On the Randić index of graphs *

C. Dalfó

Departament de Matemàtiques
Universitat Politècnica de Catalunya
Barcelona, Catalonia
cristina.dalfo@upc.edu

Abstract

For a given graph $G=(V,E)$, the degree mean rate of an edge $uv\in E$ is a half of the quotient between the geometric and arithmetic means of its end-vertex degrees $d(u)$ and $d(v)$. In this note, we derive tight bounds for the Randić index of G in terms of its maximum and minimum degree mean rates over its edges. As a consequence, we prove the known conjecture that the average distance is bounded above by the Randić index for graphs with order n large enough, when the minimum degree δ is greater than (approximately) $\Delta^{\frac{1}{3}}$, where Δ is the maximum degree. As a by-product, this proves that almost all random (Erdős-Rényi) graphs satisfy the conjecture.

Keywords: Edge degree rate, Randić index, connectivity index, mean distance.

MSC: 05C35, 05C90.

1 Background

We consider simple graphs $G=(V,E)$, with vertex set V and edge set E. Unless some distance parameters are considered, as in the next definitions, G is not necessarily connected, but we always assume that there are no

*This research is partially supported by the project 2017SGR1087 of the Agency for the Management of University and Research Grants (AGAUR) of the Government of Catalonia.

This research has also received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 734922.

isolated vertices. Given two vertices $u, v \in V$, let denote by $\mathrm{dist}(u,v)$ the distance between u and v. The *mean distance* of G is

$$\mu(G) = \frac{1}{n(n-1)} \sum_{u,v \in V} \mathrm{dist}(u,v).$$

Let $d(u)$ denote the degree of vertex u, and δ and Δ the minimum and maximum degree of G. The *Randić index* [9], also called connectivity index, of G is

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d(u)d(v)}}.$$

Fajtlowicz [6] conjectured that, for any (connected) graph G,

$$\mu(G) \leq R(G). \tag{1}$$

Besides, Caporossi and Hansen [5] generalized this conjecture by proposing the inequality

$$\mu(G) \leq R(G) - \left[\sqrt{n-1} - 2\left(1 - \frac{1}{n}\right)\right]. \tag{2}$$

Since then, some sufficient conditions have been given for these conjectures to hold. For instance, Li and Shi [7] proved that, for any $\epsilon \in (0,1)$, if G has minimum degree $\delta \geq \epsilon n$, then (1) holds for order n large enough. In fact, we show that this result is a consequence of our main theorem and the following bound for $\mu(G)$ in terms of δ (see Beezer, Riegsecker, and Smith [1]).

$$\mu(G) \leq \frac{n}{\delta + 1} + 2. \tag{3}$$

2 Bounds of the Randić index for graphs with given degree mean rate

Before giving our main result, we introduce the following concept. Given a graph $G = (V,E)$, the *degree mean rate* $\gamma(e)$ of an edge $e = uv \in E$ is a half of the quotient between the geometric and arithmetic means of its end-vertex degrees $d(u)$ and $d(v)$, that is,

$$\gamma(uv) = \frac{\sqrt{d(u)d(v)}}{d(u)+d(v)} = \frac{\sqrt{\frac{d(v)}{d(u)}}}{1 + \frac{d(v)}{d(u)}}.$$

Moreover, the maximum and minimum of this parameter over all the edges of G are denoted by

$$\Delta_E = \max_{uv \in E} \gamma(uv) \qquad \text{and} \qquad \delta_E = \min_{uv \in E} \gamma(uv).$$

Notice that

$$\frac{\sqrt{n-1}}{n} \le \delta_E \le \Delta_E \le \frac{1}{2}, \tag{4}$$

with lower and upper bounds attained, respectively, by (any edge of) the star $S_n (= K_{1,n-1})$ and a regular graph.

Theorem 2.1. *Let $G = (V, E)$ be a graph on n vertices, with given Δ_E and δ_E. Then, its Randić index $R(G)$ satisfies the following bounds:*

$$n\delta_E \le R(G) \le n\Delta_E. \tag{5}$$

Proof. Notice first that, as

$$\sum_{uv\in E}\left(\frac{1}{d(u)}+\frac{1}{d(v)}\right) = \frac{1}{2}\left(\sum_{u\in V} 1 + \sum_{v\in V} 1\right) = n,$$

for any given constant, say $\rho > 0$, the Randić index can be written as

$$R(G) = \rho + \sum_{uv\in E}\left[\frac{1}{\sqrt{d(u)d(v)}} - \frac{\rho}{n}\left(\frac{1}{d(u)}+\frac{1}{d(v)}\right)\right]. \tag{6}$$

Moreover, the function

$$z = f(x,y) = \frac{1}{\sqrt{xy}} - \frac{\rho}{n}\left(\frac{1}{x}+\frac{1}{y}\right)$$

takes zero value at the straight lines with equations $y = \alpha x$ and $y = \beta x$, where

$$\alpha = \frac{\frac{n}{2}(n - \sqrt{n^2-4\rho^2}) - \rho^2}{\rho^2};$$
$$\beta = \frac{\frac{n}{2}(n + \sqrt{n^2-4\rho^2}) - \rho^2}{\rho^2} = \alpha^{-1}.$$

Figure 1 (left) shows the function $z = f(x,y)$, when $n = 20$ and $\rho = 8$, for the region of interest $1 \le x, y \le n-1$. Besides, it happens that $f(x,y) \ge 0$ insides the region where $\alpha \le \frac{y}{x} \le \beta$ (corresponding to the regions (*II*) and (*III*) in Figure 1 (right)), and $f(x,y) \le 0$ otherwise.

Now, let us go back to (6) by taking $x = d(u)$ and $y = d(v)$ and, without loss of generality (because of the symmetry of $f(x,y)$), assume that $d(u) \ge d(v)$. If, for some $\rho > 0$, we have

$$(1 \ge)\, a = \min_{uv\in E} \frac{d(v)}{d(u)} = \alpha, \tag{7}$$

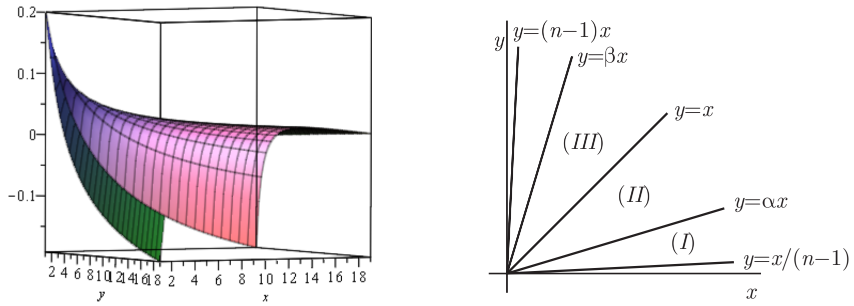

Figure 1: Left: The function $z = f(x, y)$, when $n = 20$ and $\rho = 8$, for the region of interest $1 \leq x, y \leq n-1$. Right: The different regions of $z = f(x, y)$ in the plane xy.

then all the other values of $\frac{d(v)}{d(u)}$ are inside of the cone, in the region (II) in Figure 1. Hence, $R(G) \geq \rho$. Otherwise, if, for some $\rho > 0$, we have

$$\left(\tfrac{1}{n-1} \leq\right) b = \max_{uv \in E} \frac{d(v)}{d(u)} = \alpha, \tag{8}$$

then all the other values of $\frac{d(v)}{d(u)}$ are outside of the cone, in the region (I) in Figure 1. Hence, $R(G) \leq \rho$. Then, solving for ρ (positive), we see that the conditions (7) and (8) are equivalent, respectively, to

$$\rho = \frac{n\sqrt{a}}{a+1} = n\delta_E; \tag{9}$$

$$\rho = \frac{n\sqrt{b}}{b+1} = n\Delta_E. \tag{10}$$

The above equalities are due to the fact that the function $\phi(x) = \frac{\sqrt{x}}{x+1}$ is increasing for $x \in (0, 1)$. Thus, the best lower and upper bounds in (5) are given, respectively, by (9) and (10). This completes the proof. □

Note that the graphs G that satisfy $n\delta_E = R(G) = n\Delta_E$ are those whose ratio $d(v)/d(u)$ is constant for every edge. In this case, $a = b$ (see (7) and (8)), and then $\delta_E = \Delta_E = \sqrt{a}/(1+a)$ and $R(G) = n\sqrt{a}/(1+a)$. An example is given by the complete bipartite graphs K_{n_1,n_2} having $R(K_{n_1,n_2}) = \sqrt{n_1 n_2}$. Another example is provided by the trees T_p, for $p = 1, 2, \ldots$, with sets of vertices $V_0, V_1, \ldots, V_p$, such that V_0 is a singleton with degree 2^p, and every vertex of V_i (with degree 2^{p-i}) is adjacent to one vertex of V_{i-1} and $2^{p-i} - 1$ vertices of V_{i+1}. Thus, every edge of T_p, say uv with $u \in V_i$ and $v \in V_{i+1}$, has $\frac{d(v)}{d(u)} = \frac{2^{p-i-1}}{2^{p-i}} = \frac{1}{2}$, so $\delta_E = \Delta_E = \sqrt{2}/3$ and $R(T_p) = n\sqrt{2}/3$. See the example of T_3 in Figure 2 (f).

See Table 1 for the values of the Randić index and the given bounds for the graphs of Figure 2 (a)–(e).

Graph	$n\delta_E$	$R(G)$	$n\Delta_E$
(a)	5.629	5.974	6.128
(b)	2.828	2.914	3
(c)	2.449	2.710	3.5
(d)	2.904	2.957	3
(e)	2.710	2.834	2.981

Table 1: Values of $n\delta_E$, $R(G)$ and $n\Delta_E$ for the graphs of Figure 2 (a)–(e).

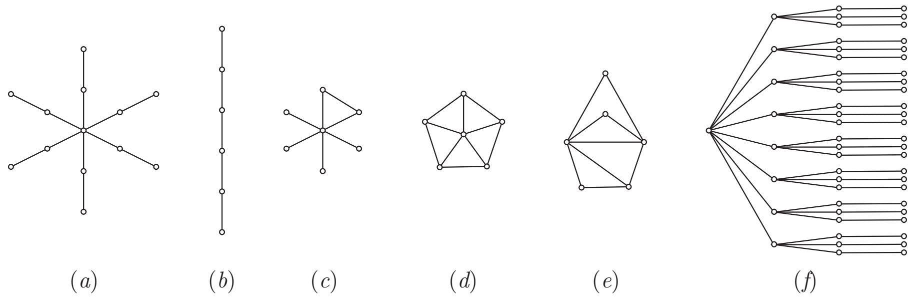

Figure 2: The graphs (a)–(e) correspond to Table 1, and (f) is the tree T_3 satisfying $n\delta_E = R(G) = n\Delta_E$.

As a corollary of Theorem 2.1, we obtain the following known result (see Bollobás and Erdős [3], or Pavlović and Gutman [8], or Caporossi, Gutman, Hansen, and Pavlović [4]).

Corollary 2.2. *The Randić index of any graph G satisfies*

$$\sqrt{n-1} \leq R(G) \leq \frac{n}{2}.$$

Moreover, the lower bound is attained if and only if $G = K_{1,n}$ (or star graph), and the upper bound is attained if and only if all components of G are regular (not necessarily with equal degree of regularity).

Proof. The lower and upper bounds come from (4). Besides, $G = K_{1,n}$ if and only if, in the proof of Theorem 2.1, $a = b = 1/(n-1)$, that is, $R(G) = n\delta_E = n\Delta_E = \sqrt{n-1}$. Analogously, all components of G are regular if and only $a = b = 1$, that is, $R(G) = n\delta_E = n\Delta_E = \frac{n}{2}$. $\square$

Another consequence of Theorem 2.1 is a sufficient condition for the conjecture $\mu(G) \leq R(G)$ to hold.

Corollary 2.3. *Let G be a graph with minimum degree δ satisfying*

$$\delta \geq \frac{n}{n\delta_E - 2} - 1. \tag{11}$$

Then, its Randić index satisfies $\mu(G) \leq R(G)$.

Proof. Apply Theorem 2.1 by using the bound for $\mu(G)$ in (3). $\square$

In particular, if $\frac{n\sqrt{\delta/\Delta}}{1+\delta/\Delta} \geq \frac{n}{\delta+1} + 2$, as $\delta_E \geq \frac{\sqrt{\delta/\Delta}}{1+\delta/\Delta}$, then we have

$$\mu(G) \leq \frac{n}{\delta+1} + 2 \leq \frac{n\sqrt{\delta/\Delta}}{1+\delta/\Delta} \leq n\delta_E \leq R(G). \tag{12}$$

So, one see that the conjecture $\mu(G) \leq R(G)$ holds, for n large enough, when δ is greater than (approximately) $\Delta^{\frac{1}{3}}$. Indeed, dividing by n the second inequality in (12), we only need to show that

$$\frac{1}{\delta+1} < \frac{\sqrt{\delta/\Delta}}{1+\delta/\Delta}$$

or, equivalently, $\sqrt{\Delta/\delta} + \sqrt{\delta/\Delta} - 1 < \delta$, which holds when $\Delta < \delta^3$ since $\delta/\Delta \leq 1$.

Moreover, Corollary 2.3 implies the result of Li and Shi [7]:

Corollary 2.4. *For any given $\epsilon \in (0,1)$, if G is a (connected) graph with order n and minimum degree $\delta \geq \epsilon n$, then its Randić index satisfies $\mu(G) \leq R(G)$ for sufficiently large n.*

Proof. Since $\delta \geq \epsilon n$ and $\Delta \leq n-1$, we have that $\delta_E \geq \frac{\sqrt{n(n-1)\epsilon}}{n(\epsilon+1)-1}$. Then, for n large enough (for the second inequality to hold), we have

$$\delta \geq n\epsilon \geq \frac{n}{n\frac{\sqrt{n(n-1)\epsilon}}{n(\epsilon+1)-1} - 2} - 1 \geq \frac{n}{n\delta_E - 2} - 1 \tag{13}$$

and Corollary 2.3 gives the result. $\square$

To have an idea about the lower bound for n, notice that the second inequality in (13) gives (approximately) $n \geq \epsilon^{-3/2}$. Indeed, for large n, such inequality holds if $n\epsilon > \frac{n}{\frac{\sqrt{n(n-1)\epsilon}}{\epsilon+1}}$, that is, $\epsilon > \frac{\epsilon+1}{n\sqrt{\epsilon}}$ or $n > \epsilon^{-1/2} + \epsilon^{-3/2}$ that, for small values of ϵ, can be approximated by $n > \epsilon^{-3/2}$, as claimed.

In Table 2 we have listed, for $\epsilon = 1/r$ and $r = 2, \ldots, 20$, the bound on n given by the second inequality in (13) considering the equality, and its approximation $\epsilon^{-3/2}$. Notice that, for $\epsilon \leq 1/13$, the latter always applies.

Now we consider a random graph G from the standard Erdős-Rényi model $\mathcal{G}(n,p)$. That is, G has n vertices and each edge appears independently with probability p. Then, the condition $\delta > \Delta^{\frac{1}{3}}$ implies the following result.

ϵ	bound on n from (13)	$\epsilon^{-3/2}$
1/2	7.4	2.8
1/3	9.6	5.2
1/4	12.2	8
1/5	15.1	11.2
1/6	18.2	14.7
1/7	21.7	18.5
1/8	25.3	22.6
1/9	29.2	27
1/10	33.3	31.6
1/11	37.6	36.5
1/12	42.1	41.6
1/13	46.8	46.9
1/14	51.7	52.4
1/15	56.8	58.1
1/16	62.1	64
1/17	67.6	70.1
1/18	73.2	76.4
1/19	79	82.8
1/20	84.9	89.4

Table 2: Comparison between the bounds for n required by the second inequality in (13) when considering the equality, and its approximation $\epsilon^{-3/2}$.

Corollary 2.5. *Given any $p > 0$ almost every graph G in $\mathcal{G}(n,p)$ satisfies $\mu(G) \leq R(G)$.*

Proof. It is known that, in the Erdős-Rényi model, almost all graphs G have maximum degree

$$\Delta(G) = p(n-1) + (2pqn\log n)^{\frac{1}{2}} + o((n\log n)^{\frac{1}{2}})$$

where $q = 1-p$. (See Bollobás [2]).

Since the minimum degree of G is $n-1$ minus the maximum degree of the complement of G, this implies that almost all graphs G in $\mathcal{G}(n,p)$ have minimum degree

$$\begin{aligned}\delta(G) &= n-1-p(n-1) - (2pqn\log n)^{\frac{1}{2}} + o((n\log n)^{\frac{1}{2}}) \\ &= q(n-1) - (2pqn\log n)^{\frac{1}{2}} + o((n\log n)^{\frac{1}{2}}).\end{aligned}$$

Now, the result follows from the fact that

$$\frac{\Delta(G)}{\delta(G)^3} \overset{n\to\infty}{\longrightarrow} 0.$$

$\square$

In a similar way as done for the Randić index, we could find lower and upper bounds for the *generalized Randić index*

$$R_\alpha(G) = \sum_{uv \in E} (d(u)d(v))^\alpha,$$

where now α is an arbitrary real number (the standard Randić index corresponds to $\alpha = -1/2$). More precisely, the same method applies from the following equality:

$$R_\alpha(G) = \rho + \sum_{uv \in E} \left[(d(u)d(v))^\alpha - \frac{\rho}{n} \left(\frac{1}{d(u)} + \frac{1}{d(v)} \right) \right].$$

References

[1] R. A. Beezer, J. E. Riegsecker, and B. A. Smith, Using minimum degree to bound average distance, *Discrete Math.* **226** (2001) 365–371.

[2] B. Bollobás, Degree sequences of random graphs, *Discrete Math.* **33** (1981) 1–19.

[3] B. Bollobás and P. Erdős, Graphs of extremal weights, *Ars Combin.* **50** (1998) 225–233.

[4] G. Caporossi, I. Gutman, P. Hansen, and L. Pavlović, Graphs with maximum connectivity index, *Comput. Biol. Chem.* **27** (2003) 85–90.

[5] G. Caporossi and P. Hansen, Variable neighborhood search for extremal graphs 1: The AutographiX system, *Discrete Math.* **212** (2000) 29–44.

[6] S. Fajtlowicz, On conjectures of Graffiti, *Discrete Math.* **72** (1988), 113–118.

[7] X. Li and Y. Shi, Randić index, diameter and average distance, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 425–431.

[8] L. Pavlović and I. Gutman, Graphs with extremal connectivity index, *Novi Sad J. Math.* **31** (2001) 53–58.

[9] M. Randić, Characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.