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Discrete Applied Mathematics 128 (2003) 447–463
DISCRETE APPLIED MATHEMATICS
www.elsevier.com/locate/dam

Randić structure of a graph

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Received 12 October 2001; received in revised form 18 April 2002; accepted 29 April 2002

Abstract

Let $\mathcal{G}$ be a collection of graphs with n vertices. We present a simple description of $[G]_\chi = \{H \in \mathcal{G}\colon \chi(H) = \chi(G)\}$ where χ denotes the Randić index. We associate to $\mathcal{G}$ a $\mathbb{Q}$-linear map $\rho : \mathbb{Q}^m \to \mathbb{Q}^k$ (for some integers k, m depending on $\mathcal{G}$) such that the kernel of ρ contains the necessary information to describe $[G]_\chi$ in terms of linear equations. These results provide precise tools for analyzing the behavior of χ on a collection of graphs.

1. Introduction

Let G be a simple graph (i.e. G does not have loops or multiple edges) with n vertices. The connectivity index of G, denoted by χ, is defined as follows:

$$\chi(G) = \sum_{1 \leqslant i \leqslant j \leqslant n-1} \frac{m_{ij}(G)}{\sqrt{ij}}, \tag{1}$$

where $m_{ij}(G)$ is the number of edges in G between vertices with degrees i and j.

Randić [15] introduced this index (known today as the Randić index) in the study of branching properties of alkanes, and it became one of the most useful graph-based molecular descriptors in applications to physical and chemical properties [10,11]. In spite of this great number of practical applications, the study of the general mathematical properties of χ started recently (see for instance [1–7,9,12–14]).

It is well known that χ does not separate non-isomorphic graphs, and of course, it does not distinguish between graphs with equal m_{ij}'s. So, given a (significant) collection

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0166-218X/03/\$ - see front matter
PII: S0166-218X(02)00505-X

of graphs $\mathcal{G}$ with n vertices and $G \in \mathcal{G}$, it would be interesting to describe the set

$$[G]_\chi = \{H \in \mathcal{G}\colon \chi(H) = \chi(G)\}.$$

To compute all graphs in this set seems a quite demanding task, since $[G]_\chi$ is complex from a combinatoric view point. In spite of all this, we will show that $[G]_\chi$ can be described very simply in terms of a system of linear equations.

In order to state our results we need the following identity for the Randić index [8]:

$$\chi(G) = \frac{n(G)}{2} - \frac{1}{2} \sum_{1 \leqslant i < j \leqslant n-1} \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{i}} \right)^2 m_{ij}(G). \tag{2}$$

Notice that the m_{ii}'s are not included. We denote by $R(G)$ the set $\{m_{ij}(G)\}_{1 \leqslant i < j \leqslant n-1}$ and called it the *Randić structure* of G. It is clear from (2) that if $R(G) = R(G')$, then $\chi(G) = \chi(G')$. Our description of $[G]_\chi$ will be in terms of the Randić structure of a graph.

The basic idea is the following. Let $\mathcal{G}$ be a collection of graphs and $G \in \mathcal{G}$. First, we express $\chi(G)$ as a linearly independent combination of certain $\sqrt{q_i}$'s, where the q_i's are positive integers which derive from the set of vertex degrees of graphs from $\mathcal{G}$. The coefficients in this linear combination, which will depend on $R(G)$, induce in a natural way a $\mathbb{Q}$-linear map $\rho\colon \mathbb{Q}^m \to \mathbb{Q}^k$ (for some integers k, m depending on $\mathcal{G}$). As we shall see, the kernel of ρ contains precise information that will lead us to characterize the set $[G]_\chi$, in terms of a system of linear equations on the m_{ij}'s. More precisely, we will show that for all $G, H \in \mathcal{G}$

$$\chi(G) = \chi(H) \Leftrightarrow R(G) - R(H) \in \ker \rho.$$

Perhaps the simplest situation, regarding the problem of describing $[G]_\chi$, is when $[G]_\chi$ consists merely of those $H \in \mathcal{G}$ such that $R(H) = R(G)$. In this case, we will say $\mathcal{G}$ has *Randić structure property* (RSP). We will show a fairly general method to generate collections with the RSP. Furthermore, it will be shown that any collection of graphs $\mathcal{G}$ can be decomposed into pairwise disjoint subcollections with the RSP. Moreover (and this is the non-trivial part of such decompositions) the subcollections are defined by linear equations on the m_{ij}'s. As an example of how these ideas can be used to get information about the behavior of χ on a collection of graphs, we will make in the last section an analysis of the collection of branch regular trees of degree 4 (i.e. trees such that every vertex has degree 1, 2 or 4).

2. The Randić matrix

Let $\mathcal{G}$ be a collection of graphs with n vertices. We would like, for a given graph $G \in \mathcal{G}$, to describe the set

$$[G]_\chi = \{H \in \mathcal{G}\colon \chi(H) = \chi(G)\}.$$

As we mentioned in Section 1, the idea is to associate to $\mathcal{G}$ a $\mathbb{Q}$-linear map $\rho\colon \mathbb{Q}^m \to \mathbb{Q}^k$ (for some integers k, m depending on $\mathcal{G}$). The kernel of ρ contains the information needed to characterize $[G]_\chi$ in terms of a system of linear equations. Heading in this direction we introduce some notation.

Let $\mathbb{D}(\mathcal{G})$ be the set of vertex degrees of graphs in $\mathcal{G}$ and

$$\mathbb{X}(\mathcal{G}) = \{i \cdot j\colon\ i, j \in \mathbb{D}(\mathcal{G}) \text{ and } i < j\}.$$

Given $x \in \mathbb{X}(\mathcal{G})$, let $x = p_1^{\alpha_1} \cdots p_r^{\alpha_r}$ be the prime decomposition and define $E(x) = \{i \in \{1, \ldots, r\}\colon\ \alpha_i \text{ is even}\}$ and $O(x) = \{i \in \{1, \ldots, r\}\colon\ \alpha_i \text{ is odd}\}$. So we can express every $x \in \mathbb{X}(\mathcal{G})$ as $x = \prod_{i \in E(x)} p_i^{\alpha_i} \prod_{i \in O(x)} p_i^{\alpha_i}$. If $y = \prod_{j \in E(y)} q_j^{\beta_j} \prod_{j \in O(y)} q_j^{\beta_j} \in \mathbb{X}(\mathcal{G})$ we define an equivalence relation over $\mathbb{X}(\mathcal{G})$ as follows:

$$x \sim y \Leftrightarrow \{p_i\colon\ i \in O(x)\} = \{q_j\colon\ j \in O(y)\}.$$

Denote by $\overline{\mathbb{X}(\mathcal{G})}$ the quotient set of $\mathbb{X}(\mathcal{G})$ modulo this equivalence relation and by $[x]$ the equivalence class of $x \in \mathbb{X}(\mathcal{G})$. Finally, let $\Psi\colon \overline{\mathbb{X}(\mathcal{G})} \to \mathbb{R}$ be the function defined as follows:

$$\Psi([x]) = \begin{cases} \sqrt{\displaystyle\prod_{i \in O(x)} p_i} & \text{if } O(x) \neq \emptyset, \\ 1 & \text{if } O(x) = \emptyset. \end{cases}$$

The following lemma is probably known, but we will sketch its proof for the sake of completeness.

Lemma 2.1. $\{\Psi([x])\}_{[x] \in \overline{\mathbb{X}(\mathcal{G})}}$ *is a linearly independent set over* $\mathbb{Q}$.

Proof. Let $p_1, \ldots, p_r$ be the set of all different prime numbers appearing as odd powers in the prime decomposition of each $[x] \in \overline{\mathbb{X}(\mathcal{G})}$. Consider the following tower of field extensions:

$$K_0 \subseteq K_1 \subseteq \cdots \subseteq K_r,$$

where for each $1 \leqslant i \leqslant r$, $K_i = K_{i-1}(\sqrt{p_i})$ (the field obtained from K_{i-1} by adjoining $\sqrt{p_i}$). Since $\{1, \sqrt{p_i}\}$ is a basis of K_i over K_{i-1} then the set

$$\mathbb{B} = \{z_1 \cdot z_2 \cdots z_r\colon\ z_i \in \{1, \sqrt{p_i}\}\}$$

forms a basis of K_r over $K_0 = \mathbb{Q}$. But clearly $\{\Psi([x])\}_{[x] \in \overline{\mathbb{X}(\mathcal{G})}} \subseteq \mathbb{B}$ which implies that $\{\Psi([x])\}_{[x] \in \overline{\mathbb{X}(\mathcal{G})}}$ is a linearly independent set over $\mathbb{Q}$. $\square$

Let $\Gamma\colon \mathbb{X}(\mathcal{G}) \to \mathbb{N}$ be the function defined by

$$\Gamma(x) = \prod_{i \in E(x)} p_i^{\alpha_i/2} \times \prod_{i \in O(x)} p_i^{(\beta_i - 1)/2}.$$

For instance, $\Gamma(2^3 \times 3^4 \times 5) = 2 \times 3^2$. In other words, $\Gamma(x)$ is the part of x that can be taken out as an integer of the square root of x.

Now, we have all we need to show a key lemma.

Lemma 2.2. *Let $\mathscr{G}$ be a collection of graphs with n vertices ($n \geqslant 5$) and χ: $\mathscr{G} \to \mathbb{R}$ the Randić function. Suppose there is $u \in \mathbb{X}(\mathscr{G}$ such that $O(u) = \emptyset$ (i.e. u is a perfect square) and let $k = \mathrm{l.c.m.}\{\mathbb{X}(\mathscr{G})\}$. Then for every $G \in \mathscr{G}$,*

$$k(2\chi(G) - n) = \sum_{ij \in [u]} A_{ij} m_{ij}(G) - \sum_{\substack{[x] \in \overline{\mathbb{X}(\mathscr{G})} \\ [x] \neq [u]}} \sum_{ij \in [x]} B_{ij} m_{ij}(G)$$

$$+ \sum_{\substack{[x] \in \overline{\mathbb{X}(\mathscr{G})} \\ [x] \neq [u]}} \left(\sum_{ij \in [x]} C_{ij} m_{ij}(G) \right) \Psi([x]),$$

where $A_{ij} = k(2\Gamma(ij) - i - j)/ij \in \mathbb{Z}, B_{ij} = k(i + j)/ij \in \mathbb{N}$ and $C_{ij} = 2k\Gamma(ij)/ij \in \mathbb{N}$.

Proof. For $G \in \mathscr{G}$ we know from (2) that

$$\chi(G) = \frac{n(G)}{2} - \frac{1}{2} \sum_{1 \leqslant i < j \leqslant n-1} \left(\frac{1}{j} + \frac{1}{i} \right) m_{ij}(G) + \sum_{1 \leqslant i < j \leqslant n-1} \frac{\sqrt{ij}}{ij} m_{ij}(G) \tag{3}$$

and

$$\sum_{1 \leqslant i < j \leqslant n-1} \frac{\sqrt{ij}}{ij} m_{ij}(G) = \sum_{[x] \in \overline{\mathbb{X}(\mathscr{G})}} \left[\sum_{ij \in [x]} \frac{\Gamma(ij)}{ij} m_{ij}(G) \right] \Psi([x])$$

$$= \sum_{ij \in [u]} \frac{\Gamma(ij)}{ij} m_{ij}(G)$$

$$+ \sum_{\substack{[x] \in \overline{\mathbb{X}(\mathscr{G})} \\ [x] \neq [u]}} \left[\sum_{ij \in [x]} \frac{\Gamma(ij)}{ij} m_{ij}(G) \right] \Psi([x]).$$

By substituting this last equation in (3) and then multiplying by $2k$ we get the result. □

The integer coefficients A_{ij}, B_{ij} and C_{ij} that appeared in Lemma 2.2 gives a natural way to associate a linear map $\rho_{\mathscr{G}}$: $\mathbb{Q}^{|\mathbb{X}(\mathscr{G})|} \to \mathbb{Q}^{|\overline{\mathbb{X}(\mathscr{G})}|}$ to every collection $\mathscr{G}$ of graphs with a fixed number of vertices as follows:

$$\rho_{\mathscr{G}} = \begin{pmatrix} [A_{ij}]_{ij \in [u]} & [-B_{ij}]_{ij \in [x_1]} & [-B_{ij}]_{ij \in [x_2]} & \cdots & [-B_{ij}]_{ij \in [x_r]} \\ [0]_{ij \in [u]} & [C_{ij}]_{ij \in [x_1]} & [0]_{ij \in [x_2]} & \cdots & [0]_{ij \in [x_r]} \\ [0]_{ij \in [u]} & [0]_{ij \in [x_1]} & [C_{ij}]_{ij \in [x_2]} & \cdots & [0]_{ij \in [x_r]} \\ \vdots & \vdots & \vdots & & \vdots \\ [0]_{ij \in [u]} & [0]_{ij \in [x_1]} & [0]_{ij \in [x_2]} & \cdots & [C_{ij}]_{ij \in [x_r]} \end{pmatrix},$$

where $\overline{\mathbb{X}(\mathscr{G})} = \{[u], [x_1], \ldots, [x_r]\}$ is ordered by the induced order of $\{\Psi([x])\}_{[x]\in\overline{\mathbb{X}(\mathscr{G})}}$ and the elements in each class of $\overline{\mathbb{X}(\mathscr{G})}$ are lexicographically ordered (viewing them as a set of two integers). We call the matrix above the *Randić matrix of* $\mathscr{G}$. For the sake of simplicity, when there is no danger of confusion about the collection $\mathscr{G}$, we will write ρ instead of $\rho_{\mathscr{G}}$.

Remark 2.3. If $\mathbb{X}(\mathscr{G})$ contains no perfect square numbers, then $k(2\chi(G)-n)$ can be expressed in a simpler way as

$$k(2\chi(G)-n) = -\sum_{[x]\in\overline{\mathbb{X}(\mathscr{G})}}\sum_{ij\in[x]} B_{ij}m_{ij}(G) + \sum_{[x]\in\overline{\mathbb{X}(\mathscr{G})}}\left(\sum_{ij\in[x]} C_{ij}m_{ij}(G)\right)\Psi([x]).$$

In this case, the Randić matrix of $\mathscr{G}$ is

$$\rho_{\mathscr{G}} = \begin{pmatrix} [-B_{ij}]_{ij\in[x_1]} & [-B_{ij}]_{ij\in[x_2]} & \cdots & [-B_{ij}]_{ij\in[x_r]} \\ [C_{ij}]_{ij\in[x_1]} & [0]_{ij\in[x_2]} & \cdots & [0]_{ij\in[x_r]} \\ [0]_{ij\in[x_1]} & [C_{ij}]_{ij\in[x_2]} & \cdots & [0]_{ij\in[x_r]} \\ \vdots & \vdots & & \vdots \\ [0]_{ij\in[x_1]} & [0]_{ij\in[x_2]} & \cdots & [C_{ij}]_{ij\in[x_r]} \end{pmatrix} \tag{4}$$

which determines a $\mathbb{Q}$-linear map $\rho_{\mathscr{G}}$: $\mathbb{Q}^{|\mathbb{X}(\mathscr{G})|} \to \mathbb{Q}^{|\overline{\mathbb{X}(\mathscr{G})}|+1}$.

It is convenient at this point to redefine the notion of the Randić structure of a graph (see Section 1) so that it includes the order of the columns of the Randić matrix.

Definition 2.4. The Randić structure of a graph G with n vertices, denoted by $R(G)$, is defined as the ordered $|\mathbb{X}(\mathscr{G})|$-tuple

$$R(G) = (m_{ij})_{ij\in\mathbb{X}(\mathscr{G})} \in \mathbb{Q}^{|\mathbb{X}(\mathscr{G})|},$$

where $ij\in\mathbb{X}(\mathscr{G})$ varies in the same order as the columns of $\rho_{\mathscr{G}}$.

In this way we have the Randić structure function $\mathscr{G}\xrightarrow{R}\mathbb{Q}^{|\mathbb{X}(\mathscr{G})|}$, defined by $R(G) = (m_{ij})_{ij\in\mathbb{X}(\mathscr{G})}$. The content of Lemma 2.2 is that, for a $G\in\mathscr{G}$, $\chi(G)$ can be expressed in terms of the Randić matrix of $\mathscr{G}$ as follows:

$$k(2\chi(G)-n) = \rho(R(G))\cdot(\Psi([u]), \Psi([x_1]), \ldots, \Psi([x_r])), \tag{5}$$

where $\cdot$ means the usual inner product.

Now we are ready to present a basic representation of $[G]_\chi$ for a general collection $\mathscr{G}$ of graphs.

Theorem 2.5. *Let $\mathscr{G}$ be a collection of graphs with n vertices and let $\rho_{\mathscr{G}}$ be the linear map associate to $\mathscr{G}$. Then the following holds for every $G, H\in\mathscr{G}$:*

$$\chi(G) = \chi(H) \Leftrightarrow R(G) - R(H) \in \ker\rho_{\mathscr{G}}.$$

Proof. For every $G \in \mathcal{G}$, we know from Eq. (5) that

$$k(2\chi(G)-n) = \rho(R(G)) \cdot (\Psi[u], \Psi[x_1], \ldots, \Psi[x_r]).$$

From this it follows that

$$\chi(G) = \chi(H) \Leftrightarrow \rho(R(G) - R(H)) \cdot (\Psi[u], \Psi[x_1], \ldots, \Psi[x_r]) = 0.$$

To finish the proof we recall that by Lemma 2.1 the $\Psi[x]$'s are all independent over $\mathbb{Q}$. $\square$

Example 2.6. Consider the collection of chemical graphs $\mathscr{C} = \mathscr{C}(n)$ (i.e. graphs in which no vertex has degree greater than 4) with n vertices. Then

$$\mathbb{X}(\mathscr{C}) = \{1\cdot 2, 1\cdot 3, 1\cdot 4, 2\cdot 3, 2\cdot 4, 3\cdot 4\}$$

and

$$\overline{\mathbb{X}(\mathscr{C})} = \{[1\cdot 4], [1\cdot 2], [1\cdot 3], [2\cdot 3]\}.$$

Let us calculate the entries of $\rho_{\mathscr{C}}$

$$A_{14} = \frac{24(2\cdot 2-5)}{4} = -6, \quad B_{12} = \frac{24(1+2)}{2} = 36, \quad B_{24} = \frac{24(2+4)}{8} = 18,$$

$$B_{13} = \frac{24(1+3)}{3} = 32, \quad B_{34} = \frac{24(3+4)}{12} = 14, \quad B_{23} = \frac{24(2+3)}{6} = 20,$$

$$C_{12} = \frac{2\cdot 24\cdot 1}{2} = 24, \quad C_{24} = \frac{2\cdot 24\cdot 2}{8} = 12, \quad C_{13} = \frac{2\cdot 24\cdot 1}{3} = 16,$$

$$C_{34} = \frac{2\cdot 24\cdot 2}{12} = 8, \quad C_{23} = \frac{2\cdot 24\cdot 1}{6} = 8.$$

and the matrix is

$$\rho_{\mathscr{C}} = \begin{pmatrix} -6 & -36 & -18 & -32 & -14 & -20 \\ 0 & 24 & 12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 16 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 \end{pmatrix}.$$

It can be easily checked that $\ker(\rho_{\mathscr{C}}) = \langle(-2,0,0,3,-6,0),(0,1,-2,0,0,0)\rangle$, where $\langle X\rangle$ denotes the subspace generated by X.

Now fix $G \in \mathscr{C}$ and let $R(G) = (m_{14}(G), m_{12}(G), m_{24}(G), m_{13}(G), m_{34}(G), m_{23}(G))$. By Theorem 2.5

$$[G]_\chi = \{H \in \mathscr{C}\colon R(H) - R(G) \in \langle(-2,0,0,3,-6,0),(0,1,-2,0,0,0)\rangle\}.$$

In other words, $H \in [G]_\chi$ if and only if there exist integers a, b such that

$$m_{14}(H) = m_{14}(G) - 2a,$$

$$m_{12}(H) = m_{12}(G) + b,$$

$$m_{24}(H) = m_{24}(G) - 2b,$$

$$m_{13}(H) = m_{13}(G) + 3a,$$

$$m_{34}(H) = m_{34}(G) - 6a,$$

$$m_{23}(H) = m_{23}(G).$$

We end this section with a couple of remarks in order to clarify the dependency of the Randić matrix on the collection $\mathscr{G}$ and also the role played by the identity (2) in our definition of ρ.

Remark 2.7. (i) The order we have been using for the columns of a Randić matrix and for the Randić structure of a graphs does not really depend on the collection $\mathscr{G}$. In fact, it only depends on n.

(ii) Given two collections $\mathscr{G}' \subset \mathscr{G}$, it is not difficult to show that $\rho_{\mathscr{G}'}$ can be easily computed from $\rho_{\mathscr{G}}$. In fact, $\rho_{\mathscr{G}'}$ is obtained by deleting the columns of $\rho_{\mathscr{G}}$ which do not correspond to elements of $\mathbb{X}(\mathscr{G}')$ and then multiplying by an appropriate integer (determined by the m.c.m used to define $\rho_{\mathscr{G}}$ and $\rho_{\mathscr{G}'}$).

(iii) There are other identities like (2) that could be used to associate a matrix to χ. The advantage of using (2) is that the number of variables used is minimal.

3. The Randić structure property

As we said in Section 1, perhaps the simplest situation, regarding the problem of describing $[G]_\chi$, is when $[G]_\chi$ consists merely of those $H \in \mathscr{G}$ such that $R(H) = R(G)$. In this section, we will present examples of such collections. We recall a concept already mentioned in Section 1.

Definition 3.1. A collection $\mathscr{G}$ of graphs with a fixed number of vertices has the Randić structure property (RSP) if for all $G, G' \in \mathscr{G}$

$$\chi(G) = \chi(G') \Leftrightarrow R(G) = R(G').$$

Notice that the implication from right to left always holds. In other words, if $\mathscr{G}$ has RSP then for every $G \in \mathscr{G}$

$$[G]_\chi = \{H \in \mathscr{G}\colon m_{ij}(H) = m_{ij}(G) \quad \text{for all } i < j \in \mathbb{D}(\mathscr{G})\}.$$

Let us define $\Delta_{\mathscr{G}}\colon \mathscr{G} \times \mathscr{G} \to \mathbb{Q}^{|\mathbb{X}(\mathscr{G})|}$ as $\Delta(G, H) = R(G) - R(H)$ for every $G, H \in \mathscr{G}$. From Theorem 2.5 we immediately get the following

Proposition 3.2. *Let $\mathscr{G}$ be a collection of graphs with n vertices and $\rho_{\mathscr{G}}$ its associated linear map. The following conditions are equivalent*:

(1) *$\mathscr{G}$ has the Randić structure property*
(2) $\mathrm{Im}(\Delta_{\mathscr{G}}) \cap \ker \rho_{\mathscr{G}} = (0)$.

In particular, if $\rho_{\mathscr{G}}$ is one to one then $\mathscr{G}$ has the RSP. Our next result characterizes collections $\mathscr{G}$ such that $\rho_{\mathscr{G}}$ is one to one.

Proposition 3.3. *Let $\mathscr{G}$ be a collection of graphs with n vertices and $\rho_{\mathscr{G}}$ its associated linear map. The following conditions are equivalent*:

(1) *$\rho_{\mathscr{G}}$ is one to one*
(2) $|\mathbb{X}(\mathscr{G})| = |\overline{\mathbb{X}(\mathscr{G})}|$.

Proof. If there exists a perfect square number $u \in \mathbb{X}(\mathscr{G})$ then $\dim(\operatorname{Im}\rho_{\mathscr{G}}) = |\overline{\mathbb{X}(\mathscr{G})}|$ since $\rho_{\mathscr{G}}$ has exactly $|\overline{\mathbb{X}(\mathscr{G})}|$ independent rows. Consequently, $\dim(\ker\rho_{\mathscr{G}}) = |\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}|$ and the result follows.

Let us assume then that $\mathbb{X}(\mathscr{G})$ has no perfect squares and so its Randić matrix has the form (4). Note that $|\overline{\mathbb{X}(\mathscr{G})}| \leqslant \dim(\operatorname{Im}\rho_{\mathscr{G}}) \leqslant |\overline{\mathbb{X}(\mathscr{G})}| + 1$ which implies

$$|\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}| - 1 \leqslant \dim(\ker\rho_{\mathscr{G}}) \leqslant |\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}| \tag{6}$$

1. $\Rightarrow$ 2. Suppose that $|\mathbb{X}(\mathscr{G})| > |\overline{\mathbb{X}(\mathscr{G})}|$. If $|\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}| \geqslant 2$ then, by (6), $\dim(\ker\rho_{\mathscr{G}}) \geqslant 1$ and so $\ker\rho_{\mathscr{G}} \neq (0)$.

Next, we show that if $\mathbb{X}(\mathscr{G})$ has no perfect squares then $|\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}| \neq 1$. If $|\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}| = 1$ then there exists $ij,\ rs \in \mathbb{X}(\mathscr{G})$ such that $\{i,j\} \neq \{r,s\}$ and $ij \sim rs$. Consequently, we have expressions of the form

$$ij = \prod_{k=1}^{u} p_k^{e_k} \times \prod_{k=1}^{v} q_k^{o_k}, \quad rs = \prod_{k=1}^{u} p_k^{e'_k} \times \prod_{k=1}^{v} q_k^{o'_k},$$

where for all k, e_k and e'_k are even (possibly zero) natural numbers and o_k and o'_k are odd natural numbers. Let

$$i = \prod_{k=1}^{u} p_k^{\alpha_k} \times \prod_{k=1}^{v} q_k^{\beta_k}, \quad j = \prod_{k=1}^{u} p_k^{\gamma_k} \times \prod_{k=1}^{v} q_k^{\delta_k},$$

$$r = \prod_{k=1}^{u} p_k^{\alpha'_k} \times \prod_{k=1}^{v} q_k^{\beta'_k}, \quad s = \prod_{k=1}^{u} p_k^{\gamma'_k} \times \prod_{k=1}^{v} q_k^{\delta'_k},$$

where for each k

$$\begin{aligned} &\alpha_k + \gamma_k = e_k, \quad \beta_k + \delta_k = o_k,\\ &\alpha'_k + \gamma'_k = e'_k, \quad \beta'_k + \delta'_k = o'_k. \end{aligned} \tag{7}$$

We claim that $ir \sim js$. In fact

$$ir = \prod_{k=1}^{u} p_k^{\alpha_k+\alpha'_k} \times \prod_{k=1}^{v} q_k^{\beta_k+\beta'_k}, \quad js = \prod_{k=1}^{u} p_k^{\gamma_k+\gamma'_k} \times \prod_{k=1}^{v} q_k^{\delta_k+\delta'_k},$$

where by (7)

$$(\alpha_k + \alpha'_k) + (\gamma_k + \gamma'_k) = e_k + e'_k,$$

$$(\beta_k + \beta'_k) + (\delta_k + \delta'_k) = o_k + o'_k.$$

Since $e_k + e'_k$ and $o_k + o'_k$ are even, we deduce that

$$(\alpha_k + \alpha'_k) \text{ is even} \Leftrightarrow (\gamma_k + \gamma'_k) \text{ is even},$$

$$(\beta_k + \beta'_k) \text{ is even} \Leftrightarrow (\delta_k + \delta'_k) \text{ is even}.$$

Consequently, $ir \sim js$.

Now, since $|\mathbb{X}(\mathscr{G})| - |\overline{\mathbb{X}(\mathscr{G})}| = 1$ we must have $r = j$ or $i = s$. Assume $r = j$. Then for all k, $\alpha'_k = \gamma_k$ and $\beta'_k = \delta_k$, which implies by (7)

$$\alpha_k + \alpha'_k = e_k, \quad \beta_k + \beta'_k = o_k,$$

$$\alpha'_k + \gamma'_k = e'_k, \quad \beta'_k + \delta'_k = o'_k.$$

Hence

$$\alpha_k \text{ is even} \Leftrightarrow \gamma'_k \text{ is even},$$

$$\beta_k \text{ is even} \Leftrightarrow \delta'_k \text{ is even}.$$

This clearly implies that $\alpha_k + \gamma'_k$ and $\beta_k + \delta'_k$ are even for all k. Finally, since

$$is = \prod_{k=1}^{u} p_k^{\alpha_k + \gamma'_k} \times \prod_{k=1}^{v} q_k^{\beta_k + \delta'_k},$$

we conclude that is is a perfect square, but this is a contradiction. Similarly, $i = s$ implies rj is a perfect square which also yields a contradiction.

(2) $\Rightarrow$ (1): This is an immediate consequence of (6). $\square$

An application of Propositions 3.2 and 3.3 gives the following examples

Example 3.4. Let $\mathscr{P}_n$ be the collection of all graphs with n vertices such that all vertex degrees are prime numbers or 1. Then clearly the condition $|\mathbb{X}(\mathscr{P}_n)| = |\overline{\mathbb{X}(\mathscr{P}_n)}|$ is satisfied for all n. Hence $\mathscr{P}_n$ has the Randić structure property.

For example, if $\mathscr{G} = \mathscr{B}_n$ is the set of benzenoid systems with n vertices or $\mathscr{G} = \mathscr{R}_3(n)$, the set of all graphs of maximal degree 3 and n vertices, then $\mathscr{G}$ has RSP.

Example 3.5. Let $\mathscr{G} = \mathscr{R}_\delta(n)$ be the set of all branch regular trees of degree δ and n vertices (see [14]). We recall that $G \in \mathscr{R}_\delta(n)$ if and only if all branching vertices of G have degree δ. It can be easily checked that for all values of δ, except when δ is a perfect square or an odd power of 2, $|\mathbb{X}(\mathscr{R}_\delta(n))| = |\overline{\mathbb{X}(\mathscr{R}_\delta(n))}|$. It follows that for these values of δ, $\mathscr{R}_\delta(n)$ has RSP.

In what follows, given a graph G, $k_i = k_i(G)$ denotes the number of vertices of G of degree i.

In general, if δ is a perfect square or an odd power of 2, $\mathscr{R}_\delta(n)$ has not the RSP. Let us analyze $\mathscr{R}_4 = \mathscr{R}_4(n)$. In this case, $\mathbb{X}(\mathscr{R}_4) = \{1 \cdot 2, 1 \cdot 4, 2 \cdot 4\}$. Since $1 \cdot 2$ and $2 \cdot 4$ are equivalent, then $\overline{\mathbb{X}(\mathscr{R}_4)} = \{[1 \cdot 4], [1 \cdot 2]\}$ and $k = 8$. The associated

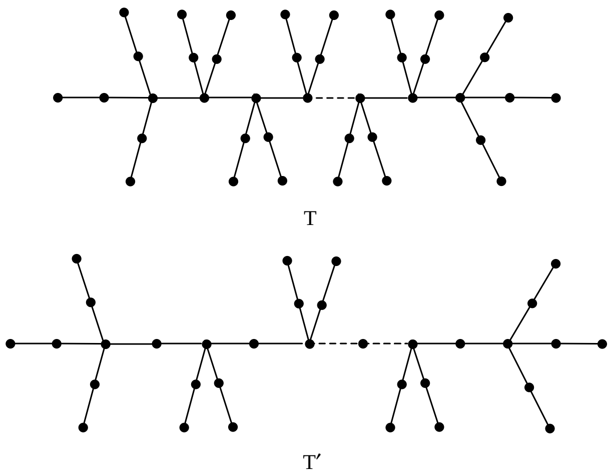

Fig. 1.

matrix $\rho = \rho_{\mathscr{R}_4}$ is

$$\rho = \begin{pmatrix} -2 & -12 & -6 \\ 0 & 8 & 4 \end{pmatrix}. \tag{8}$$

The kernel of ρ can be easily shown to be generated by $(0, 1, -2)$. We next show that $\mathrm{Im}(\Delta_{\mathscr{R}_4}) \cap \ker \rho \neq (0)$. In fact, we will construct trees $T, T' \in \mathscr{R}_4$ such that $(0) \neq R(T) - R(T') \in \ker \rho$. We are looking for trees whose structure is shown in Fig. 1.

Let k_4 and k_4' denote the number of branching vertices of T and T', respectively. Then

$$m_{14} = 0, \quad m_{14}' = 0,$$

$$m_{12} = 2k_4 + 2, \quad m_{12}' = 2k_4' + 2,$$

$$m_{24} = 2k_4 + 2, \quad m_{24}' = 4k_4'$$

and so $R(T) - R(T') = (0, 2(k_4 - k_4'), 2k_4 + 2 - 4k_4') = (0, u, -2u)$ for $u \in \mathbb{Z}$. If $u = 2l$ then we obtain the equations

$$2(k_4 - k_4') = 2l,$$

$$2k_4 + 2 - 4k_4' = -4l$$

which gives the relations

$$k_4' = 3l + 1,$$

$$k_4 = 4l + 1.$$

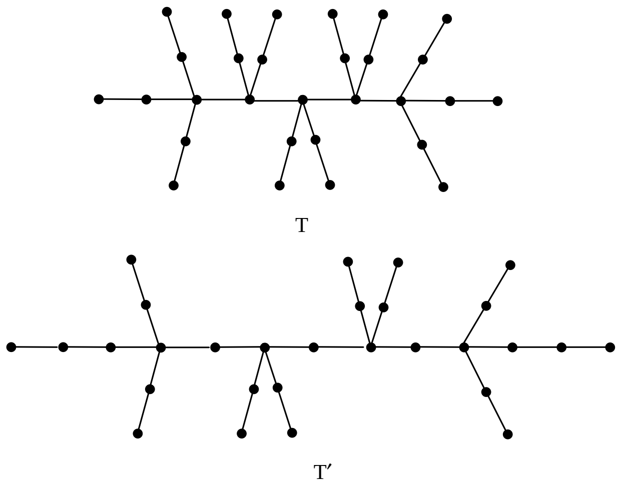

Fig. 2.

In this way, for each positive integer l (and n large enough) we can construct pairs of trees T and T' as in Fig. 1 such that $\chi(T) = \chi(T')$ but $R(T) \neq R(T')$. For example, $l = 1$ gives the pair of trees shown in Fig. 2.

In the case that δ is an odd power of 2, for example $\mathscr{R}_8$, an analogous argument using $\ker \rho_{\mathscr{R}_8}$, gives that for every positive integer l, the trees shown in Fig. 3, such that $k_8 = 178l + 1$ and $k_8' = 177l + 1$, have equal connectivity index but different Randić structure.

Up to now all examples of RSP collections $\mathscr{G}$ have $\ker(\rho_{\mathscr{G}}) = (0)$. As we will see in our next example this is not always the case.

Example 3.6. Let $\mathscr{S}_4 = \mathscr{S}_4(n)$ be the collection of all starlike trees of degree 4 and n vertices. Recall that $T \in \mathscr{S}_4$ if and only if T has a unique branching vertex of degree 4. Since $\mathbb{X}(\mathscr{S}_4) = \mathbb{X}(\mathscr{R}_4)$ then

$$\rho_{\mathscr{S}_4} = \begin{pmatrix} -2 & -12 & -6 \\ 0 & 8 & 4 \end{pmatrix}$$

and again, $\ker(\rho_{\mathscr{S}_4}) = \langle(0, 1, -2)\rangle$. Now, for every $S \in \mathscr{S}_4$ the following relations hold:

$$m_{12}(S) = m_{24}(S) = 4 - m_{14}(S).$$

Consequently

$$\Delta_{\mathscr{S}_4}(S, S') = R(S) - R(S') = (m_{14} - m'_{14}, m_{12} - m'_{12}, m_{24} - m'_{24}) \subseteq \langle(1, -1, -1)\rangle.$$

Since $\langle(1, -1, -1)\rangle \cap \ker(\rho_{\mathscr{S}_4}) = (0)$, we deduce that $\mathrm{Im}(\Delta_{\mathscr{S}_4}) \cap \ker(\rho_{\mathscr{S}_4}) = (0)$. It follows by Proposition 3.2, that $\mathscr{S}_4$ has RSP.

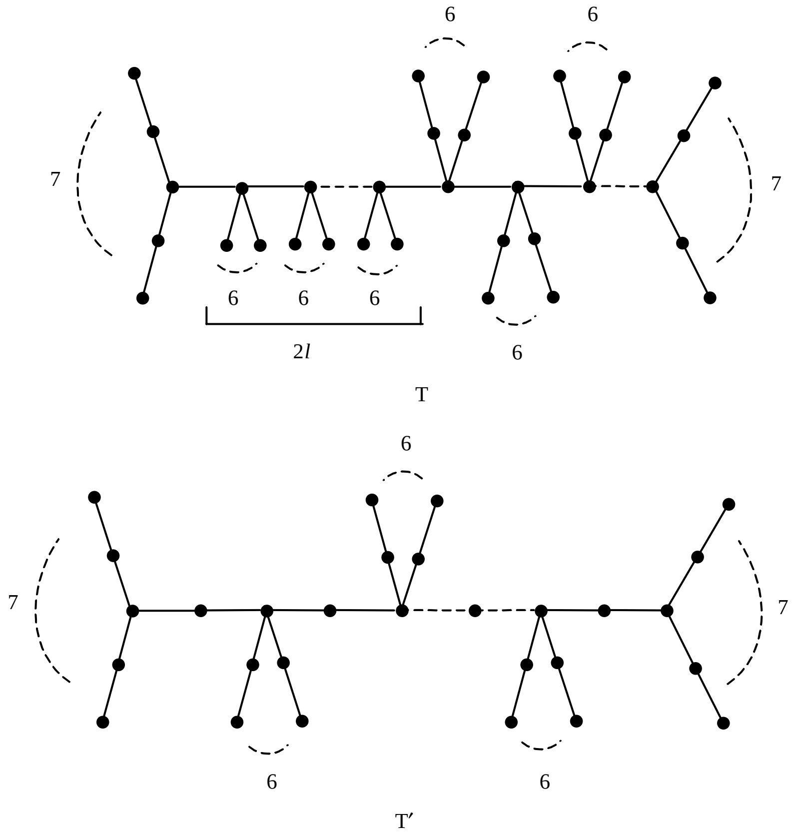

Fig. 3.

4. Decomposition of a collection of graphs into disjoint RSP subcollections

Even though collections with RSP might seem hard to find, we will show in this section a fairly general method to generate them. Furthermore, we will show that every collection $\mathscr{G}$ can be decomposed as a disjoint union of RSP subcollections.

Let $\mathscr{G}$ be a collection of graphs with a fixed number of vertices and $\rho_{\mathscr{G}}$: $\mathbb{Q}^{|X(\mathscr{G})|} \to \mathbb{Q}^{|\overline{X(\mathscr{G})}|}$ its associated $\mathbb{Q}$-linear map. It is clear from Proposition 3.2 that a subcollection $\mathscr{G}' \subseteq \mathscr{G}$ has the RSP if and only if $\rho_{\mathscr{G}}$ is one-to-one in $\{R(G)\colon G \in \mathscr{G}'\}$. The basic idea for getting the above-mentioned decomposition of $\mathscr{G}$ is first to decompose $\mathbb{Q}^{|X(\mathscr{G})|}$ into disjoint pieces where $\rho_{\mathscr{G}}$ is one-to-one and then pull back with R^{-1} such decomposition into $\mathscr{G}$.

Lemma 4.1. *Let ρ: $\mathbb{Q}^m \to \mathbb{Q}^k$ and σ: $\mathbb{Q}^m \to \mathbb{Q}^{m-k}$ be $\mathbb{Q}$-linear maps and consider the $\mathbb{Q}$-linear map (ρ,σ): $\mathbb{Q}^m \to \mathbb{Q}^m$, defined by $(\rho,\sigma)(Z)=(\rho(Z),\sigma(Z))$ for every $Z \in \mathbb{Q}^m$. If (ρ,σ) is invertible then* $\ker(\sigma)$ *is a complementary direct summand of* $\ker(\rho)$ *in $\mathbb{Q}^m$.*

Proof. It is clear that $(0)=\ker((\rho,\sigma))=\ker(\rho)\cap\ker(\sigma)$. Now choose $Z\in\mathbb{Q}^m$. Since (ρ,σ) is onto there exists $Y\in\mathbb{Q}^m$ such that $(\rho,\sigma)(Y)=(0,\sigma(Z))$. Consequently, $Y\in\ker(\rho)$, $Z-Y\in\ker(\sigma)$ and $Z=Y+(Z-Y)$. □

Proposition 4.2. *Let* σ: $\mathbb{Q}^{|X(\mathscr{G})|}\to\mathbb{Q}^{|X(\mathscr{G})|-|\overline{X(\mathscr{G})}|}$ *be a* $\mathbb{Q}$*-linear map such that* $(\rho_{\mathscr{G}},\sigma)$ *is invertible and* $\mathscr{G}_0$ *a subcollection of* $\mathscr{G}$. *If* $\sigma\circ\Delta_{\mathscr{G}_0}=(0)$ *then* $\mathscr{G}_0$ *has the RSP.*

Proof. Let $G,G'\in\mathscr{G}_0$ and suppose that $\chi(G)=\chi(G')$. Then by Theorem 2.5, $R(G)-R(G')\in\ker(\rho_{\mathscr{G}})$. On the other hand $R(G)-R(G')\in\ker(\sigma)$ since $\sigma\circ\Delta_{\mathscr{G}_0}=(0)$. It follows from Lemma 4.1 that $R(G)=R(G')$ and so $\mathscr{G}_0$ has the RSP. □

Theorem 4.3. *Let* $\mathscr{G}$ *be a collection of graphs with a fixed number of vertices. Then* $\mathscr{G}$ *can be decomposed into pairwise disjoint RSP subcollections.*

Proof. Choose a complementary direct summand W of $\ker(\rho_{\mathscr{G}})$ in $\mathbb{Q}^{|X(\mathscr{G})|}$. Consider the projection π: $\mathbb{Q}^{|X(\mathscr{G})|}=W\oplus\ker(\rho_{\mathscr{G}})\to\ker(\rho_{\mathscr{G}})\cong\mathbb{Q}^{|X(\mathscr{G})|-|\overline{X(\mathscr{G})}|}$. Clearly $(\rho_{\mathscr{G}},\pi)$: $\mathbb{Q}^{|X(\mathscr{G})|}\to\mathbb{Q}^{|X(\mathscr{G})|}$ is an invertible $\mathbb{Q}$-linear map. For each $k\in\mathrm{Im}(\pi\circ R)$ define $\mathscr{G}_k=\{G\in\mathscr{G}\colon R(G)\in W+k\}$. Then for every $G,G'\in\mathscr{G}_k$ we have $R(G)-R(G')\in W$ and consequently, $\pi(R(G)-R(G'))=0$. Hence $\pi\circ\Delta_{\mathscr{G}_k}=(0)$ and so, by Proposition 4.2, $\mathscr{G}_k$ has the RSP. Finally, it is clear that the $\mathscr{G}_k$'s are pairwise disjoint and $\mathscr{G}=\bigcup_{k\in\mathrm{Im}(\pi\circ R)}\mathscr{G}_k$. □

Let us look at a concrete example. Consider the collection $\mathscr{R}_\delta(n)$ of branch regular graphs of degree δ and n vertices. We analyze the case where δ is a perfect square.

Let $\delta=q^2$. Then $\mathbb{X}(\mathscr{R}_\delta)=\{1\cdot 2,1\cdot\delta,2\cdot\delta\}$, $\overline{\mathbb{X}(\mathscr{R}_\delta)}=\{[1\cdot\delta],[1\cdot 2]\}$ and $k=2\delta$. The associated matrix is

$$\rho=\begin{pmatrix}-2(q-1)^2 & -3q^2 & -(q^2+2)\\ 0 & 2q^2 & 2q\end{pmatrix}.$$

Recall that the columns correspond to the following pairs $1\cdot\delta,1\cdot 2,2\cdot\delta$ in this order. Consider the following completion of ρ

$$(\rho,\sigma)=\begin{pmatrix}-2(q-1)^2 & -3q^2 & -(q^2+2)\\ 0 & 2q^2 & 2q\\ 1 & 1 & 0\end{pmatrix},$$

where σ: $\mathbb{Q}^3\to\mathbb{Q}$ is defined by $\sigma(x_{1\delta},x_{12},x_{2\delta})=x_{1\delta}+x_{12}$. Notice that (ρ,σ) is invertible. Recall that for a given a graph G, we denote by $k_i=k_i(G)$ the number of vertices of G of degree i. For each positive integer $r\geqslant 1$ consider the subcollection

$$\mathscr{R}_\delta^r=\{G\in\mathscr{R}_\delta\colon k_\delta(G)=r\},\tag{9}$$

of $\mathscr{R}_\delta$. Since for every $G \in \mathscr{R}_\delta$, $m_{12}(G)+m_{1\delta}(G)=k_1(G)=(\delta-2)k_\delta(G)+2$, we deduce that $m_{12}(G)+m_{1\delta}(G)=(\delta-2)r+2$ for every $G \in \mathscr{R}_\delta^r$. Consequently, if $G, G' \in \mathscr{R}_\delta^r$

$$\sigma(R(G)-R(G')) = \sigma((m_{1\delta}-m'_{1\delta}, m_{12}-m'_{12}, m_{2\delta}-m'_{2\delta}))$$
$$= (m_{1\delta}-m'_{1\delta}) + (m_{12}-m'_{12}) = 0.$$

In other words, $\sigma \circ \Delta_{\mathscr{R}_\delta^r} = (0)$. It follows from Proposition 4.2 that $\mathscr{R}_\delta^r$ has the RSP for every r. Moreover, an easy induction shows that $k_\delta.(\delta-1) \leqslant n-2$. Therefore

$$\mathscr{R}_\delta = \bigcup_{r=1}^{[(n-2)/(\delta-1)]} \mathscr{R}_\delta^r \tag{10}$$

is a disjoint union of RSP subcollections of $\mathscr{R}_\delta$.

Note that $\mathscr{R}_\delta^1$ is the set of all starlike trees of degree δ. In particular, Example 3.6 can be deduced from here since $\mathscr{S}_4 = \mathscr{R}_4^1$.

The case in which δ is an odd power of 2 is similar.

We will present one more example. It will show that such decompositions into RSP pieces can be more complex than in the previous example. In particular, they could depend on more than one parameter (due to the dimension of the kernel of the Randić matrix).

Consider the collection of all chemical graphs $\mathscr{C}$ with n vertices. We have already computed in Example 2.6 its Randić matrix ρ. Consider the following completion of ρ:

$$(\rho, \sigma) = \begin{pmatrix} -6 & -36 & -18 & -32 & -14 & -20 \\ 0 & 24 & 12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 16 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix},$$

where σ: $\mathbb{Q}^6 \to \mathbb{Q}^2$ is defined by $\sigma(x_{14}, x_{12}, x_{24}, x_{13}, x_{34}, x_{23}) = (x_{14}+x_{12}+x_{13}, x_{24})$. For each pair of integers $0 \leqslant r \leqslant n$ and $0 \leqslant s \leqslant n$, let

$$\mathscr{C}_{r,s} = \{G \in \mathscr{C}\colon\ m_{12}(G)+m_{13}(G)+m_{14}(G) = r \ \&\ m_{24}(G) = s\}.$$

Proposition 4.2 says that each $\mathscr{C}_{r,s}$ has the RSP (notice that some of the $\mathscr{C}_{r,s}$'s are empty). Finally, it is clear that these subcollections form a partition of $\mathscr{C}$.

5. A finer analysis of $\mathscr{R}_4$

In this section, we will see how the ideas presented in previous sections can be used to make a finer analysis of the collection of branch regular trees. We will restrict our analysis to $\mathscr{R}_4$.

The key fact for all our analysis is the following lemma. It tells, in terms of the number of branching vertices, where we have to look to find two trees in $\mathscr{R}_4$ with equal χ. Notice the crucial role played by the equations of the kernel of $\rho_{\mathscr{R}_4}$.

Lemma 5.1. *Let $T, T' \in \mathscr{R}_4$ with $\chi(T) = \chi(T')$. Then*

(a) $\frac{3k_4+1}{4} \leqslant k_4' \leqslant \frac{4k_4-1}{3}$
(b) $m_{44} - m_{44}' = 4(k_4 - k_4')$

where, as usual, k_4 is the number of vertices of degree 4 (all variables with $'$ corresponds to T' and the others to T).

Proof. (a) We use the matrix $\rho_{\mathscr{R}_4}$ and its kernel computed in (8). Since $\chi(T) = \chi(T')$ then by Theorem 2.5 we know that

$$m_{14} = m_{14}',$$

$$2m_{12} + m_{24} = 2m_{12}' + m_{24}'. \tag{11}$$

For every branch regular tree we have $m_{12} + m_{1\delta} = (\delta - 2)k_\delta + 2$ and since $m_{14} = m_{14}'$ then

$$m_{12}' = 2k_4' + 2 - m_{14}. \tag{12}$$

Let $r(T) = 2m_{12} + m_{24}$. By substituting (12) in (11) we get

$$m_{24}' = r(T) - 4k_4' - 4 + 2m_{14}. \tag{13}$$

Now, for every tree in $\mathscr{R}_4$ we have that $m_{12}' \leqslant m_{24}'$. This inequality together with (11) gives the following:

$$3m_{24}' \geqslant r(T).$$

From this and (13) we get

$$k_4' \leqslant \frac{r(T)}{6} + \frac{m_{14}}{2} - 1.$$

Since $m_{12} + m_{14} = 2k_4 + 2$, we immediately get

$$k_4' \leqslant \frac{2}{3}k_4 + \frac{m_{14} + m_{24}}{6} - \frac{1}{3}. \tag{14}$$

Since $m_{14} + m_{24} + 2m_{44} = 4k_4$, then $m_{14} + m_{24} \leqslant 4k_4$. This last inequality together with (14) gives the right-hand side of part (a) of our claim. The other inequality follows by symmetry.

(b) Since $m_{14} + m_{24} + 2m_{44} = 4k_4$, and $m_{14} = m_{14}'$ then we get

$$4(k_4 - k_4') = 2(m_{44} - m_{44}') + m_{24} - m_{24}'. \tag{15}$$

From (11) we get

$$2(k_4 - k_4') = m_{44} - m_{44}' + m_{12}' - m_{12}. \tag{16}$$

Since $m_{12} + m_{14} = 2k_4 + 2$ and $m_{14} = m_{14}'$, then we immediately get that $m_{12}' - m_{12} = -2(k_4 - k_4')$. From this and (16) we are done. $\square$

Recall from Section 4 the partition of $\mathcal{R}_4$ given by the $\mathcal{R}_4^r$'s.

Proposition 5.2. *The following collection has the RSP for every $r \geqslant 4$*

$$\mathcal{R}_4^1 \cup \mathcal{R}_4^2 \cup \mathcal{R}_4^3 \cup \mathcal{R}_4^r.$$

Proof. This is a straightforward application of Lemma 5.1(a). We will show the claim in three steps. First we show that $\mathcal{R}_4^1 \cup \mathcal{R}_4^r$ has the RSP for every $r \geqslant 2$. Second we show that $\mathcal{R}_4^2 \cup \mathcal{R}_4^r$ has the RSP for every $r \geqslant 3$ and then we show that $\mathcal{R}_4^3 \cup \mathcal{R}_4^r$ has the RSP for every $r \geqslant 4$.

(i) Let $T \in \mathcal{R}_4^1$ and $T' \in \mathcal{R}_4^r$ with $\chi(T) = \chi(T')$. Then $k_4 = 1$ and $k_4' = r$. By Lemma 5.1 we know that $r \leqslant 4 - 1/3 = 1$. Therefore $T' \in \mathcal{R}_4^1$ and we are done as $\mathcal{R}_4^1$ has the RSP.

(ii) Let $T \in \mathcal{R}_4^2$ and $T' \in \mathcal{R}_4^r$ with $\chi(T) = \chi(T')$. Then from Lemma 5.1 we know that $r \leqslant \frac{8-1}{3} < 3$. Therefore $T' \in \mathcal{R}_4^1 \cup \mathcal{R}_4^2$ and we are done as we just saw that this collection has the RSP.
Notice that from (i) and (ii) we can conclude that $\mathcal{R}_4^1 \cup \mathcal{R}_4^2 \cup \mathcal{R}_4^3$ has the RSP.

(iii) Let $T \in \mathcal{R}_4^3$ and $T' \in \mathcal{R}_4^r$ with $\chi(T) = \chi(T')$. Then from Lemma 5.1 we know that $r \leqslant \frac{12-1}{3} < 4$. Therefore $T' \in \mathcal{R}_4^1 \cup \mathcal{R}_4^2 \cup \mathcal{R}_4^3$ and we are done as we just saw that this collection has the RSP. □

We have already seen that the previous result is best possible, since $\mathcal{R}_4$ does not have the RSP (for large enough n) and the smallest pair of counterexamples given in Section 3 have k_4 equal to 4 and 5, respectively (see Fig. 2). But we can nevertheless get sharper results if we take into account the number of vertices. Recall that for branch regular trees we have that $k_\delta \leqslant (n-2)/(\delta - 1)$. In particular, for $\delta = 4$, we have that $k_4 \leqslant (n-2)/3$. It is not difficult to see from 5.1 that the smallest pair of trees in $\mathcal{R}_4$ with equal χ and different R have size 19. Thus we have the following

Proposition 5.3. (i) *For $n < 19$, $\mathcal{R}_4$ has the RSP.*

(ii) *For $19 \leqslant n < 20$, $\mathcal{R}_4$ does not have the RSP but it is the union of two subcollections with the RSP, namely $\mathcal{R}_4^1 \cup \mathcal{R}_4^2 \cup \mathcal{R}_4^3 \cup \mathcal{R}_4^4$* and *$\mathcal{R}_4^5$.*

(iii) *For $20 \leqslant n < 23$, $\mathcal{R}_4$ does not have the RSP but it is the union of two subcollections with the RSP, namely $\mathcal{R}_4^1 \cup \mathcal{R}_4^2 \cup \mathcal{R}_4^3 \cup \mathcal{R}_4^4 \cup \mathcal{R}_4^6$ and $\mathcal{R}_4^5$.*

Remark. Let us define an equivalence relation $=_R$ by letting $G =_R G'$ when $R(G) = R(G')$. A way of understanding the previous result is by noticing that the number of RSP pieces gives a bound to the number of $=_R$ equivalence classes that form $[G]_\chi$. In particular, for $G \in \mathcal{R}_4$ (with $n < 23$), there is at most one more Randić structure different than $R(G)$ corresponding to a tree $H \in \mathcal{R}_4$ with $\chi(G) = \chi(H)$.

Of course, we can continue the previous analysis to get a quite sharp picture of $\mathcal{R}_4$ in terms of the smallest number of RSP pieces which are necessary to cover it all. This analysis would give further information about the behavior of χ over $\mathcal{R}_4$. For instance, given k, it is now easy to construct (for large enough n) a set of k trees in $\mathscr{R}_4$ with equal χ and different Randić structures.

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