2 Edge realizability of simple graphs

Let $G = (V, E)$ be a graph with vertex set V and edge set E. We denote by $G[W]$ the subgraph of G induced by a subset $W \subseteq V$ of vertices, by $d_G(v)$ the degree of v in G, and by $\Delta(G)$ the maximum degree in G. Let e_{uv} be the number of edges linking u with v in G. The number $\mu(G)$ of multiple edges in G is defined as $\mu(G) = \sum_{u \neq v} \max\{e_{uv} - 1, 0\}$. Hence, $\mu(G) = 0$ if and only if G does not contain any multiple edge.

Given a symmetric $r \times r$ matrix $M = [m_{ij}]$, an M-graph is a graph G with $\Delta(G) = r$ and such that the number of edges with end-vertex degrees i and j is equal to m_{ij}. 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.

Let Γ_M be the set of simple M-graphs (i.e., the set of M-graph without loops or multiple edges). We now characterize the symmetric matrices M for which Γ_M is non-empty.

Theorem 1 *Let $M = [m_{ij}]$ be a symmetric $r \times r$ matrix of non-negative integers. $\Gamma_M \neq \emptyset$ if and only if the following conditions hold:*

(C1) $n_i = \frac{1}{i}(\sum_{j=i}^{r} m_{ij} + \sum_{j=1}^{i} m_{ji})$ *is an integer for all* $i = 1, \ldots, r$;

(C2) $m_{ii} \leq \frac{1}{2}(n_i(n_i - 1))$ *for all* $i = 2, \ldots, r$ *such that* $1 \leq n_i \leq i$.

(C3) $m_{ij} \leq n_i n_j$ *for all* $2 \leq i < j \leq r$ *such that* $1 \leq n_i < j$ *and* $1 \leq n_j < i$.

Proof. *Necessity.* Let G be a simple M-graph. The number n_i of vertices of degree i in G is of course an integer, and is equal to $\frac{1}{i}(\sum_{j=i}^{r} m_{ij} + \sum_{j=1}^{i} m_{ji})$. Also, since G is a simple graph, the number m_{ii} of edges that connect vertices of degree i is at most equal to $\frac{1}{2}(n_i(n_i-1))$.

- If $i=1$, condition (C1) imposes $m_{11} \leq \frac{1}{2}n_1 \leq \frac{1}{2}n_1(n_1-1)$ when $n_1 \geq 2$, and $m_{11}=0$ when $n_1 \leq 1$.
- If $i>1$, condition (C1) imposes $m_{ii} \leq \frac{in_i}{2} \leq \frac{1}{2}(n_i(n_i-1))$ when $n_i \geq i+1$ or $n_i = 0$.

Hence, it is sufficent to impose $m_{ii} \leq \frac{1}{2}(n_i(n_i-1))$ for $i=2,\ldots,r$ and $n_i = 1,\ldots,i$. The number m_{ij} of edges with end-degrees i and j is at most equal to n_in_j, and it is sufficient to impose this constraint when $n_i \leq j-1$ and $n_j \leq i-1$, since (C1) imposes $m_{ij} \leq in_i \leq n_in_j$ when $n_j \geq i$ or $n_i = 0$, and $m_{ij} \leq jn_j \leq n_in_j$ when $n_i \geq j$ or $n_j = 0$.

Sufficiency We first prove that the three conditions are sufficient for the existence of a non-necessarily simple M-graphs (i.e., an M-graph in which loops and multiple edges are permitted). Let $V_1,\ldots,V_r$ be r sets (possibly empty) of distinct vertices, with $|V_i| = n_i$, and let $\mathcal{G}_\mathcal{M}$ be the set of graphs with vertex set $V = \cup_{i=1}^{r} V_i$, such that every vertex in V_i $(i=1,\ldots,r)$ has degree at most i, and there are at most m_{ij} edges with end-vertex degrees i and j, $1 \leq i \leq j \leq r$. Note that $\mathcal{G}_\mathcal{M}$ is not empty since it contains the empty graph (i.e., the graph $G=(V,E)$ with $E=\emptyset$). Consider now a graph G in $\mathcal{G}_\mathcal{M}$ with maximum number of edges. Let m'_{ij} be the number of edges of G with end-vertex degrees i and j. It is sufficient to prove that $m'_{ij} = m_{ij}$ for $1 \leq i \leq j \leq r$. Assume, by contradition, that there are two integers i and j such that $m'_{ij} < m_{ij}$.

- If $i=j$, then
$$\sum_{v\in V_i} d_G(v) = 2m'_{ii} + \sum_{j\neq i} m'_{ij} \leq 2(m_{ii}-1) + \sum_{j\neq i} m_{ij} = i|V_i| - 2.$$
Hence, either there are two vertices u,v in V_i with $d_G(u) < i$ and $d_G(v) < i$, in which case we can add an edge between u and v. Otherwise, a vertex $v \in V_i$ has degree at most $i-2$, while all other vertices in V_i have degree i, and we can add a loop at vertex v. Both cases contradict the maximality of G in $\mathcal{G}_\mathcal{M}$.
- If $i<j$, then
$$\sum_{v\in V_i} d_G(v) = 2m'_{ii} + \sum_{k\neq i} m'_{ik} \leq 2m_{ii} + (\sum_{k\neq i} m_{ik} - 1) = i|V_i| - 1.$$
Similarly, we have $\sum_{v\in V_j} d_G(v) \leq j|V_j| - 1$. Hence, there are at least one vertex $u \in V_i$ and one vertex $v \in V_j$ such that $d_G(u) < i$ and $d_G(v) < j$. We can therefore add an edge between u and v, which contradicts the maximality of G in $\mathcal{G}_\mathcal{M}$.

We now show how to remove loops and multiple edges in G. We start with loops. Assume there is a loop at a vertex $u \in V_i$. If there is a loop at a vertex $v \neq u$ in V_i, then we replace the loops at u and v by two parallel edges between u and v. Otherwise, condition (C2) implies $n_i \geq 2$, and there is therefore another vertex $v \neq u$ in V_i. Since u and v both have degree i, there is a vertex w with $e_{vw} > e_{uw}$; we remove a loop at u as well as an edge between v and w, and we add an edge between u and w and another one between u and v. By repeating this process, we get an M-graph without loops, and we now show how to remove multiple edges.

Assume G contains two vertices $u \in V_i$ and $v \in V_j$ with $e_{uv} > 1$ (where i is possibly equal to j). We show how to construct an M-graph G' with $\mu(G') < \mu(G)$. We distinguish three cases.

(a) If there is a vertex $w \neq v$ in V_j that is not linked to u, then there is a vertex q such that $e_{vq} < e_{wq}$ (since both v and w have degree j). We remove one edge linking u with v as well as one edge linking w with q, and we add an edge between u and w, and another one between v and q. Clearly, the resulting graph G' is still an M-graph and $\mu(G') < \mu(G)$.

(b) If u is linked to all vertices in V_j and there is a vertex $w \neq u$ in V_i that is not linked to v, we proceed as in the previous case (by permuting the roles of u and v) to get a graph G' with $\mu(G') < \mu(G)$.

(c) If u is linked to all vertices in V_j and v is linked to all vertices in V_i, we have $i \neq j$. Indeed, with $i=j$, we would have $m_{ii} > \frac{1}{2}(n_i(n_i-1)$, which is forbidden by condition (C1) (if $n_i \geq i+1$) or (C2) (if $n_i \leq i$). Moreover, there exist two non-adjacent vertices $u' \in V_i$ and $v' \in V_j$, else we would have $m_{ij} > n_in_j$, which is forbidden by condition (C1) (if $n_i \geq j$ or $n_j \geq i$) or (C3) (if $n_i \leq j-1$ and $n_j \leq i-1$). We can assume that u is linked to v' and v to u' by single edges, else we would be in case (a) or (b). Since u

and u' both have degree i, there is a vertex $x \notin \{u, u', v, v'\}$ such that $e_{ux} < e_{u'x}$. Similarly, there is a vertex $y \notin \{u, u', v, v'\}$ (possibly equal to x) such that $e_{vy} < e_{v'y}$. We remove one edge linking u with v, one edge linking u' with x and one edge linking v' with y, and we add one edge between u' and v', one edge between u and x and one edge between v and y. Again, the resulting graph G' is an M-graph with $\mu(G') < \mu(G)$.

In all cases, we can construct an M-graph with a stricly smaller number of multiple edges. By repeating this process, we can therefore construct an M-graph with no mulitple edges. □

3 Edge realizability of connected simple graphs

Let $\Gamma'_M \subseteq \Gamma_M$ be the set of simple M-graphs with minimum number of connected components. We now characterize the symmetric matrices M for which there exists a simple connected M-graph G. In other words, we give necessary and sufficient conditions on M so that all graphs in Γ'_M are connected. In comparison with Theorem 1, we will show that a fourth condition has to be added. We first need to introduce some notations.

For a graph G, let $D(G)$ be the set of integers i such that there is at least one vertex v with $d_G(v) = i$ that lies on a cycle in G. Also, let $D'(G)$ be the set of integers $i \notin D(G)$ such that there is at least one vertex w with $d_G(w) = i$ that lies on a path P in G whose endpoints u and v have the same degree $d_G(u) = d_G(v) \in D(G)$. Finally, let $H(G)$ be the subgraph of G induced by the vertices with degree $i \in D(G) \cup D'(G)$ in G. For example, considering the graphs in Figure 1, we have $D(G) = \{3, 4\}$ in (a), (b), (c), $D(G) = \emptyset$ in (d), $D'(G) = \{2\}$ in (a), $D'(G) = \{2, 6\}$ in (b), and $D'(G) = \emptyset$ in (c) and (d). The black vertices are those with a degree $i \in D(G)$, while the grey ones are those with a degree $i \in D'(G)$. The vertices of $H(G)$ are the black and grey ones, and the edges of $H(G)$ are those represented with bold lines.

We now prove a useful lemma, and we will then illustrate it with the graphs on Figure 1.

Lemma 1 *Let G be a graph in Γ'_M with maximum value $|D(G) \cup D'(G)|$. If two vertices u and v in G have the same degree $i \in D(G) \cup D'(G)$, then they belong to the same connected component of $H(G)$.*

Proof. Consider two vertices u and v with the same degree $i \in D(G) \cup D'(G)$, and assume, by contradiction, that u and v belong to two different connected components of $H(G)$.

Case 1: $i \in D(G)$. Vertices u and v belong to two different connected components of G, else $H(G)$ would contain all vertices of every path linking u to v, and u and v would therefore belong to the same connected component of $H(G)$. So let C be a cycle that contains a vertex w (possibly equal to u or v) with $d_G(w) = i$. At least one of u and v, say u, does not belong to the same connected component of G as w. Let p be a neighbor of w on C, and let q be any neighbor of u in G. By replacing the edges uq and wp by wq and up we get a new simple M-graph with a smaller number of connected components. We therefore have $G \notin \Gamma'_M$, a contradiction.

Case 2: $i \in D'(G)$. There is a vertex x (possibly equal to u or v) in G with $d_G(x) = i$ on a path P whose endpoints w_1 and w_2 have the same degree $d_G(w_1) = d_G(w_2) \in D(G)$. At least one of u and v, say u does not belong to the same connected component of $H(G)$ as P. We distinguish two cases.

Case 2.1: u and x belong to two different connected components of G. Let p be a neighbor of x on P, and let q be a neighbor of u. By replacing the edges uq and xp by xq and up we get a new simple M-graph G' with at most as many connected components as G, which implies $G' \in \Gamma'_M$. Since x does not belong to a cycle in G (else $i \in D(G)$), we know that w_1 and w_2 belong to two different connected components of G', and it follows from Case 1 that $G' \notin \Gamma'_M$, a contradiction.

Case 2.2: u and x belong to the same connected component of G. Let P' be a shortest path linking u to x in G, let p be a vertex in $P \setminus P'$ adjacent to x, and let q be a neighbor of u not on P'. Let $G' \in \Gamma'_M$ be the graph obtained from G by replacing the edges xp and uq by xq and up. By using $P' \cup \{up\}$ and $P' \cup \{xq\}$ in G' instead of xp and uq in G to connect vertices, we have:

- $D(G) \subseteq D(G')$. Indeed, if a vertex is on a cycle in G, then it belongs to a cycle in G'.
- $D'(G) \subset D'(G')$. Indeed, if a vertex w is on a path in G that links two vertices y_1 and y_2 with the same degree in $D(G)$, then w is on a path in G' linking y_1 to y_2 (which proves $D'(G) \subseteq D'(G')$). Moreover, all vertices on P' belong to $H(G')$ since $(P \cup P') \setminus \{xp\}$ is a path linking w_1 to w_2 in G'. Since at least one vertex on P' does not belong to $H(G)$ (else u and x would belong to the same connected component of $H(G)$), we have $D'(G) \subset D'(G')$.

Hence, G' is a graph in Γ'_M with $|D(G') \cup D'(G')| > |D(G) \cup D'(G)|$, a contradiction.

□

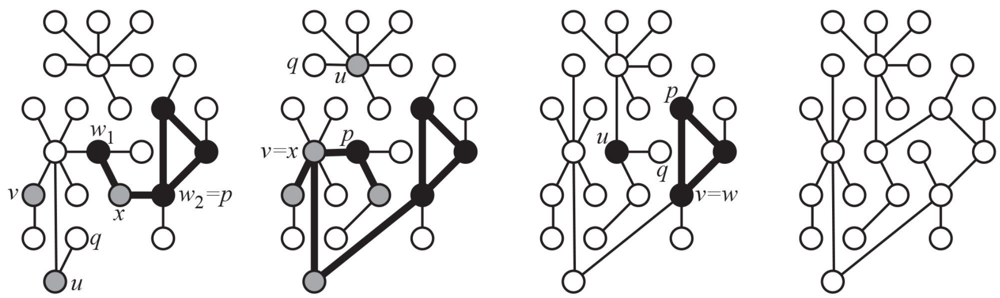

Figure 1: Illustration of Lemma 1.

Consider the graph in Figure 1(a). Cases 1 and 2.1 do not apply since all vertices of $H(G)$ belong to the same connected component of G. By applying the edge exchange of Case 2.2, we obtain the graph in Figure 1(b) with one more integer in $D'(G)$. The graph in Figure 1(b) has two vertices u and v with the same degree $6 \in D'(G)$, but in different connected components of G. By applying the edge exchange of Case 2.1, one gets the graph in Figure 1(c) with the same number of connected components, but in which the edge exchange of Case 1 can be applied to obtain the graph in Figure 1(d) which is now connected.

We now introduce some additional notations. Let $\mathcal{P}_r$ be the set containing all partitions of all subsets of $\{2, \ldots, r\}$. For example, for $r = 4$, $\mathcal{P}_4$ contains the 15 following partitions:

- the 5 non-empty partitions of $\{2,3,4\}$: $\big\{\{2\},\{3\},\{4\}\big\}$,$\big\{\{2\},\{3,4\}\big\}$, $\big\{\{3\},\{2,4\}\big\}$, $\big\{\{4\},\{2,3\}\big\}$, and $\big\{\{2,3,4\}\big\}$;
- the 2 non-empty partitions of $\{2,3\}$: $\big\{\{2\},\{3\}\big\}$,$\big\{\{2,3\}\big\}$;
- the 2 non-empty partitions of $\{2,4\}$: $\big\{\{2\},\{4\}\big\}$,$\big\{\{2,4\}\big\}$;
- the 2 non-empty partitions of $\{3,4\}$: $\big\{\{3\},\{4\}\big\}$,$\big\{\{3,4\}\big\}$;
- the 3 non-empty partitions of $\{2\}$, $\{3\}$ and $\{4\}$: $\big\{\{2\}\big\}$,$\big\{\{3\}\big\}$,$\big\{\{4\}\big\}$;
- the empty partition.

Also, for a partition $p \in \mathcal{P}_r$, let $E_r(p)$ be the set of all integers that appear in a subset of p (i.e., $E_r(p) = \cup_{s \in p}\, s$, and let $\overline{E_r(p)} = \{2, \ldots, r\} \setminus E_r(p)$. For example, for $p = \{\{2,3\},\{5\}\}$, we have $E_6(p) = \{2,3,5\}$ and $\overline{E_6(p)} = \{4,6\}$.

Now, let $I(M)$ be the set of integers i in $\{2, \ldots, r\}$ such that $m_{ii} + \sum_{j=1}^{r} m_{ij} \geq 1$. For a partition $p \in \mathcal{P}_r$, we denote by $|p|_M$ be the number of subsets $s \in p$ such that $s \cap I(M) \neq \emptyset$. For example, for $I(M) = \{2,3,5,6,8\}$ and $p = \{\{2,4\},\{3\},\{5,8\},\{7\}\}$, we have $|p|_M = 3$.

There is a bijection between $\mathcal{P}_r$ and the set of partitions of $\{1, \ldots, r\}$. Indeed, to every partition $p \in \mathcal{P}_r$, we can associate a partition of the set $\{1, \ldots, r\}$ by adding the bloc $\overline{E_r(p)} \cup \{1\}$ to p. Hence, the total number of partitions in $\mathcal{P}_r$ is the r^{th} *Bell number* B_r (sequence A000110 in OEIS [15]).

We are now ready to prove the main theorem that characterizes those matrices M for which there is a simple connected M-graph G.

Theorem 2 *Let $M = [m_{ij}]$ be a symmetric $r \times r$ matrix of non-negative integers. There is a simple connneted M-graph G if and only if the following conditions hold:*

(C1) $n_i = \frac{1}{i}(\sum\limits_{j=i}^{r} m_{ij} + \sum\limits_{j=1}^{i} m_{ji})$ *is an integer for all* $i = 1, \dots, r$;

(C2) $m_{ii} \leq \frac{1}{2}(n_i(n_i - 1))$ *for all* $i = 2, \dots, r$ *such that* $1 \leq n_i \leq i$.

(C3) $m_{ij} \leq n_i n_j$ *for all* $2 \leq i < j \leq r$ *such that* $1 \leq n_i < j$ *and* $1 \leq n_j < i$.

(C4) $\sum\limits_{\substack{s \neq s' \\ s,s' \in p}} \sum\limits_{\substack{i \in s \\ j \in s'}} m_{ij} + \sum\limits_{\substack{i \in E_r(p) \\ j \in \overline{E_r(p)}}} m_{ij} + \sum\limits_{\substack{i \leq j \\ \{i,j\} \subseteq \overline{E_r(p)}}} m_{ij} - m_{11} \geq \sum\limits_{i \in \overline{E_r(p)}} n_i + |p|_M - 1 \; \forall p \in \mathcal{P}_r$.

Proof. *Necessity.* Let G be a simple connected M-graph. It follows from Theorem 1 that conditions (C1)–(C3) hold. Moreover, condition (C1) implies that $I(M)$ is the set of all integers $i \in \{2, \dots, r\}$ such that $n_i \geq 1$. Let p be any partition in $\mathcal{P}_r$, and let us prove that condition (C4) also holds. For this purpose, we construct a new (not necessarily simple) graph G' from G as follows: we first remove all vertices of degree 1; then, for every $s \in p$ with $s \cap I(M) \neq \emptyset$, we contract all vertices of degree $i \in s$ in G to a single vertex v_s; finally, we remove all loops. Clearly, G' is also connected, and contains $|p|_M$ vertices that result from contractions, as well as all vertices of G with a degree $i \notin E_r(p)$. Let n' be the number of vertices in G', and let m' be its number of edges. We then have:

$$n' = \sum_{i \in \overline{E_r(p)}} n_i + |p|_M; \tag{a}$$

$$m' = \sum_{\substack{s \neq s' \\ s,s' \in p}} \sum_{\substack{i \in s \\ j \in s'}} m_{ij} + \sum_{\substack{i \in E_r(p) \\ j \in \overline{E_r(p)}}} m_{ij} + \sum_{\substack{i \leq j \\ \{i,j\} \subseteq \overline{E_r(p)}}} m_{ij}. \tag{b}$$

It remains to prove that $m' - m_{11} \geq n' - 1$.

- If $m_{11} > 0$, then G contains only two vertices (since it is connected), and $m_{11} = 1$. Hence, $n' = m' = 0$, which implies $m' - m_{11} = n' - 1$.
- If $m_{11} = 0$, then $m' \geq n' - 1$ (since G' is connected), which is equivalent to $m' - m_{11} \geq n' - 1$.

Sufficiency. Assume M satisfies conditions (C1)–(C4). We know from Theorem 1 that Γ_M is not empty. So let G be a simple M-graph in Γ'_M with maximum value $|D(G) \cup D'(G)|$. It remains to prove that G is connected. Let $H_1, \dots, H_k$ be the connected components of $H(G)$, and let s_j be the set of integers $i \in D(G) \cup D'(G)$ such that H_j contains at least one vertex of degree i. It follows from Lemma 1 that $p = \{s_1, \dots, s_k\}$ is a partition of $D(G) \cup D'(G)$.

Let G' be the (not necessarily simple) graph obtained from G by contracting all vertices in H_j ($j = 1, \dots, k$) to a single vertex v_j, and by removing all loops. It is sufficient to prove that G' is connected, since this implies that the original graph G is also connected.

Let n' and m' denote, respectively, the number of vertices and edges in G'. We have

$$n' = n_1 + \sum_{i \in \overline{E_r(p)}} n_i + |p|_M; \tag{a'}$$

$$m' = \sum_{i=1}^{r} m_{1i} + \sum_{\substack{s \neq s' \\ s,s' \in p}} \sum_{\substack{i \in s \\ j \in s'}} m_{ij} + \sum_{\substack{i \in E_r(p) \\ j \in \overline{E_r(p)}}} m_{ij} + \sum_{\substack{i \leq j \\ \{i,j\} \subseteq \overline{E_r(p)}}} m_{ij}. \tag{b'}$$

Condition (C4) then implies $m' - \sum_{i=1}^{r} m_{1i} - m_{11} \geq n' - n_1 - 1$, which is equivalent to $m' \geq n' - 1$ since $n_1 = m_{11} + \sum_{i=1}^{r} m_{1i}$ (by condition (C1)).

Assume, by contradiction, that G' is not connected. Since $m' \geq n' - 1$, it contains a cycle or multiple edges. If a vertex $u \notin H(G)$ is connected to a v_j ($1 \leq j \leq k$) by multiple edges in G', then two vertices of H_j

are adjacent to u in G. But since H_j is connected, this means that u belongs to a cycle in G, and hence $u \in H(G)$, a contradiction.

Also, if two vertices v_i and v_j $(1 \le i < j \le k)$ are connected by multiple edges in G', then there are (not necessarily distinct) vertices $u_{i,1}$ and $u_{i,2}$ in H_i and (not necessarily distinct, unless $u_{i,1} = u_{i,2}$) vertices $u_{j,1}$ and $u_{j,2}$ in H_j such that $u_{i,1}$ is adjacent to $u_{j,1}$ and $u_{i,2}$ is adjacent to $u_{j,2}$ in G. Since both H_i and H_j are connected, this means that G contains a cycle with vertices in H_i and H_j, which contradicts the fact that H_i and H_j are different connected components of $H(G)$.

We have thus proven that G' does not contains any multiple edge, which means that there is a cycle $C = w_0w_2 \dots w_tw_0$ in G' (since $m' \ge n' - 1$). Every edge on C that links w_i to w_{i+1} (indices being taken modulo $t+1$) corresponds to an edge in G that links a vertex x_i to a vertex y_{i+1}. If $w_i \notin \{v_1, \dots, v_k\}$, then $w_i = x_i = y_i$. If $w_i \in \{v_1, \dots, v_k\}$, then x_i and y_i belong to the same connected component of $H(G)$, which means that there is a path (with possibly only one vertex) connecting x_i to y_i in G. Hence, G contains a cycle with a vertex $w_i \notin H(G)$, or with two vertices x_i and y_{i+1} in two different connected components of $H(G)$, a contradiction. □

While conditions (C4) of Theorem 2 are numerous, particularly for large values of r, they may prove to be useful in the case of chemical graphs, where $r = \Delta(G) \le 4$. Indeed, as already observed, $\mathcal{P}_4$ contains only 15 partitions.

4 An integer programming model

Let n and m be two positive integers. In this section, we show how to determine a symmetric $r \times r$ matrix $M = [m_{ij}]$ of non-negative integers that satisfies all conditions of Theorem 2 as well as the two following conditions:

(C5) $n = \sum_{i=1}^{r} n_i$
(C6) $m = \sum_{1 \le i \le j \le r} m_{ij}$.

An M-graph with such a matrix M has n vertices and m edges. Finding such a matrix can be done using an Integer Linear Programming (ILP) model. Since M has to be symmetric, we consider non-negative integer variables m_{ij} for all $1 \le i \le j \le r$. The ILP also uses non-negative integer variables n_i $(i = 1, \dots, r)$ which are constrained as follows, to satisfy condition (C1) :

$$\sum_{j=i}^{r} m_{ij} + \sum_{j=1}^{i} m_{ji} = in_i \quad \forall i = 1, \dots, r \tag{1}$$

In order to impose condition (C2), we consider new Boolean variables x_{ik} defined for $i = 1, \dots, r$ and $k = 1, \dots, i$, and impose

$$n_i \ge (k+1)(1 - x_{ik}) \qquad \forall i = 2, \dots, r, \forall k = 1, \dots, i \tag{2}$$

$$m_{ii} + x_{ik}m \le \frac{k(k-1)}{2} + m \qquad \forall i = 2, \dots, r, \forall k = 1, \dots, i \tag{3}$$

Constraints (2) imply that $x_{ik} = 1$ when $n_i \le k$, while x_{ik} can take value 0 or 1 otherwise. Consider any $i \in \{2, \dots, r\}$:

- if $n_i > i$, constraints (3) do not impose any restriction since x_{ik} can be set equal to 0 for all $k = 1, \dots, i$;
- if $n_i = 0$, constraints (3) impose a series of upper bounds on m_{ii}, the strongest one being obtained with $k = 1$. We thus get $m_{ii} \le 0$, which is already imposed by constraints (1);
- if $1 \le n_i \le i$, constraints (3) impose a series of upper bounds on m_{ii}, the strongest one being obtained with $k = n_i$ (i.e., $m_{ii} \le \frac{1}{2}n_i(n_i - 1)$), which corresponds to condition (C2).

Condition (C3) is imposed in a similar way:

$$m_{ij} + mx_{jk} \leq kn_i + m \qquad \forall 2 \leq i < j \leq r, \forall k = 1, \ldots, i-1 \tag{4}$$

$$m_{ij} + mx_{ik} \leq kn_j + m \qquad \forall 2 \leq i < j \leq r, \forall k = 1, \ldots, j-1 \tag{5}$$

Indeed, consider any i, j such that $2 \leq i < j \leq r$:

- if $n_i \geq j$ and $n_j \geq i$, no constraint is imposed since x_{jk} in (4) and x_{ik} in (5) can be set equal to 0 for all considered values of k;
- if $n_i = 0$ or $n_j = 0$, constraints (4) and (5) are not more restrictive than constraints (1) which impose $m_{ij} = 0$;
- if $n_i \geq j$ and $1 \leq n_j \leq i-1$, constraints (4) impose $m_{ij} \leq n_i n_j$, which is not more restrictive then $m_{ij} \leq jn_j$ imposed by constraints (1) (while constraints (5) do not impose any restriction);
- if $n_j \geq i$ and $1 \leq n_i \leq j-1$, constraints (5) impose $m_{ij} \leq n_i n_j$, which is not more restrictive then $m_{ij} \leq in_i$ imposed by constraints (1).
- if $1 \leq n_j \leq i-1$ and $1 \leq n_i \leq j-1$, both (4) and (5) impose condition (C3).

For imposing condition (C4), the only difficulty is the term $|p|_M$ since M is not known. By definition, $I(M)$ is the set of integers i in $\{2, \ldots, r\}$ such that $m_{ii} + \sum_{j=1}^{r} m_{ij} \geq 1$, and it follows from constraints (1) that this is equivalent to say that $I(M)$ is the set of integers i in $\{2, \ldots, r\}$ such that $n_i \geq 1$. Hence, given a partition $p \in \mathcal{P}_r$ and a set $s \in p$, we have $s \cap I(M) \neq \emptyset$ if and only if there exists $i \in s$ with $n_i \geq 1$. We therefore define Boolean variables q_s for all non-empty subsets s of $\{2, \ldots, r\}$ so that

$$q_s = \begin{cases} 1 & \text{if there is an integer } i \in s \text{ such that } n_i \geq 1 \\ 0 & \text{otherwise.} \end{cases}$$

This is done by imposing the following constraints:

$$\sum_{i \in s} n_i \leq nq_s \qquad \forall \text{ non-empty } s \subseteq \{2, \ldots, r\} \tag{6}$$

$$\sum_{i \in s} n_i \geq q_s \qquad \forall \text{ non-empty } s \subseteq \{2, \ldots, r\} \tag{7}$$

Since $|p|_M = \sum_{s \in p} q_s$, we can now impose Condition (C4) as follows. For a partition $p \in \mathcal{P}_r$, let $A(p)$ be the set of pairs (i, j) such that $i < j$ and there are two distinct sets s, s' in p with $i \in s$ and $j \in s'$. Also, let $B(p)$ the the set of pairs (i, j) such that $i < j$ and either $i \in E_r(p)$ and $j \in \overline{E_r(p)}$, or $j \in E_r(p)$ and $i \in \overline{E_r(p)}$. Condition (C4) is then imposed by the following constraint:

$$\sum_{(i,j) \in A(p) \cup B(p)} m_{ij} + \sum_{\substack{i \leq j \\ \{i,j\} \subseteq \overline{E_r(p)}}} m_{ij} - m_{11} \geq \sum_{i \in \overline{E_r(p)}} n_i + \sum_{s \in p} q_s - 1 \quad \forall p \in \mathcal{P}_r \tag{8}$$

Clearly, conditions (C5) and (C6) are imposed as follows, where n and m are fixed integers.

$$\sum_{i=1}^{r} n_i = n \tag{9}$$

$$\sum_{1 \leq i \leq j \leq r} m_{ij} = m \tag{10}$$

Finally, the following constraints define the possible values of all variables:

$$m_{ij} \in \mathbb{N} \qquad \forall i = 1, \ldots, r, \forall j = i, \ldots, r \tag{11}$$

$$n_i \in \mathbb{N} \qquad \forall i = 1, \ldots, r \tag{12}$$

$$x_{ik} \in \{0, 1\} \qquad \forall i = 2, \ldots, r, \forall k = 1, \ldots, i \tag{13}$$

$$q_s \in \{0, 1\} \qquad \forall \text{ non-empty } s \subseteq \{2, \ldots, r\} \tag{14}$$

A simple calculation shows that there are $2^{r-1} + r(r+2) - 2$ variables and $2^r + \frac{r}{2}(r^2 - r + 6) - 4 + B_r$ constraints (where B_r denotes the r^{th} Bell number).

4.1 Finding more than one matrix

Given any matrix M produced by the ILP of the previous section, we now show how to generate a different one (if any) that also satisfies conditions (C1)–(C6). This is done as follows. Let $\{M_{ij}\}$ denote the values of the matrix obtained using the ILP of the previous section. For all $1 \le i \le j \le r$ with $M_{ij} > 0$, we define a Boolean variable y_{ij} so that $y_{ij} = 1$ if and only if $M_{ij} < m_{ij}$. This is done by imposing the following constraints:

$$M_{ij} + my_{ij} \ge m_{ij} \qquad \forall 1 \le i \le j \le r \text{ with } M_{ij} > 0 \tag{15}$$

$$y_{ij}(M_{ij} + 1) \le m_{ij} \qquad \forall 1 \le i \le j \le r \text{ with } M_{ij} > 0 \tag{16}$$

$$y_{ij} \in \{0, 1\} \qquad \forall 1 \le i \le j \le r \text{ with } M_{ij} > 0 \tag{17}$$

In a similar way, we consider, we consider Boolean variable z_{ij} so that $z_{ij} = 1$ if and only if $M_{ij} > m_{ij}$:

$$M_{ij} + m(1 - z_{ij}) \ge m_{ij} + 1 \qquad \forall 1 \le i \le j \le r \text{ with } M_{ij} > 0 \tag{18}$$

$$(1 - z_{ij})M_{ij} \le m_{ij} \qquad \forall 1 \le i \le j \le r \text{ with } M_{ij} > 0 \tag{19}$$

$$z_{ij} \in \{0, 1\} \qquad \forall 1 \le i \le j \le r \text{ with } M_{ij} > 0 \tag{20}$$

In order to generate a new matrix different from the previous one, it is then sufficient to add the constraint that at least one the y_{ij} and z_{ij} variables must be equal to 1. This is simply done as follows:

$$\sum_{i=1}^{r}\sum_{j=i}^{r}(y_{ij} + z_{ij}) \quad \ge \quad 1 \tag{21}$$

5 Constructing simple connected graphs that optimize a given invariant

The construction of a simple M-graph or a simple connected M-graph can be done as described in Sections 2 and 3. More precisely, given a matrix M that satisfies conditions (C1)–(C3), Algorithm 1 in Table 1 constructs a simple M-graph, following the proof of Theorems 1. Instructions 2–13 build an M-graph, instructions 15–18 remove loops, and instructions 19–25 remove multiple edges. Note that we do not consider the case where two vertices with the same degree i have a loop, since such a situation never occurs with the construction phase in 2–13. Also, cases (a) and (b) of Theorem 1 correspond to instructions 20–21, while case (c) is treated in 22–23.

Similarly, given a matrix M that satisfies conditions (C1)–(C4), Algorithm 2 in Table 2 constructs a simple connected M-graph, following the proof of Theorems 2. A is the set of vertices that belong to a cycle, while B contains all vertices with a degree $i \in D(G)$. Also, A' is the set of vertices that belong to a path linking two vertices of B with the same degree, while B' contains all vertices with a degree $i \in D'(G)$. Vertex b_v that appears in instructions 16, 21 and 26, is a neighbor of $v \in A'$ on a path linking two vertices of B with the same degree. The edge exchange in instructions 8–10 corresponds to Case 1 of Theorem 2, while instuctions 20–22 are for Case 2.1, and instructions 25–27 for Case 2.2.

6 Extremal graphs for some Adriatic indices

For a graph G, let $\mathcal{I}(G)$ be an invariant that can be written as a function linear in the numbers n_i of vertices of degree i and in the numbers m_{ij} of edges with end-degrees i and j. For example the first and second Zagreb indices [7] and the Randić index [14] are defined as follows :

$$\text{First Zagreg index of } G \quad : \quad \sum_{i=1}^{r} n_i i^2$$

$$\text{Second Zagreg index of } G \quad : \quad \sum_{i=1}^{r}\sum_{j=i}^{r} m_{ij} ij$$

$$\text{Randić index of } G \quad : \quad \sum_{i=1}^{r}\sum_{j=i}^{r}\frac{m_{ij}}{\sqrt{ij}}$$

Such indices belong to the set of Adriatic indices studied in [22]. In this section, we show how to determine simple graphs and simple connected graphs that optimize (i.e., minimize of maximize) these invariants.

Given two integers n and m, finding a simple connected graph G with optimal value $\mathcal{I}(G)$ can be done by solving the following ILP, and then building a simple connected M-graph (with Algorithm 2), using the matrix M produced by the ILP:

Minimize or maximize the graph invariant $\mathcal{I}$

Subject to constraints (1)–(14)

Algorithm 3 in Table 3 generates a set of simple connected graphs with n vertices and m edges that optimize $\mathcal{I}(G)$. The algorithm first generate a set of optimal matrices M, and a simple connected M-graph for each such matrix M. Finally, additional graphs are added using a procedure that transforms a simple connected M-graph into another one. We conjecture that Alogrithm 3 generates all simple connected graphs G with optimal value $\mathcal{I}(G)$.

Conjecture *Given any two numbers n and m and a graph invariant $\mathcal{I}$, Algorithm 3 generates all simple connected graphs G with optimal value $\mathcal{I}(G)$.*

In order to generate the set of simple connected graphs with second-minimum value, or any k^{th}-minimal value, $k > 1$, it is sufficient to change the stopping criteria at Step 9 of Algorithm 3. Note that in order to determine, in Step 16, whether G' belongs to S, we use McKay algorithm [11] to store only non-isomorphic graphs in S.

We illustrate the use of the models and algorithms of Sections 4 and 5 by considering *chemical trees*, i.e., trees with maximum degree $r \leq 4$. We therefore solve the ILP by setting $r = 4$ and $m = n - 1$. As already mentioned in Section 4, the ILP has $2^{r-1} + r(r+2) - 2$ variables and $2^r + \frac{r}{2}(r^2 - r + 6) - 4 + B_r$ constraints, which gives a total of 30 variables and 63 constraints for $r = 4$, regardless of the number of vertices in the considered chemical trees. We first identify all simple chemical trees with $6 \leq n \leq 15$ vertices having minimum, second-minimum, third-ninimum, fourth minimum, and fifth-minimum value of the Randić index. The set of extremal chemical trees is shown in Figure 3.

For comparison, a similar study was performed in [6] and [10], where the authors analyse chemical trees with minimum, second minimum and third minimum Randić index. They give one example of such extreme graphs for every $n = 6, 7, \ldots, 24$. A careful comparison of the these studies shows that three graphs presented in [6] and [10] (at page 87) are not correct: their second-minimum and third-minimum for $n = 11$, and their third minimum for $n = 14$ have a Randić index strictly larger than our fifth-minimum. For example, the graphs shown in Figure 3 with $n = 11$ have a Randić index of 4.5, 4.62, 4, 65, 4.66, and 4.69, while the graph presented in [6] and [10] as second-minimum, and drawn in Figure 2, has value 4.71.

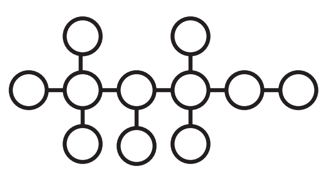

Figure 2: Chemical tree with 11 vertices and presented in [6] and [10] as second-minimum for the Randić index.

Condition (C4) is essential to ensure the connectivity. For comparison, we show in Figure 4 the simple graphs having maximum degree $r \leq 4$, $m = n - 1$ edges, $4 \leq n \leq 13$ vertices, and minimum Randić index. These graphs were obtained by replacing constraint (9) by the inequality $\sum_{i=1}^{r} n_i \leq n$ to allow isolated vertices, by removing constraints (6), (7), and (8), by using Algorithm 1 instead of Algorithm 2 at Step 5 of Algorithm 3, and by removing the connectivity condition at Step 16 of Algorithm 3.

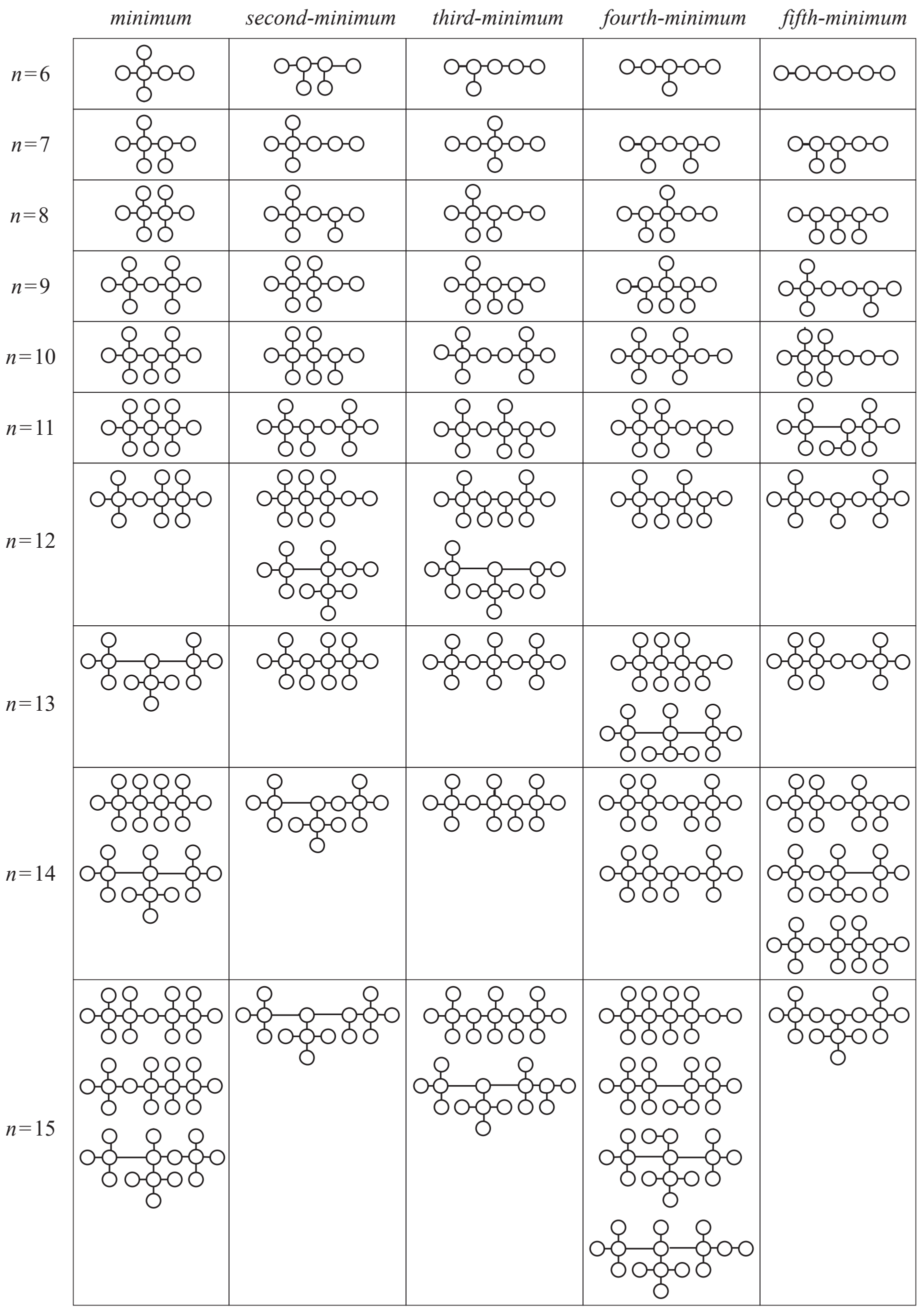

Figure 3: Extremal chemical trees for the Randić index.

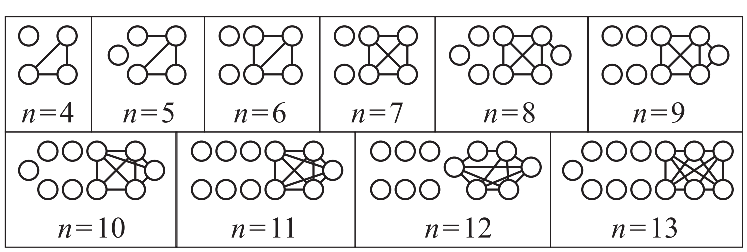

Figure 4: Graphs with minimum Randić index and $n-1$ edges.

Let R_n be the minimum Randić index of a chemical tree with n vertices, and let R^*_n be the minimum Randić index of a simple graph with n vertices, $m-1$ edges and maximum degree $r \leq 4$. Clearly, $R_n \geq R^*_n$. The difference $R_n - R^*_n$ is somehow a *price of connectivity* [3] which we represent in Figure 5 for $n \leq 99$. The curve indicates a regular shape for all $n \geq 11$. By analysing the extreme graphs for R^*_n, we have observed that they all have $\frac{n-1}{2}$ vertices of degree 4, and $\frac{n+1}{2}$ isolated vertices if n is odd, and $\frac{n-2}{2}$ vertices of degree 4, 1 vertex of degree 2, and $\frac{n}{2}$ isolated vertices if n is even. The regular shape of the curve in Figure 5 is due to the fact that for all $n \geq 11$, we have

$$R_n - R^*_n = \begin{cases} \frac{n}{6} & \text{if } n \mod 6 = 0 \\ \frac{n-1}{6} + \frac{\sqrt{3}-1}{2} & \text{if } n \mod 6 = 1 \\ \frac{n+4}{6} - \frac{\sqrt{2}}{2} & \text{if } n \mod 6 = 2 \\ \frac{n-3}{6} + \frac{\sqrt{2}}{2} & \text{if } n \mod 6 = 3 \\ \frac{n-4}{6} + \frac{1+\sqrt{3}-\sqrt{2}}{2} & \text{if } n \mod 6 = 4 \\ \frac{n+1}{6} & \text{if } n \mod 6 = 5. \end{cases}$$

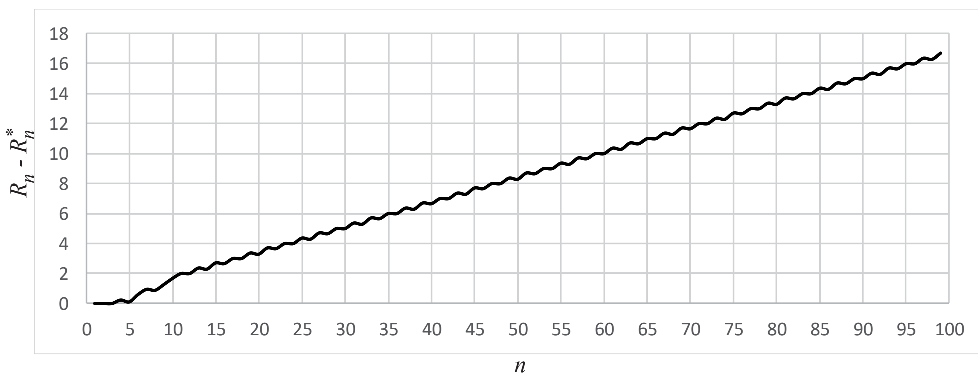

Figure 5: Price of connectivity for the Randić index of chemical trees.

As final illustration of the use of the proposed methods, we give in Figure 6 all simple chemical trees with $6 \leq n \leq 12$ vertices having minimum, second-minimum, third-ninimum, fourth-minimum, and fifth-minimum value of the second Zageb index.

While this was not the case for the Randić index, it happens several times that an extremal value of the second Zagreg index in reached with more than one M-matrix. Extreme graphs having the same value, but different M-matrices are separated with a dotted line in Figure 6. For example, for $n = 10$, there are 4 graphs with fourth-minimum value of the the second Zagreg index. The first one was obtained from a first M-matrix, while the three others were obtained from a second M-matrix.

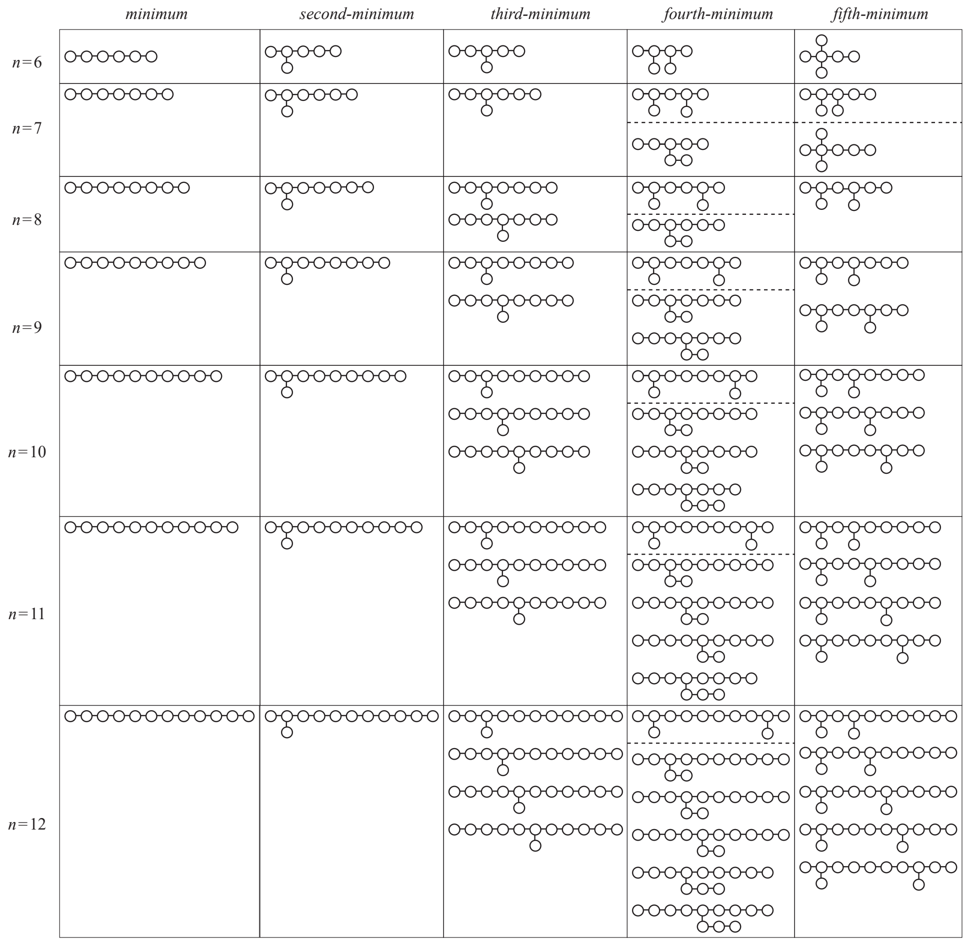

Figure 6: Extremal chemical trees for the second Zagreb index.

Conclusion

We have given necessary and sufficient conditions on the numbers m_{ij} of edges with end-degrees i and j for the existence of a simple graph or a simple connected graph with fixed maximum degree. These conditions can be imposed by an integer programming model, and graphs with these m_{ij} values can be generated using the proposed algorithms.

We have shown that these models and algorithms are very helpful to determine all extremal graphs of Adriatic indices that linearly depend on the the n_i and m_{ij} values.

Table 1: Construction of a simple M-graph.

Algorithm 1: Construction of a simple M-graph for a matrix M satisfying conditions (C1)–(C3)

CONSTRUCTION OF AN M-GRAPH
Create r sets V_i $(i = 1, \cdots, r)$ of distinct vertices, with $|V_i| = n_i$;
Set $m'_{ij} = 0 \ \forall\ 1 \leq i \leq j \leq r$ and $I = \{(i, j) \mid i \leq j$ and $m'_{ij} < m_{ij}\}$;
while $I \neq \emptyset$ **do**
    Choose a pair $(i, j) \in I$;
    if i=j **then**
        if *there are two vertices* u, v *of degree* $< i$ *in* V_i **then**
            add an edge between u and v;
        else
            choose $u \in V_i$ of degree $< i$, and add a loop at u;
    else
        choose $u \in V_i$ of degree $< i$ and $v \in V_j$ of degree $< j$, and add an edge between u and v;
end
REMOVAL OF LOOPS and MULTIPLE EDGES
while *the graph contains loops* **do**
    Choose u, v in the same V_i such that there is a loop at u;
    choose $w \neq u$ adjacent to v; replace a loop at u and an edge between v and w, by an edge between u and v, and one between u and w;
end
while *the graph contains multiple edges* **do**
    if *there are* u, v, w *such that* $e_{uv} > 1$, $e_{v,w} = 0$, *and* v *and* w *belong to the same* V_i **then**
        choose q with $e_{vq} < e_{wq}$, remove an edge between u and v and one between w and q, and add an edge between u and w as well as one between v and q;
    else
        Determine u, v, u', v' such that u, u' belong to the same V_i, v, v' belong to the same V_j, $e_{uv} > 1$, and $e_{u'v'} = 0$;
        choose x and y so that $e_{ux} < e_{u'x}$ and $e_{vy} < e_{v'y}$, remove one edge between u with v, one between u' and x and one between v' and y; add an edge between u' and v', one between u and x, and one between v and y;
end

Table 2: Construction of a simple connected M-graph.

Algorithm 2: Construction of a simple connected M-graph for a matrix M satisfying conditions (C1)–(C4)

Use Algorithm 1 to construct a simple M-graph G;
while G *is not connected* **do**
    Determine a cycle basis of G and let A be the set of vertices that belong to at least one cycle ot that basis;
    foreach *vertex* $v \in A$ **do**
        Set C_v equal to a cycle of the basis that contains v;
    end
    Determine the set $B \supseteq A$ of vertices with the same degree as at least one vertex in A;
    if *there are* $u \in B$ *and* $v \in A$ *with the same degree, and belonging to two different connected components of* G **then**
        Choose q adjacent to u and p on C_v adjacent to v;
        Replace the edges uq and vp by up and vq;
    else
        set $A' = \emptyset$;
        foreach *vertex* $v \notin B$ **do**
            Let $u_1,\ldots,u_r$ be the neighbors of v in G and let G_j $(1 \leq j \leq r)$ be the connected component of $G - v$ that contains u_j;
            if *there are* $x \in G_i \cap B$ *and* $y \in G_j \cap B$ *with the same degree, and with* $i \neq j$ **then**
                Choose one such pair x, y of vertices, set $b_v = x$, and add v to A';
        end
        Determine the set $B' \supseteq A'$ of vertices having the same degree as at least one vertex in A';
        if *there are* $u \in B'$ *and* $v \in A'$ *with the same degree, and belonging to two different connected components of* G **then**
            Choose a vertex q adjacent to u;
            Replace the edges uq and vb_v by ub_v and vq;
        else
            Let H be the subgraph induced by the vertices in $B \cup B'$;
            Determine $u \in B'$ and $v \in A'$ with the same degree, and belonging to two different connected components of H;
            Choose a vertex q adjacent to u;
            Replace the edges uq and vb_v by ub_v and vq;
end

Table 3: Construction of a set of simple connected graphs which optimize an invariant.

Algorithm 3: Construction of a set S of simple connected graphs G with n vertices, m edges, and optimal value $\mathcal{I}(G)$

Minmize of maximize the invariant $\mathcal{I}$ under constraints (1)-(14);
Let $\mathcal{I}^*$ be the resulting optimal value, and M the optimal matrix;
Set $S = \emptyset$;
repeat
    Build a simple connected M-graph G with Algorithm 2;
    Add G to S;
    Add constraints (15)-(21) of Section 4.1 to the Integer Linear Program to avoid generating M again;
    Solve the new Integer Linear Program, set M equal to the new optimal matrix, and let $\mathcal{I}'$ be the resulting optimal value;
until $\mathcal{I}' \neq \mathcal{I}^*$;
Consider all graphs in S as not marked;
while *S contains non-marked graphs* **do**
    Choose a non-marked graph G in S;
    foreach *quadruple (u, v, x, y) of vertices* **do**
        if *u and v have the same degree, u is linked to x but not to y, and v is linked to y but not to x* **then**
            Construct a graph G' from G by replacing the edges linking u to x and v to y by edges linking u to y and v to x;
            if *G' is connected and not yet in S* **then**
                add G' to S, and consider G' as non-marked;
    end
    mark G;
end

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