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On Randić Spread

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Abstract

A new spectral graph invariant spr_R, called Randić spread, is defined and investigated. This quantity is equal to the maximal difference between two eigenvalues of the Randić matrix, disregarding the spectral radius. Lower and upper bounds for spr_R are deduced, some of which depending on the Randić index of the underlying graph.

1 Notation and preliminaries

In this paper G stands for an undirected simple graph on n vertices and m edges. Its vertex set and edge set are $V(G)$ and $E(G)$, respectively. The vertices of G are assumed to be labeled by $1, 2, \ldots, n$. If $e \in E(G)$ has end vertices i and j, then we say that i and j are adjacent ($i \sim j$) and that $e = ij$. The set $N_i = \{j \in V(G) : ij \in$

$E(G)\}$ is the set of neighbors of $i \in V(G)$ and its cardinality is the degree d_i of the vertex i. In this work an isolated vertex of G (i.e., a vertex of degree zero) is called a singleton.

A p-regular graph G is a graph in which every vertex has degree p , $p \geq 0$.

A graph G is bipartite if there exists a nonempty disjoint decomposition $V(G) = X \cup Y$ such that each edge $ij \in E(G)$ has an end vertex in X and the other one in Y. The sets X, Y are called a bipartition of G.

The adjacency matrix $\mathbf{A} = \mathbf{A}(G)$ of the graph G is the 0–1 matrix of order n whose (i,j)-entry is equal to 1 if $ij \in E(G)$, and 0 otherwise. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\mathbf{A}$ are usually referred to as the eigenvalues of the graph G (see [10]). Moreover, if G is a connected graph, then the matrix $\mathbf{A}$ is nonnegative and irreducible (see [10]).

For a real symmetric matrix $\mathbf{M}$ associated to the graph G, we denote by $\lambda_i(\mathbf{M})$ its i-th greatest eigenvalue. The spectrum (the multiset of eigenvalues) of $\mathbf{M}$ is denoted by $\sigma(\mathbf{M}) = \sigma(\mathbf{M}(G))$. The multiplicity s of an eigenvalue λ in this spectrum will be denoted by $\lambda^{(s)}$.

The Laplacian matrix is $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$, where $\mathbf{D}(G)$ is the diagonal matrix of the vertex degrees. Its spectrum is called the Laplacian spectrum of G. Recall that $\mathbf{L}(G)$ is a positive semidefinite matrix (see [10]). Moreover, 0 is always a Laplacian eigenvalue with $\mathbf{e}$, the all-one vector, as a corresponding eigenvector. Its multiplicity corresponds to the number of connected components of G.

In what follows, K_n and $\overline{K_n}$ denote the complete graph on n vertices and its complement, respectively. We denote by $\mathbf{I}_n$, or simply $\mathbf{I}$ the identity matrix of order n, or of appropriate order, respectively.

2 The Randić matrix

The graph matrix that nowadays is referred to as the *Randić matrix* has a long history. First of all, in 1975 Milan Randić [32] invented a molecular structure descriptor (topological index) that he called "branching index", and which later became known under the name “connectivity index” or “Randić index”. It is defined as[1]

$$\chi = \chi(G) = \sum_{ij \in E(G)} \frac{1}{\sqrt{d_i\, d_j}} \,. \tag{1}$$

The plethora of chemical and pharmacological applications of the Randić index, as well as its numerous mathematical investigations are well known and much documented; see [18, 22–24, 26, 33] and the references cited therein. The Randić index happens to be the first in a long series of vertex–degree based structure descriptors encountered and studied in contemporary mathematical chemistry; for details see [15, 17, 20].

Bearing in mind Eq. (1), it would be straightforward to conceive a graph matrix $\mathbf{R} = \mathbf{R}(G) = (r_{ij})$, where $r_{ij} = 1/\sqrt{d_i\, d_j}$ if $ij \in E(G)$, and zero otherwise. The obvious name for $\mathbf{R}$ would be Randić matrix.

However, the actual history of the matrix $\mathbf{R}$ is almost independent of Randić's Eq. (1). This matrix (without any name and without any mention of the Randić index) is found already in the seminal book by Cvetković, Doob and Sachs [10] (p. 26).

As before, let $\mathbf{D} = \mathbf{D}(G)$ be the diagonal matrix of the vertex degrees of the graph G. For graphs without singletons, the diagonal matrix $\mathbf{D}^{-1/2}$ is well defined. Then $\mathcal{L} = \mathcal{L}(G) = \mathbf{D}^{-1/2}\,\mathbf{L}(G)\,\mathbf{D}^{-1/2}$ is the “normalized Laplacian matrix” and an entire spectral theory based on it has been elaborated (see [9]). It is easy to see that

$$\mathcal{L}(G) = \mathbf{I}_n - \mathbf{R}(G)$$

implying that the eigenvalues of the Randić matrix are closely related with those of the normalized Laplacian matrix. In particular, λ is a Randić eigenvalue of G if and only if $1-\lambda$ is a normalized Laplacian eigenvalue of G. The normalized Laplacian matrix is positive semidefinite (see [9]). This implies that $\lambda = 1$ is the greatest Randić eigenvalue of any graph with at least one edge. Moreover, a standard verification shows that $\mathbf{D}^{1/2}\,\mathbf{e}$ is an eigenvector of the Randić matrix for the eigenvalue $\lambda = 1$ and also of the normalized Laplacian matrix for eigenvalue $\lambda = 0$. If G is connected,

[1] In the contemporary mathematical and mathematico–chemical literature, the Randić index is usually denoted by R (see [15, 17, 18, 20, 23, 24, 26]). Because in our paper this symbol is used for the Randić matrix, we return here to Randić's original notation χ [32].

then $\mathbf{R}(G)$ is a nonnegative irreducible matrix and by the Perron–Frobenius theorem its spectral radius is the unique eigenvalue with an associated positive eigenvector. From all the above results, for an arbitrary graph G, the multiplicity of $1 \in \sigma(\mathbf{R}(G))$ corresponds to the number of connected components of G which are not singletons.

In connection with the Randić index, the matrix $\mathbf{R}$ seems to be first time used in 2005 by Rodríguez, who referred to it as the "weighted adjacency matrix" [34] and the "degree adjacency matrix" [35]. In 2010, a systematic study of spectral properties of the Randić matrix started [2–5, 14, 19, 27, 36, 37], mainly motivated by the newly conceived concept of *Randić energy* [25], equal to the sum of absolute values of the eigenvalues of $\mathbf{R}$. Independently, based on the matrix $\mathcal{L}$, the "normalized Laplacian energy" was put forward [8], which is exactly the same as the Randić energy.

3 The Randić spread

In this section we introduce the concept of *Randić spread* and deduce upper and lower bounds for this spectral invariant. Some of these bounds are in terms of the Randić index of the underlying graph.

Generally, the spread of an $n \times n$ complex matrix $\mathbf{M}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ is defined by

$$s(\mathbf{M}) = \max_{i,j} |\lambda_i - \lambda_j|$$

where the maximum is taken over all pairs of eigenvalues of $\mathbf{M}$. There is a considerable literature related with this parameter, see for instance [1, 21, 29–31]. The following lower bound for the spread of a Hermitian matrix $\mathbf{M} = (m_{ij})$ was given in [1] and [29]:

$$s(\mathbf{M}) \geq \max_{i,j} \left((m_{jj} - m_{ii})^2 + 2 \sum_{s \neq j} |m_{js}|^2 + 2 \sum_{s \neq i} |m_{is}|^2 \right)^{1/2} . \tag{2}$$

This is one of the best lower bounds for symmetric matrices.

Recently, the spread of a graph (defined as the spread of its adjacency matrix) has been extensively studied. In [16] lower and upper bounds for this spectral graph invariant were obtained. In fact, the authors of [16] showed that the path is the unique graph with minimal spread among all connected graphs of a given order and, as the maximal spread is still unknown, some conjectures were presented.

In the case of the Laplacian and normalized Laplacian matrices, the smallest eigenvalue is always equal to zero. In the case of the Randić matrix, the greatest eigenvalue is always equal to unity. Because of this, the concept of spread of these matrices is trivial and uninteresting: $s(\mathbf{L})$ and $s(\mathcal{L})$ are equal to the spectral radii of the respective matrices;[2] $s(\mathbf{R})$ is equal to 1 minus the smallest Randić eigenvalue, and, in addition, is equal to $s(\mathcal{L})$. Even worse, for all bipartite graphs, $s(\mathbf{R}) = 2$.

In order to overcome these difficulties, the spread concept of $\mathbf{L}$, $\mathcal{L}$, and $\mathbf{R}$ has been somewhat modified.

Taking into account that the smallest eigenvalue of the Laplacian matrix of a graph G is zero, and that the second smallest eigenvalue is the algebraic connectivity of G (which is an important algebraic measure of the connectivity of a graph [11,13]), the "Laplacian spread" was defined as [12]

$$spr_{\mathbf{L}}(G) = \max\left\{|\lambda_i(\mathbf{L}) - \lambda_j(\mathbf{L})| : \lambda_i(\mathbf{L}), \lambda_j(\mathbf{L}) \in \sigma(\mathbf{L}(G)) \setminus \{0\}\right\}. \tag{3}$$

In an analogous manner, the normalized Laplacian spread of G is

$$spr_{\mathcal{L}}(G) = \max\left\{|\lambda_i(\mathcal{L}) - \lambda_j(\mathcal{L})| : \lambda_i(\mathcal{L}), \lambda_j(\mathcal{L}) \in \sigma(\mathcal{L}(G)) \setminus \{0\}\right\}. \tag{4}$$

In parallel with Eqs. (3) and (4), we now define the Randić spread as:

$$spr_{\mathbf{R}}(G) = \max\left\{|\lambda_i(\mathbf{R}) - \lambda_j(\mathbf{R})| : \lambda_i(\mathbf{R}), \lambda_j(\mathbf{R}) \in \sigma(\mathbf{R}(G)) \setminus \{1\}\right\}. \tag{5}$$

¿From (4) and (5) follows that for graphs G having no singletons, $spr_{\mathbf{R}}(G)$ coincides with $spr_{\mathcal{L}}(G)$. For instance, if $G \cong K_n$, then

$$\sigma(\mathbf{R}(K_n)) = \left\{1, \left(-\frac{1}{n-1}\right)^{(n-1)}\right\} \qquad \text{and} \qquad \sigma(\mathcal{L}(K_n)) = \left\{\left(\frac{n}{n-1}\right)^{(n-1)}, 0\right\}.$$

Therefore, $spr_{\mathbf{R}}(K_n) = spr_{\mathcal{L}}(K_n) = 0$.

In the literature concerned with the localization of eigenvalues of nonnegative square matrices, special attention has been devoted to upper bounds on the second greatest modulus of an eigenvalue [37,38]. We shall need the following result.

[2] Recall that in the literature there are many results on the greatest eigenvalues of $\mathbf{L}$ and $\mathcal{L}$, i.e., on their spectral radii, especially upper bounds (see for instance [28,37]).

Lemma 1. [37] *Let G be an undirected simple and connected graph. For $i \in V(G)$, let N_i be the set of first neighbors of the vertex i of G. If $\lambda(\mathbf{R})$ is an eigenvalue with greatest modulus among the negative Randić eigenvalues of G, then*

$$|\lambda(\mathbf{R})| \leq 1 - \min_{i \sim j} \left\{ \frac{|N_i \cap N_j|}{\max\{d_i, d_j\}} \right\}$$

where the minimum is taken over all pairs (i,j) , $1 \leq i < j \leq n$, such that the vertices i and j are adjacent.

Since $1 \in \sigma(\mathbf{R}(G))$, by using Lemma 1 we directly arrive at:

Theorem 2. *Let G be an undirected simple and connected graph whose Randić matrix is $\mathbf{R}(G)$. Then*

$$spr_{\mathbf{R}}(G) = \lambda_2(\mathbf{R}(G)) - \lambda_n(\mathbf{R}(G)) \leq 2 - \min_{i \sim j} \left\{ \frac{|N_i \cap N_j|}{\max\{d_i, d_j\}} \right\} \tag{6}$$

where the minimum is taken over all pairs (i,j) , $1 \leq i < j \leq n$, such that the vertices i and j are adjacent.

The next theorem is due to Brauer [6] and relates the eigenvalues of an arbitrary matrix and the matrix resulting from a rank-one additive perturbation.

Theorem 3. [6] *Let $\mathbf{M}$ be an arbitrary $n \times n$ matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Let x_k be an eigenvector of $\mathbf{M}$ associated with the eigenvalue λ_k, and let q be any n-dimensional vector. Then the matrix $\mathbf{M} + x_k\, q^t$ has eigenvalues*

$$\lambda_1, \ldots, \lambda_{k-1}\, ,\, \lambda_k + x_k^t\, q\, ,\, \lambda_{k+1}, \ldots, \lambda_n \ .$$

Let G be an arbitrary graph of order n with m edges and $pq \in E(G)$. Then the matrix

$$\mathbf{R}_{pq} = \begin{pmatrix} 0 & (d_p\, d_q)^{-1/2} \\ (d_p\, d_q)^{-1/2} & 0 \end{pmatrix}$$

is a principal submatrix of order 2 of $\mathbf{P}\,\mathbf{R}(G)\,\mathbf{P}^t$, where $\mathbf{P}$ is an appropriate permutation matrix of order n.

The smallest eigenvalue of $\mathbf{R}_{pq}$ is $\lambda_{pq} = -1/\sqrt{d_p\, d_q}$. By the Cauchy interlacing theorem (see [10]), we have

$$\lambda_n(\mathbf{R}(G)) \leq \lambda_{pq} \leq \lambda_2(\mathbf{R}(G)) \ . \tag{7}$$

On the other hand, the average of these values

$$\frac{1}{m}\sum_{p\sim q}\lambda_{pq} = \frac{1}{m}\sum_{p\sim q}\left(-\frac{1}{\sqrt{d_p\,d_q}}\right) = -\frac{\chi(G)}{m}$$

also has the property (7), namely

$$\lambda_n(\mathbf{R}(G)) \leq -\frac{\chi(G)}{m} \leq \lambda_2(\mathbf{R}(G)) \ . \tag{8}$$

Now, if

$$w = \mathbf{D}^{1/2}\,\mathbf{e} = \left(\sqrt{d_1},\ldots,\sqrt{d_n}\right)^t$$

is an eigenvector corresponding to the Randić eigenvalue 1, and if

$$\beta_{pq} = -\frac{1}{2m}\left[\frac{1}{\sqrt{d_p\,d_q}} + 1\right] \tag{9}$$

then by Theorem 3, the matrix

$$\mathbf{B}_{pq} = \mathbf{R}(G) + \beta_{pq}\,w\,w^t \tag{10}$$

has spectrum

$$\begin{aligned}\sigma(\mathbf{B}_{pq}) &= \sigma(\mathbf{R}(G)) \setminus \{1\} \cup \left\{1 + \beta_{pq}\,w^t\,w\right\} \\ &= \sigma(\mathbf{R}(G)) \setminus \{1\} \cup \left\{1 - \left((d_p\,d_q)^{-1/2} + 1\right)\right\} = \sigma(\mathbf{R}(G)) \setminus \{1\} \cup \{\lambda_{pq}\}\,.\end{aligned}$$

Remark 1. *By Theorem 3, for any given value* ξ *such that* $\lambda_n(\mathbf{R}(G)) \leq \xi \leq \lambda_2(\mathbf{R}(G))$*, the equality* $spr_{\mathbf{R}}(G) = s(\mathbf{B}_\xi)$ *holds, where* $\mathbf{B}_\xi = \mathbf{R}(G) + \kappa\,w\,w^t$ *with*

$$\kappa = \frac{1}{2m}\,(\xi - 1) \ . \tag{11}$$

Note that $\kappa = \kappa(\xi)$ and in this case, β_{pq} in (9) is equal to $\kappa\left(-1/\sqrt{d_p\,d_q}\right)$.

Let κ be as in 11 and let $\mathbf{C} = \mathbf{R}(G) + \kappa\,w\,w^t$. If $\mathbf{C} = (c_{ij})$, then

$$c_{ij} = \begin{cases} \kappa\,d_i & \text{if } i = j \\ \frac{1}{\sqrt{d_i\,d_j}} + \kappa\sqrt{d_i\,d_j} & \text{if } ij \in E(G) \\ \kappa\sqrt{d_i\,d_j} & \text{if } ij \notin E(G)\ . \end{cases}$$

In what follows, using the suggestion in Remark 1, we deduce some lower bounds for the Randić spread (and for the spread of a rank-one perturbed Randić matrix).

An obvious consequence of the inequality (8) is the following.

Theorem 4. *Let G be an undirected simple graph without singletons whose Randić matrix is* $\mathbf{R}(G)$. *Then*

$$\max\left\{\left|\frac{\chi(G)}{m}+\lambda_n(\mathbf{R}(G))\right|\ ,\ \frac{\chi(G)}{m}+\lambda_2(\mathbf{R}(G))\right\}\leq spr_{\mathbf{R}}(G)\ . \tag{12}$$

It should be noted that if $spr_{\mathbf{R}}(G)=0$, then

$$\chi(G)=-m\,\lambda_2(\mathbf{R}(G))=-m\,\lambda_n(\mathbf{R}(G))\ .$$

Let

$$\mathbf{B}=\mathbf{R}(G)+\beta\,w\,w^t \tag{13}$$

with

$$\beta=-\frac{1}{2m}\left(\frac{\chi}{m}+1\right). \tag{14}$$

By Theorem 3, the spectrum of $\mathbf{B}$ satisfies

$$\begin{aligned}\sigma(\mathbf{B}) &= \sigma(\mathbf{R}(G))\setminus\{1\}\cup\{1+\beta\,w^t\,w\}\\ &= \sigma(\mathbf{R}(G))\setminus\{1\}\cup\left\{1-\left(\frac{\chi}{m}+1\right)\right\}=\sigma(\mathbf{R}(G))\setminus\{1\}\cup\left\{-\frac{\chi}{m}\right\}.\end{aligned}$$

Then

$$spr_{\mathbf{R}}(G)=s(\mathbf{B})=s(\mathbf{B}_{pq}) \tag{15}$$

where $\mathbf{B}_{pq}$ and $\mathbf{B}$ are the matrices defined by Eqs. (10) and (13), respectively.

Remark 2. *Let G be a graph as specified in Theorem 4. Let λ_{pq}^{min} and λ_{pq}^{max} be, respectively, the minimum and the maximum values of λ_{pq} for $pq\in E(G)$. Then*

$$\max\left\{\lambda_{pq}^{max}-\lambda_n(\mathbf{R}(G))\,,\,\lambda_2(\mathbf{R}(G))-\lambda_{pq}^{min}\right\}\leq spr_{\mathbf{R}}(G)\ . \tag{16}$$

Furthermore,

$$\max\left\{\left|\frac{\chi}{m}+\lambda_n(\mathbf{R}(G))\right|,\frac{\chi}{m}+\lambda_2(\mathbf{R}(G))\right\}\leq\max\left\{\lambda_{pq}^{max}-\lambda_n(\mathbf{R}(G))\,,\,\lambda_2(\mathbf{R}(G))-\lambda_{pq}^{min}\right\}.$$

In fact, when $d_p\,d_q$ is constant for all $pq\in E(G)$, for example when G is a bipartite graph, then the lower bounds coincide. If, however, $d_p\,d_q$ is not constant, then the lower bound (16) is better than the lower bound (12).

Lemma 5. *Let G be a graph of order n. Then $\lambda_2(\mathbf{R}(G))<0$ if and only if $G\cong K_n$.*

Proof. ¿From an example given above, we know that $\lambda_2(\mathbf{R}(K_n)) = -1/(n-1)$. Thus, if $G \cong K_n$, then $\lambda_2(\mathbf{R}(G)) < 0$. If $G \ncong K_n$ and $\lambda_2(\mathbf{R}(G)) < 0$, then there exist vertices $v, w \in V(G)$ such that $vw \notin E(G)$. Then, for a suitable permutation matrix $\mathbf{P}$, the matrix $\mathbf{P}\,\mathbf{R}(G)\,\mathbf{P}^t$ has a zero square submatrix of order 2. Then by the Cauchy interlacing theorem, $0 \leq \lambda_2(\mathbf{R}(G))$, which is a contradiction. □

Corollary 6. *Let G be a graph with n vertices. Then $spr_{\mathbf{R}}(G) = 0$ if and only if $G \cong K_n$.*

Proof. If $G \cong K_n$, then, as we have already seen, $spr_{\mathbf{R}}(G) = 0$. If $spr_{\mathbf{R}}(G) = 0$, then $\lambda_2(\mathbf{R}(G)) = \lambda_n(\mathbf{R}(G)) < 0$. Then by Lemma 5, we have $G \cong K_n$. □

The following result was proven by Merikoski and Kumar.

Lemma 7. [29] *Let $\mathbf{M} = (m_{ij})$ be a normal matrix of order n. Then*

$$s(\mathbf{M}) \geq \frac{1}{n-1} \left| \sum_j \sum_{k \neq j} m_{jk} \right| .$$

Corollary 8. *Let G be a regular graph of order n and degree p. If $spr_{\mathbf{R}}(G)$ is defined as in (5), then*

$$spr_{\mathbf{R}}(G) \geq \frac{1}{p} - \frac{1}{n-1} \ . \tag{17}$$

Equality holds if $G \cong K_n$.

Proof. Replace the matrix $\mathbf{M}$ in Lemma 7 by the matrix $\mathbf{B}$, defined via (13). □

Corollary 9. *Let G be a graph of order n such that $G \ncong K_n$. If $spr_{\mathbf{R}}(G)$ is defined as in (5), then*

$$spr_{\mathbf{R}}(G) \geq \frac{2\chi}{n-1} - 1 + \lambda_2(\mathbf{R}(G)) \ . \tag{18}$$

Proof. Considering $\mathbf{M} = \mathbf{R}(G)$ in Lemma 7, we have

$$1 - \lambda_n(\mathbf{R}(G)) \geq \frac{2\chi}{n-1} \ . \tag{19}$$

The inequality (18) is obtained by adding $\lambda_2(\mathbf{R}(G)) - 1$ at both sides of (19), and using the result in Lemma 5. □

The following result provides a connection between the Randić and Laplacian spreads of regular graphs.

Theorem 10. *Let G be a regular graph of order n and degree p. Let $spr_{\mathbf{L}}(G)$ and $spr_{\mathbf{R}}(G)$ be defined as in (3) and (5). Then $spr_{\mathbf{L}}(G) = p \cdot spr_{\mathbf{R}}(G)$.*

Proof. We know that for graphs G without singletons $spr_{\mathbf{R}}(G)$ and $spr_{\mathcal{L}}(G)$ coincide. Since $\mathcal{L}(G) = D^{-1/2}L(G)D^{-1/2}$ and G is a regular graph of degree p, $\mathbf{L}(G) = p\,\mathcal{L}(G)$. Then if ξ is a normalized Laplacian eigenvalue of G, $p\,\xi$ is a Laplacian eigenvalue of G. Therefore, $p \cdot spr_{\mathbf{R}}(G) = p \cdot spr_{\mathcal{L}}(G) = spr_{\mathbf{L}}(G)$. □

Corollary 11. *Let G be a regular graph of order n and degree p. Then*

$$spr_{\mathbf{L}}(G) \geq 1 - \frac{p}{n-1}\ .$$

Equality holds if $G \cong K_n$.

In order to use inequality (2) for obtaining another lower bound for the Randić spread, define

$$\Gamma(j) = \sum_{s \sim j} \frac{1}{d_s}$$

for $1 \leq j \leq n$. Note that if G is a regular graph, then $\Gamma(j) = 1$ for all $1 \leq j \leq n$.

Taking into account (2), we arrive at:

Theorem 12. *Let G be an arbitrary graph with n vertices and m edges. Then*

$$spr_{\mathbf{R}}(G)^2 \geq \max_{i<j} \left\{ 4\kappa\,(d_j + d_i)(1+\kappa m) - \kappa^2\,(d_j+d_i)^2 + \frac{2}{d_j}\,\Gamma(j) + \frac{2}{d_i}\,\Gamma(i) \right\} \qquad (20)$$

where κ is equal to the right–hand side of either Eq. (9) or Eq. (14) or also satisfying the requisite of Remark 1.

Proof. For simplicity we set $\mathbf{C} = \mathbf{R}(G) + \kappa\, w\, w^t$. Because of equalities (15), it is sufficient to show that $s(\mathbf{C})$ satisfies the inequality (20). By (2), we get

$$\begin{aligned} s(\mathbf{C})^2 \;\; &\geq \;\; \kappa^2\,(d_j - d_i)^2 + 2\sum_{s \sim j} \frac{(1+\kappa\, d_s\, d_j)^2}{d_s\, d_j} \\ &+ \;\; 2\kappa^2\, d_j \sum_{s \nsim j} d_s + 2\sum_{s \sim i} \frac{(1+\kappa\, d_s\, d_i)^2}{d_s\, d_i} + 2\kappa^2\, d_i \sum_{s \nsim i} d_s \end{aligned}$$

$$\begin{aligned}
&= \kappa^2\,(d_j-d_i)^2 + 2\kappa^2\,d_j \sum_{s\sim j} d_s + \frac{2}{d_j}\sum_{s\sim j}\frac{1}{d_s} + 4d_j\,\kappa + 2\kappa^2\,d_j \sum_{s\nsim j} d_s \\
&+ \; 2\kappa^2\,d_i \sum_{s\sim i} d_s + \frac{2}{d_i}\sum_{s\sim i}\frac{1}{d_s} + 4d_i\,\kappa + 2\kappa^2\,d_i \sum_{s\nsim i} d_s \\
&= \kappa^2\,(d_j-d_i)^2 + 2\kappa^2\,d_j\,(2m-d_j) + 2\kappa^2\,d_i\,(2m-d_i) \\
&+ \; 4\kappa\,(d_j+d_i) + \frac{2}{d_j}\,\Gamma(j) + \frac{2}{d_i}\,\Gamma(i) \\
&= 4\kappa\,(d_j+d_i)(1+\kappa\,m) - \kappa^2\,(d_j+d_i)^2 + \frac{2}{d_j}\,\Gamma(j) + \frac{2}{d_i}\,\Gamma(i)\;.
\end{aligned}$$

Due to the symmetry of the latter formula, we can impose $i<j$. □

Remark 3. *If G is a regular graph of order n and degree p, then the lower bound (20) becomes*

$$spr_{\mathbf{R}}(G) \geq \frac{2}{np}\,\sqrt{(n-1-p)(pn+p+1)}\;.$$

Thus

$$spr_{\mathbf{L}}(G) \geq \frac{2}{n}\,\sqrt{(n-1-p)(pn+p+1)}\;.$$

Note that for $G \cong K_n$ the equality holds for both expressions.

Remark 4. *Let G be an arbitrary graph with n vertices and m edges. For $\kappa<0$ define the auxiliary function*

$$\begin{aligned}
f(\kappa) &= 4\kappa\,(d_j+d_i)(1+\kappa m) - \kappa^2\,(d_j+d_i)^2 + \frac{2}{d_j}\,\Gamma(j) + \frac{2}{d_i}\,\Gamma(i) \\
&= \frac{d_i+d_j}{4m-(d_i+d_j)}\,\left[(4m-(d_i+d_j))\,\kappa+2\right]^2 \\
&+ \; \frac{2}{d_j}\,\Gamma(j) + \frac{2}{d_i}\,\Gamma(i) - \frac{4}{4m-(d_i+d_j)}\;.
\end{aligned}$$

Its global minimum is at

$$\kappa_{\min} = -\frac{2}{4m-(d_i+d_j)}\;.$$

Note that if $G \cong K_n$, then $\kappa_{\min} = \beta_{pq} = \beta$ where β_{pq} and β are defined by Eqs. (9) and (14), respectively. Thus, a simple method to improve an obtained lower bound is to use either the smallest κ or the greatest known κ.

Remark 5. *If $\lambda_n(\mathbf{R}(G)) \leq \xi \leq \lambda_2(\mathbf{R}(G))$, then by replacing κ in (20) by the expression (11), we get*

$$spr_{\mathbf{R}}(G)^2 \geq \max_{i<j} \left\{ \frac{\xi^2-1}{m}(d_j+d_i) - \frac{1}{4m^2}(\xi-1)^2\,(d_i+d_j)^2 + \frac{2}{d_j}\Gamma(j) + \frac{2}{d_i}\Gamma(i) \right\}.$$

For $G \ncong K_n$ and $\xi = 0$, this lower bound becomes

$$spr_{\mathbf{R}}(G)^2 \geq \max_{i<j} \left\{ \frac{2}{d_j}\Gamma(j) + \frac{2}{d_i}\Gamma(i) - \frac{d_j+d_i}{m}\left(1+\frac{1}{4m}(d_i+d_j)\right) \right\}. \tag{21}$$

Example 1. *Let $K_{r,s}$, $r,s \geq 1$, denote the complete bipartite graph with bipartition X (of cardinality r) and Y (of cardinality s). Then*

$$\sigma(\mathbf{R}(K_{r,s})) = \left\{1\,,\,0^{(r+s-2)}\,,\,-1\right\}.$$

By Remark 1, we may take either the least or the second greatest eigenvalue. In this way κ is defined as

$$\kappa(-1) = \frac{1}{2rs}(-1-1) = -\frac{1}{rs}\,.$$

Then

$$\Gamma(j) = \begin{cases} s/r & \text{if } j \in X \\ r/s & \text{if } j \in Y \end{cases}$$

for all $1 \leq j \leq n$. Suppose that $i \in X$ and $j \in Y$. By evaluating the lower bound in Theorem 12 we get

$$\begin{aligned} spr_{\mathbf{R}}(K_{r,s}) &\geq \sqrt{\frac{2(r+s)}{r^2\,s^2}\left(2rs - \frac{r+s}{2}\right) - \frac{4(r+s)}{rs} + \frac{2}{r}\cdot\frac{r}{s} + \frac{2}{s}\cdot\frac{s}{r}} \\ &= \sqrt{-\left(\frac{r+s}{rs}\right)^2 + \frac{2}{s} + \frac{2}{r}} = \sqrt{\left(\frac{1}{s}+\frac{1}{r}\right)\left(2-\frac{1}{s}-\frac{1}{r}\right)}\,. \end{aligned}$$

By setting $r = s$,

$$spr_{\mathbf{R}}\left(K_{r,r}\right) \geq 2\sqrt{\frac{1}{r}-\frac{1}{r^2}}\,. \tag{22}$$

By setting $r = 1$ and $s = n-1$, we arrive at the expression for the Randić spread of the n-vertex star:

$$spr_{\mathbf{R}}\left(K_{1,n-1}\right) \geq \sqrt{1-\frac{1}{(n-1)^2}}\,.$$

If we use

$$\kappa(0) = \frac{1}{2rs}(-1) = -\frac{1}{2rs}$$

then by (21) we obtain

$$spr_{\mathbf{R}}(K_{r,s}) \geq \sqrt{\left(\frac{1}{s}+\frac{1}{r}\right)\left(1-\frac{1}{4}\left(\frac{1}{s}+\frac{1}{r}\right)\right)}$$

and

$$spr_{\mathbf{R}}(K_{r,r}) \geq \sqrt{\frac{2}{r}\left(1-\frac{1}{2r}\right)} = \sqrt{\frac{2}{r}-\frac{1}{r^2}}$$

which, for $r \geq 2$*, is a weaker lower bound than (22).*

4 Comparing the bounds for Randić spread

In this section, we compare the estimates obtained by Theorem 2 (upper bound (6)), Theorem 4 (lower bound (12)), Theorem 12 (lower bound (15)), and Corollary 8 (lower bound (17)), with the actual Randić spread. Our values pertain to complete bipartite graphs, $K_{r,s}$. In the following table, ee is the relative error, defined as usual:

$$ee = \frac{|spr_{\mathbf{R}}(G) - bound|}{spr_{\mathbf{R}}(G)}$$

G	$spr_{\mathbf{R}}(G)$	(6)	ee	(12)	ee	(15)	ee	(17)	ee
$K_{1,4}$	1	2	1	0.5	0.500	**0.8268**	0.173	−−	0.688
$K_{1,5}$	1	2	1	0.5528	0.447	**0.8283**	0.172	−−	0.668
$K_{1,7}$	1	2	1	0.6220	0.378	**0.8283**	0.172	−−	0.644
$K_{7,8}$	1	2	1	**0.8664**	0.134	0.5144	0.486	−−	0.937
$K_{11,13}$	1	2	1	**0.9164**	0.084	0.4164	0.584	−−	0.958
$K_{3,4}$	1	2	1	0.7113	0.289	**0.7333**	0.267	−−	0.874
$K_{100,200}$	1	2	1	**0.9929**	0.007	0.1411	0.859	−−	0.968
$K_{6,6}$	1	2	1	**0.8333**	0.167	0.5521	0.448	0.0758	0.924
$K_{15,15}$	1	2	1	**0.9333**	0.067	0.3590	0.641	0.0322	0.968
$K_{31,31}$	1	2	1	**0.9677**	0.032	0.2519	0.748	0.0159	0.984

Analyzing the above examples, we observe the following:

- In the class of stars (i.e., $r = 1, s = n - 1$), the lower bound (15), given by Theorem 12, is the best.
- In the class of the regular graphs (i.e., $r = s$), the best results are obtained by formula (12) of Theorem 4.

- In any case, the approximation given by the best lower bound is better, when $r+s=n$ is greater.

5 Randić matrix and spread of join of two graphs

Let G_1 and G_2 be two graphs with disjoint vertex sets. Their join, denoted by $G_1 \vee G_2$, is the graph obtained from the union of G_1 and G_2, by joining all vertices of G_1 with all vertices of G_2.

Example 2. *For $i=1,2$, let G_i be a p_i-regular graph on n_i vertices with $p_i \geq 0$, $n_i \geq 1$. Then*

$$\mathbf{R}(G_1 \vee G_2) = \begin{pmatrix} \frac{1}{p_1+n_2}\mathbf{A}(G_1) & \frac{\mathbf{e}_{n_1}\mathbf{e}_{n_2}^t}{\sqrt{(p_1+n_2)(p_2+n_1)}} \\ \frac{\mathbf{e}_{n_2}\mathbf{e}_{n_1}^t}{\sqrt{(p_1+n_2)(p_2+n_1)}} & \frac{1}{p_2+n_1}\mathbf{A}(G_2) \end{pmatrix}.$$

It is easy to obtain

$$\chi(G_1 \vee G_2) = \frac{1}{2}\left(\frac{n_1 p_1}{p_1+n_2} + \frac{n_2 p_2}{p_2+n_1} + \frac{2n_1 n_2}{\sqrt{(p_1+n_2)(p_2+n_1)}}\right).$$

Because $G_1 \vee G_2$ is connected, the Randić spectral radius 1 is a simple eigenvalue whose corresponding eigenvector is

$$w = \left(\sqrt{p_1+n_2}\,\mathbf{e}_{n_1}^t \quad \sqrt{p_2+n_1}\,\mathbf{e}_{n_2}^t\right)^t.$$

A short calculation shows that

$$ww^t = \begin{pmatrix} (p_1+n_2)\,\mathbf{e}_{n_1}\mathbf{e}_{n_1}^t & \sqrt{(n_2+p_1)(n_1+p_2)}\,\mathbf{e}_{n_1}\mathbf{e}_{n_2}^t \\ \sqrt{(n_2+p_1)(n_1+p_2)}\,\mathbf{e}_{n_2}\mathbf{e}_{n_1}^t & (p_2+n_1)\,\mathbf{e}_{n_2}\mathbf{e}_{n_2}^t \end{pmatrix}.$$

Let

$$\mathbf{S} = \begin{pmatrix} \frac{p_1}{p_1+n_2} & \frac{\sqrt{n_1 n_2}}{\sqrt{(p_1+n_2)(p_2+n_1)}} \\ \frac{\sqrt{n_1 n_2}}{\sqrt{(p_1+n_2)(p_2+n_1)}} & \frac{p_2}{p_2+n_1} \end{pmatrix}.$$

Then

$$\sigma(\mathbf{S}) = \{1, \det \mathbf{S}\}.$$

By applying a lemma of Fiedler (see [7]*), the spectrum of $R(G_1 \vee G_2)$ becomes*

$$\sigma\left(\frac{1}{p_1+n_2}\mathbf{A}(G_1)\right) \cup \sigma\left(\frac{1}{p_2+n_1}\mathbf{A}(G_2)\right) \cup \sigma(S) \setminus \left\{\frac{p_1}{p_1+n_2}, \frac{p_2}{p_2+n_1}\right\}. \tag{23}$$

Lemma 13. *Let G_1 and G_2 be graphs of order n_1 and n_2, respectively. Then*

$$\lambda_2(\mathbf{R}(G_1 \vee G_2)) = \max\left\{\lambda_2\left(\frac{1}{p_1+n_2}\,\mathbf{A}(G_1)\right),\ \lambda_2\left(\frac{1}{p_2+n_1}\,\mathbf{A}(G_2)\right)\right\}. \qquad (24)$$

Proof. If $G_1 \ncong K_{n_1}$ or if $G_2 \ncong K_{n_2}$, then by Lemma 5, $\lambda_2(\mathbf{R}(G_1 \vee G_2)) \geq 0$. Since

$$\det \mathbf{S} = \frac{p_1\,p_2 - n_1\,n_2}{(p_1+n_2)(p_2+n_1)}\ .$$

is negative, by using (23) the result follows. On the other hand if $G_1 \cong K_{n_1}$ and $G_2 \cong K_{n_2}$ then $G_1 \vee G_2 \cong K_{n_1+n_2}$ and

$$\lambda_2(\mathbf{R}(G_1 \vee G_2)) = \lambda_2\left(\frac{1}{p_1+n_2}\,\mathbf{A}(G_1)\right) = \lambda_2\left(\frac{1}{p_2+n_1}\,\mathbf{A}(G_2)\right) = -\frac{1}{n_1+n_2-1}\ .$$

□

Theorem 14. *For $i = 1,2$, let G_i be a p_i-regular graph on n_i vertices with $p_i \geq 0$, $n_i \geq 1$. If*

$$\widetilde{\delta}_1 = \left|\lambda_2\left(\frac{1}{p_1+n_2}\,\mathbf{A}(G_1)\right) - \frac{p_1\,p_2 - n_1\,n_2}{(p_1+n_2)\,(p_2+n_1)}\right|$$

$$\widetilde{\delta}_2 = \left|\lambda_2\left(\frac{1}{p_2+n_1}\,\mathbf{A}(G_2)\right) - \frac{p_1\,p_2 - n_1\,n_2}{(p_1+n_2)\,(p_2+n_1)}\right|$$

then

$$spr_{\mathbf{R}}\,(G_1 \vee G_2) \geq \max\left\{\widetilde{\delta}_1, \widetilde{\delta}_2\right\}.$$

Proof. The result follows from (24) by noting that by (23), $\det \mathbf{S} = \frac{p_1\,p_2 - n_1\,n_2}{(p_1+n_2)(p_2+n_1)}$ is a Randić eigenvalue of $G_1 \vee G_2$. □

Remark 6. *If $G \cong K_{r,s}$, then $G \cong \overline{K}_r \vee \overline{K}_s$. In this case, $\widetilde{\delta}_1 = \widetilde{\delta}_2 = 1 = spr_R(K_{r,s})$.*

Concluding this paper, we offer a few examples, aimed at comparing the bounds in Lemma 7 and Theorem 14, calculated for $G_1 \vee G_2$. Our results are presented by the 4-tuple $\mathbf{g} = (g_1, g_2, g_3, g_4)$, where g_1 is the Randić spread of $G_1 \vee G_2$, g_2 is the lower bound of Theorem 12 by taken κ as a function of the least Randić eigenvalue of $G_1 \vee G_2$, g_3 is the lower bound of Theorem 12 by taken κ as a function of the Randić index χ, and g_4 is the lower bound obtained in Theorem 14.

$\mathbf{A}(G_1)$	$\mathbf{A}(G_2)$	$\mathbf{g}$
$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$	(0.7024 , 0.4853 , 0.4440 , 0.7024)
$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}$	(0.6111 , 0.4179 , 0.3532 , 0.5000)
$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$	(0.5415 , 0.3961 , 0.3756 , 0.5415)
$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$	(0.4000 , 0.3770 , 0.3383 , 0.2667)
$\begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix}$	(0.5000 , 0.3354 , 0.3166 , 0.5000)

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