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The Randić index and other Graffiti parameters of graphs

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Abstract

Many graph parameters are of interest for both chemists and mathematicians, especially when they are related to the degrees, the distances, or the eigenvalues of the adjacency matrix of the graph. Fajtlowicz developed a program called Graffiti which proposes conjectures obtained by comparing such parameters. We prove or disprove some of these conjectures and give a short survey on general results concerning one of them, the Randić index.

1. Introduction

Graphs are mathematical objects which can modelize various kinds of problems. In chemistry, they are used to represent molecular structures. In particular it has been observed that there is a relationship between the value of some graph parameters and physical or chemical properties of the molecule represented by the graph. For instance, Wiener [14, 15] and later Randić [12] observed a correlation between the boiling point of some hydrocarbons and the geometrical structure of their molecule, more precisely their "branching degree" (with the intuitive meaning that a star is more branched than a path). This led them to propose a graph parameter (the sum of all the distances, also called Wiener index, or the branching index, later called Randić index), as a measure of the branching degree of a tree. These parameters, as many others, are also of interest for mathematicians who extend their study from chemical graphs to all graphs (see for instance [4, 7, 11]). As the Wiener index or the Randić index, most of them are related to the degrees or the distances in the graph.

From 1984, Fajtlowicz developed an automated system named *Graffiti*. This program makes conjectures by comparing simple functions of graph parameters. They are tested on a data basis consisting of some families of graphs. When a new family disproves a conjecture, it is added to the data basis. Among the conjectures having successfully passed the test, those which are trivial consequences of other ones are eliminated. The remaining ones constitute a list called *Written on the Wall* which can be found in [9]. Note that for material reasons explained in the introduction of [9], some conjectures of the list, among them some conjectures which are proved or disproved in sections 2 and 3, do not appear in the last version. They can be found in earlier versions of Written on the Wall.

Many papers directly or undirectly related to Graffiti conjectures have already been published (see a bibliography in [9]). In Sections 2 and 3 of this paper we respectively prove or disprove some of them. In Section 4, specially devoted to the Randić index, we resume some known results and open problems concerning this parameter.

We first give below some definitions and notation related to a vector or to a graph.

Let $A = (a_1, \ldots, a_n)$ be a vector with real coordinates a_i. The *sum* of A is equal to $a_1 + a_2 + \cdot + a_n$ and its *mean* is $\text{sum}(A)/n$. The *deviation* of A is the square root of its *variance* where $\text{variance}(A) = (\sum_{1\le i\le n} (a_i - \text{mean}(A))^2)/n$. A classical probability formula is $\text{variance}(A) = \text{mean}(A^2) - (\text{mean}(A))^2$. The *length* of A is equal to $\sqrt{\sum_{1\le i\le n} a_i^2}$. The *inverse* of A is the sum of the inverses of the non-zero coordinates. The *range* of A is the number of distinct coordinates. The *scope* of A is the difference between the largest coordinate and the smallest one. A *mode* of A is a coordinate which occurs most often and the *maximal frequency* is the frequency of any mode. When a sentence contains the word "mode", it is necessary to specify if we consider a particular mode or any mode of A. All these parameters related to the vector A only depend on the collection of the coordinates of A and not on their order.

Let $G = (V, E)$ be a simple undirected connected graph where V is the set of vertices and E the set of edges. The order n of G is the cardinality of V, its size m is the cardinality of E. The neighbourhood of a vertex i is $N(i) = \{j \in V;$ the edge ij is in $E\}$. The *complement* $\overline{G}$ of G has the same vertex set V as G and ij an edge of $\overline{G}$ if and only if it is not an edge of G. An *independent set* of G is a set of mutually non-adjacent vertices and a *clique* is a set of mutually adjacent vertices. The maximum cardinalities of an independent set and of a clique are respectively denoted by α and ω. Note that $\omega(G) = \alpha(\overline{G})$. The *chromatic number* χ of G is the smallest number of classes in a partition of V into independent sets. A *matching* of G is a set of mutually non-adjacent edges. The *matching number* ν is the size of a largest matching. A *perfect matching* of G is a matching spanning V.

The *degree* $d(i)$ or d_i of a vertex i is the number of neighbours of i. It can be easily seen that in any graph

$$\sum_{i\in V} d_i = 2m \qquad \text{and} \qquad \sum_{i\in V} d_i^2 = \sum_{ij\in E} (d_i + d_j) \qquad (1).$$

The *dual degree* $d^*(i)$ or d_i^* of the vertex i is the mean of the degrees of the neighbours of i. Again it can be seen that in any graph

$$d_i d_i^* = \sum_{j\in N(i)} d_j \text{ for every vertex } i \quad \text{and} \quad \sum_{i\in V} d_i d_i^* = \sum_{ij\in E} (d_i + d_j) \qquad (2).$$

The *deficiency* $df(i)$ of a vertex is the number of non-edges in the graph induced by the neighbours of i. The *temperature* of a vertex i is $t_i = d_i/(n - d_i)$. The vector *Dual Degree* (*Deficiency*, *Temperature*, respectively) of G has for components the n numbers d_i^* (df(i), t_i respectively). The *residue* R of a graph G of degree sequence $S:\ d_1 \geq d_2 \geq ... \geq d_n$ is the number of zeros obtained by the iterative process consisting, while $d_1 \neq 0$, in deleting the first term d_1 of S , subtracting 1 from the d_1 following ones and sorting down the new sequence. The *depth* is the number $n - R$ of steps in this algorithm. If we stop the process as soon as the sequence only contains the values 1 and 0 (the number of 1 being then necessarily even), this last sequence is a vector called the *1-Residue*. Note that R is equal to the number of 0 of the 1-Residue plus half its number of 1. If we stop the process at step number $\lfloor \text{depth}/2 \rfloor$, the resulting degree sequence is called the *Mid-Degree*.

A weight is often defined on the edges of a graph in relation to the degrees of the endvertices of the edges. The most usual ones are the inverse of the arithmetic mean and the inverse of the geometric mean of these degrees. This allows to define the *Harmonic* of G as $Hc = \sum_{xy\in E} \frac{2}{d(x) + d(y)}$ and its *Randić index* (also called *connectivity index* by some authors) as $Rc = \sum_{xy\in E} \frac{1}{\sqrt{d(x)d(y)}}$.

The *distance* $d(i,j)$ between two vertices i and j is the length of a shortest path joining i and j. The *mean distance* μ of a connected graph G is the average value of the distances between the $n(n-1)$ pairs of vertices. For a vertex i, *even(i)* is the number of vertices at even distance (including 0) from i and *odd(i)* is the number of vertices at odd distance from i. Clearly, even(i) + odd(i) = n for every vertex. The vector *Even* (*Odd* respectively) has the n numbers even(i) (odd(i) respectively) as coordinates. The *diameter* of G is $D = \max\{d(i,j);\ i,j \in V\}$ and its *radius* is $r = \min_{i\in V}\max_{j\in V} d(i,j)$. The *girth* of a graph is the length of a smallest cycle.

For a labelling $1,\dots,n$, of the vertices of G, the *adjacency matrix* A of G is the symmetric matrix with entries $a_{ij} = 1$ or 0 according as ij is or is not an edge of G. The *eigenvalues* of G are those of A. Note that their set does not depend on the chosen labelling of the vertices. Since A is real and symmetric these eigenvalues are real numbers which constitute the coordinates of the vector *Eigenvalue*. We denote them $\lambda_1 \geq \cdots \geq \lambda_n$. For any graph of size $m > 0$, they satisfy

$$\lambda_n < 0 < \lambda_1, \quad \sum_{1\leq i\leq n} \lambda_i = 0 \quad \text{and} \quad \lambda_1 \geq |\lambda_i| \quad \text{for} \quad 2 \leq i \leq n \qquad (3).$$

2. Proved conjectures

It is worth noting that the proofs of several conjectures of this section are corollaries of stronger results, sometimes involving simpler parameters than the conjecture itself.

Conjecture 546 Every graph G of size m satisfies mean(Deficiency) $\leq m/2$.

This is a corollary of the following result.

Theorem: Let G be a graph of order n and size m and let T be the number of induced subgraphs of G isomorphic to K_3. Then $\sum_{i\in V} df(i) \leq nm/2 - m - 3T/2$.

Proof Let t_i denote the number of triangles containing the vertex i and t_{ij} the number of triangles containing the edge ij. For any vertex i, we have $df(i) = \frac{d_i(d_i-1)}{2} - t_i$ thus $\sum_{i\in V} df(i) = 1/2\sum_{i\in V} d_i^2 - m - 3T$. Since $\sum_{i\in V} d_i^2 = \sum_{ij\in E}(d_i + d_j)$ from (1), and $d_i + d_j \leq n + t_{ij}$ for every edge ij of G, we get $\sum_{i\in V} d_i^2 \leq nm + 3T$ which gives the result. ■

Conjecture 140 Every graph G satisfies deviation(Eigenvalue) $\leq Hc$.

Proof Since deviation(Eigenvalue)$= \sqrt{(\sum_{i=1}^n \lambda_i^2)/n - ((\sum_{i=1}^n \lambda_i)/n)^2} = \sqrt{2m/n}$, we have to prove $Hc \geq \sqrt{2m/n}$. As any degree is at most $n-1$, $Hc = \sum_{ij\in E} \frac{2}{d_i + d_j} \geq \frac{m}{n-1}$. So the conjecture is true if $m/(n-1) \geq \sqrt{2m/n}$, that is if $m = 0$ or $m \geq 2n - 4 + 2/n$. Hence it is true in particular for $m = 0$, for $n = 2$ and for $m \geq 2n-3$. Suppose now $n \geq 3$ and $1 \leq m \leq 2n-4$. This implies $2m/n \leq 4m/(m+4)$. For every edge ij of any graph G we ave $d_i + d_j \leq m + 1$. Therefore $Hc \geq 2m/(m+1) \geq 2\sqrt{m/(m+4)} \geq \sqrt{2m/n}$. ■

Conjecture 288 Every graph G of girth ≥ 5 satisfies mean(Deficiency) $\leq \nu(\overline{G})$.

Proof Since the girth of G is at least 5, the neighbours of any vertex i form an independent set and i is their only common neighbour. As a consequence we obtain for any vertex i, $df(i) = d_i(d_i - 1)/2$, and thus mean(Deficiency)= $(\sum_{i \in V} d_i^2 - 2m)/2n$, and $\sum_{j \in N(i)} d_j \leq n - 1$. From (1) and (2), we get $d_i d_i^* = \sum_{j \in N(i)} d_j$ for every vertex i and since $\sum_{i \in V} d_i^2 = \sum_{i \in V} d_i d_i^*$, $\sum_{i \in V} d_i^2 \leq n(n-1)$. Therefore mean(Deficiency)$\leq \frac{1}{2n}(n(n-1) - 2m)$. On the other hand, by Vizing's Theorem, there exists a partition of the edges of $\overline{G}$ into at most $\Delta(\overline{G}) + 1$ matchings. Hence $\nu\overline{G} \geq \frac{m(\overline{G})}{\Delta(\overline{G}) + 1} = \frac{n(n-1) - 2m}{2(n - \delta)}$. The result follows with equality if and only if $\delta = 0$. ■

Conjecture 586 Every tree satisfies mean(Deficiency) $\leq$ max(Dual Degree).

Since in a tree, $m = n - 1$, this conjecture is a corollary of the following result.

Theorem Every K_3-free graph of maximum dual degree Δ^* satisfies

$$\text{mean(Deficiency)} \leq \frac{m}{n}(\Delta^* - 1) .$$

Proof As in the previous proof, the neighbourhood of any vertex is independent and mean Deficiency $= \frac{1}{2n}(\sum_{i \in V} d_i^2 - 2m) = \frac{1}{2n}(\sum_{i \in V} d_i d_i^* - 2m)$. Then we get by (1),

mean Deficiency $\leq \frac{1}{2n}(\Delta^* \sum_{i \in V} d_i - 2m) = \frac{m}{n}(\Delta^* - 1)$. ■

Conjecture 668 Every graph G such that sum(Even) $\leq$ sum(Odd) satisfies

$$\text{mean(Even)} \leq n - \nu .$$

Proof Since odd(x) + even(x) $= n$ for every vertex of G, the hypothesis is equivalent to the inequality sum(Even)$\leq n^2/2$, which implies mean(Even)$\leq n/2$. The result follows as $\nu(G) \leq n/2$ for any graph G. ■

Conjecture 687 Every graph G such that sum(Even) $\geq$ sum(Odd) satisfies

$$\text{mean(Even)} \geq \sqrt{m/n} .$$

This is a corollary of the following result.

Theorem Every graph G such that sum(Even) $\geq$ sum(Odd) satisfies

$$\text{mean(Even)} \geq \sqrt{m}\ .$$

Proof In any graph, odd(x) $\geq d(x)$ for every vertex x, thus implying sum(Odd)$\geq \sum_{x\in V} d(x) = 2m$. If sum(Even) $\geq$ sum(Odd) then sum(Odd)$\leq n^2/2$. Hence in this class, $m \leq n^2/4$ and mean(Even)$\geq n/2 \geq \sqrt{m}$. ■

Conjecture 272 Every graph satisfies deviation(Temperature) $\leq$ Max(Odd)/2.

Since max(Odd) $\geq \Delta$, this is an obvious corollary of the following result.

Theorem Every graph satisfies deviation(Temperature) $\leq \Delta/2$.

Proof Since the variance of any vector remains unchanged by translation, variance(Temperature)=variance(Temperature $-\Delta/2$). The coordinates t_i of the vector Temperature take their values in the interval $[\delta/(n-\delta),\ \Delta/(n-\Delta)] \subset [0,\Delta]$. Hence the coordinates $(t_i - \Delta/2)^2$ of the vector (Temperature$-\Delta/2)^2$ take their values in the interval $[0,(\Delta/2)^2]$. Therefore variance(Temperature $-\Delta/2$) $\leq$ mean((Temperature $-\ \Delta/2)^2$) $\leq \Delta^2/4$ and deviation(Temperature)= $\sqrt{\text{variance(Temperature)}} \leq \Delta/2$. ■

3. Disproved conjectures

All the conjectures which are disproved in this section are refuted by arbitrarily large graphs.

Conjecture 267 In any graph G, $\sqrt{\text{length(Dual Degree)}} \leq \chi(G) + \chi(\overline{G})$.

Counterexample Let G_p be a complete $p-$partite graph consisting of p independent sets, each of order p, along with all the edges joining them. This graph is $p(p-1)-$regular of order $n = p^2$. The dual degree of each vertex is thus $p(p-1)$ and length(Dual Degree)= $\sqrt{\sum_{1\leq i\leq n}(d_i^*)^2} = p(p-1)\sqrt{n} = p^2(p-1)$. Hence $\sqrt{\text{length(Dual Degree)}} = p\sqrt{p-1}$. On the other hand, $\chi(G_p) = \chi(\overline{G_p}) = p$. The graph G_p disproves Conjecture 267 as soon as $p > 5$. Moreover, the difference $\sqrt{\text{length(Dual Degree)}} - (\chi(G)+\chi(\overline{G}))$ can take arbitrarily large values.

Conjecture 599 In any K_3-free graph G, $n - \alpha(G) \leq \chi(G) + \chi(\overline{G})$.

It is known (proof of Conjecture 595) that in any K_3-free graph G, $\chi(\overline{G}) = n - \nu(G)$. Hence Conjecture 599 is equivalent to the following: in any K_3-free graph, $\nu(G) \leq \chi(G) + \alpha(G)$.

Counterexample Let H be any connected cubic graph of order $h \geq 8$. From H we construct another graph G as follows: we replace each vertex x of H by a graph $P'(x)$ isomorphic to a Petersen graph minus one vertex y and attach in a one-to-one correspondence the edges of H incident to x to the three neighbours of y in $P'(x)$. An example is shown in Figure 1. G is connected, triangle-free and cubic of order $n = 9h > 4$. Hence by Brooks' theorem, $\chi(G) \leq 3$. The edges of G coming from those of H form a matching and in every P' we can choose three more independent edges. Therefore $\nu(G) = \frac{n}{2}$. On the other hand $\alpha(G) \leq 4h$ since an independent set of G cannot countain more than four vertices of each P'. Hence $\nu(G) - (\chi(G) + \alpha(G)) \geq 9h/2 - (4h + 3)$ which is positive for $h > 6$ and can be arbitrarily large.

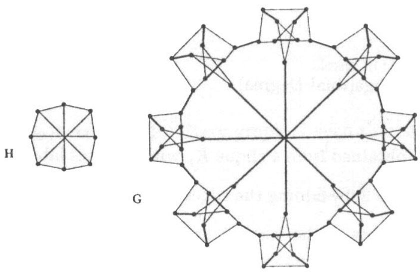

Figure 1

Conjecture 285 Every graph of girth $g \geq 5$ satisfies

$$\text{inverse(Dual Degree)} \leq \text{maximal frequency(Even)}.$$

Counterexample Let us consider the graph G_p of order $5p + 15$ consisting of p cycles C_5 of vertex sets $\{x_i u_i y_i w_i v_i\}$, $1 \leq i \leq p$, one cycle C_6 of vertex set $\{a_1 a_2 b_1 a_3 a_4 b_2\}$, one cycle C_7 of vertex set $= \{e_1 f_1 f_2 e_2 f_3 g f_4\}$ and two other vertices c and d along with the extra edges $(cb_i)_{i=1,2}$, cx_1 , $(y_i x_{i+1})_{1 \leq i \leq p-1}$, $y_p d$, $(de_i)_{i=1,2}$ (see Figure 2). The dual degrees of the vertices are respectively $d^*(c) = d^*(d) = d^*(u_i) = 3$, $d^*(b_i) = d^*(x_i) = d^*(y_i) = d^*(e_i) = 7/3$. $d^*(a_i) = d^*(v_i) = d^*(w_i) = d^*(f_i) = 5/2$ and $d^*(g) = 2$. Hence inverse(Dual Degree)$= \frac{p+2}{3} + \frac{3(2p+4)}{7} + \frac{2(2p+8)}{5} + \frac{1}{2} = \frac{418p+1277}{210}$. Let us now fix $p = 2k$ even with $k \geq 3$. By an easy calculation we can determine even(z) for each vertex z. We get even(a_i) = even(x_{2i-1}) = even(y_{2i-1}) = even$(d) = 5k + 7$, even(b_i) = even(u_{2i-1}) = even$(e_i) = 5k + 9$, even(c) = even(x_{2i}) = even(y_{2i}) = even(u_{2i}) = even$(g) = 5k + 8$. even(v_{2i}) = even(w_{2i-1}) = even$(f_i) = 5k + 6$, and even(v_{2i-1}) =

even(w_{2i}) $= 5k + 10$. Since $k \geq 3$, maximal frequency(Even)=$3k + 2$ (attained by the value $5k + 8$). Therefore inverse(Dual Degree)−maximal frequency(Even)= $(103p + 857)/210 > 0$, which disproves Conjecture 285. Moreover this difference can take arbitrarily large values.

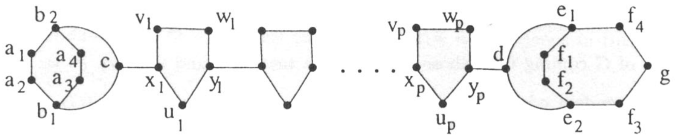

Figure 2

Conjecture 395 Every graph with $\alpha \leq 2$ satisfies

$$\text{range(Deficiency)} \leq \text{range(dual Degree)}.$$

Counterexample Let us consider the graph G_p obtained from a clique K_p with vertices labelled i, $1 \leq i \leq p$ and two other vertices labelled $p+1$, $p+2$ by adding the edges $(p+2, p+1)$, $(p+2, 1)$ and all the edges $(i, p+1)_{2 \leq i \leq p-2}$. The dual degrees of the vertices are $d^*(1) = d^*(p+1) = d^*(p+2) = p - 1$, $d^*(i) = p - \frac{4}{p}$ for $2 \leq i \leq p-2$, $d^*(p-1) = d^*(p) = p - \frac{1}{p-1}$. Thus range(Dual Degree)= 3 if $p \geq 5$. On the other hand $df(1) = p - 1$, $df(2) = \cdots = df(p-2) = 3$, $df(p-1) = df(p) = 0$, $df(p+1) = p - 3$, $df(p+2) = 1$ and range(Deficiency)= 5 if $p \geq 7$. Therefore for $p \geq 7$, the graph G_p is a counterexample to Conjecture 395.

Conjecture 678 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\text{mode(Degree)} \leq \chi(G) + \chi(\overline{G}).$$

Counterexample Let q be an even integer ≥ 10 and let G_q be obtained from the complete bipartite graph $K_{3q,2q}$ by adding the edges of a perfect matching in each of the two classes, A of order $3q$ and B of order $2q$. This graph has order $n = 5q$ and size $m = 6q^2 + 5q/2$. Since its diameter is 2, odd(v) $= d(v)$ and even(v) $= n - d(v)$ for every vertex v. Therefore sum(Odd)= $2m$ and sum(Even)= $n^2 - 2m$. Since $4m \leq n^2$ from $q \geq 10$, G_q satisfies sum(Odd) $\leq$ sum(Even). On the other hand, for the $3q$ vertices x of A, $d(x) = 2q + 1$, and for the $2q$ vertices y of B, $d(y) = 3q + 1$. Hence the vector Degree has a unique mode which is equal to $2q + 1$. Moreover,

$\chi(G) = 4$ and $\chi(\overline{G}) = 3q/2$. Therefore mode(Degree) $- (\chi(G) + \chi(\overline{G})) = q/2 - 3$ which is positive for $q \geq 10$ and can take arbitrarily large values.

We define now some infinite families of graphs, each of them is used to refute several conjectures.

Family A_p

Let A_p be the cartesian product $K_p \times K_3$, that is the graph obtained from three cliques K_p of respective vertex sets $\{x_i\}_{1 \leq i \leq p}$, $\{y_i\}_{1 \leq i \leq p}$, $\{z_i\}_{1 \leq i \leq p}$ by adding all the edges x_iy_i, y_iz_i, z_ix_i for $1 \leq i \leq p$.

Conjecture 185 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\text{length(Degree)} \geq m/\alpha.$$

Conjecture 191 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\text{min(Deficiency)} \leq m/\omega.$$

Counterexamples to Conjectures 185 and 191

The graph $G = A_p$ with $p \geq 13$ is vertex-transitive of degree $p + 1$ and order $n = 3p$. Its size is $m = 3p(p+1)/2$. Since its diameter is 2, sum(Odd)$= 2m$ and sum(Even)$= n^2 - 2m$ as already observed above, and thus sum(Odd)$\leq$ sum(Even). On the other hand, $\alpha = 3$ and $\omega = p$. Moreover, since $p \geq 13$, length(Degree)$= \sqrt{\sum_{i \in V} d_i^2} = (p+1)\sqrt{3p} < p(p+1)/2 = m/\alpha$ and the deficiency of any vertex is $df(x) = 2(p-1) > 3(p+1)/2 = m/\omega$. Hence for $p \geq 13$, A_p is a counterexample to Conjectures 185 and 191.

Family B_p

Let p be an integer ≥ 3 and let B_p be the graph consisting of a clique K_{2p-1}, an independent set $\overline{K}_p$ and a vertex x dominating all the other vertices. This graph has order $n = 3p$ and size $m = 2p^2$. Since its diameter is 2, sum(Odd)$= 2m$ and sum(Even)$= n^2 - 2m$ as observed above, and the vectors Degree and Odd are the same. Therefore B_p satisfies sum(Odd)$\leq$sum(Even) since $4m \leq n^2$. Moreover B_p has one vertex of degree $3p - 1$, p vertices of degree 1 and $2p - 1$ vertices of degree $2p - 1$. Hence the vector Degree have a unique mode which is equal to $2p - 1$, and mode(Even)$= n - (2p - 1) = p + 1$.

Conjecture 676 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\text{mode(Degree)} \leq n/2 .$$

Conjecture 679 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\text{mode(Degree)} \leq \text{mode(Even)} .$$

Conjecture 677 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\text{mode(Degree)} \leq n - \alpha .$$

Counterexamples to Conjectures 676 - 679 - 677

In the graph B_p, mode(Degree)$-n/2 = p/2 - 1$ and mode(Degree)$-$mode(Even)$= p - 2$. Since $p \geq 3$, B_p disproves Conjectures 676 and 679. Moreover, this graph shows that in the class under consideration, mode(Degree) $- n/2$ and mode(Degree)$-$mode(Even) can be arbitrarily large.

Let B'_p be the graph obtained from B_p by deleting one edge in the clique K_{2p-1}. In this operation, sum(Even)$-$sum(Odd) increases by 4 and B'_p still satisfies sum(Odd) $\leq$ sum(Even). Moreover, in B'_p, mode(Degree) remains equal to $2p - 1$ if $p > 6$, and $\alpha = p + 2$. Therefore $n - \alpha = p - 2 <$ mode(Degree), which disproves Conjecture 677.

<u>Family J_p</u>

Let J_p be the graph obtained from the disjoint union of a clique K_p and a star $K_{1,p}$ by adding a vertex x dominating all the other vertices. This graph has order $n = 2p + 2$ and diameter 2. The degrees of its vertices are respectively $d(x) = 2p + 1$, $d(y) = p$ for the vertices of the clique K_p, $d(u) = p + 1$ for the center u of the star and $d(z) = 2$ for the endvertices of the star. An easy calculation gives as dual degrees $d^*(x) = (p^2 + 3p + 1)/(2p + 1)$, $d^*(y) = (p^2 + p + 1)/p$ for all the vertices y of the clique K_p, $d^*(u) = (4p + 1)/(p + 1)$ and $d^*(z) = (3p + 2)/2$ for all the other vertices of the star. Hence, if $p \geq 2$, min(Dual Degree)$= d^*(u) = (4p + 1)/(p + 1)$ and scope(Dual Degree)$= d^*(z) - d^*(u) = 3p(p - 1)/2(p + 1)$. Note that min(Dual Degree)< 4.

Conjecture 544 For any graph,

$$\text{scope(Dual Degree)} \leq \text{number of components of Mid-Degree}.$$

Conjecture 623 For any graph of diameter 2,

$$\text{mean of Mid-Degree} \leq \text{min(Dual Degree)}.$$

Counterexamples to Conjectures 544 and 623

Let us consider the graph J_p for $p \equiv 0 \pmod 4$ and let $p = 4k$ with $k \geq 15$. The degree sequence of J_p is $2p+1, p+1, p$ (p times), 2 (p times). We leave the reader check that the process which determines the residue gives $R = 2k+2$ and depth $= n - R = 6k$. At the $(\text{depth}/2)^{th}$ step, the Mid-Degree is the sequence of $n - 3k = 5k+2 = 2+5p/4$ terms among them one is equal to $k+1$, $k+1$ are equal to $p-\text{depth}/2 = k$ and $p = 4k$ are equal to 1. Since $2+5p/4 < 3p(p-1)/2(p+1)$ for $p \geq 60$, this graph refutes Conjecture 544.

Moreover, mean of Mid-Degree= $(k^2+6k+1)/(5k+2) > 4 >$min(Dual Degree) for $k \geq 15$. Hence Conjecture 623 is also refuted.

Family H_p

Let H_p be the graph obtained from a star $K_{1,2p+1}$ of center x and endvertices $z, y_1, y'_1, \ldots, y_p, y'_p$ by adding the $2p$ edges xy_i, xy'_i with $1 \leq i \leq p$. This graph has diameter 2 and satisfies $n = 2p+2$, $\alpha(H_p) = p+1 = n/2$, $\nu(H_p) = p+1 = n/2$, $\chi(H_p) = 3$ and $\chi(\overline{H_p}) = p+1$. Therefore $\chi(\overline{H_p}) = n - \nu(H_p)$.

Conjecture 642 Every graph such that $\chi(\overline{G}) = n - \nu(G)$ satisfies

$$\text{scope(Dual Degree)} \leq \alpha(G).$$

Conjecture 643 Every graph such that $\chi(\overline{G}) = n - \nu(G)$ satisfies

scope(Dual Degree)$\leq$ number of components of Mid-Degree.

Conjecture 625 Every graph of diameter 2 satisfies length(1-Residue)$\leq \chi(G)$.

Counterexamples to Conjectures 642 - 643 - 625 Let us consider the graph H_p for p odd ≥ 5. The dual degrees of its vertices are respectively $d^*(x) = (4p+1)/(2p+1)$, $d^*(y_i) = d^*(y'_i) = (2p+3)/2$ for $1 \leq i \leq p$ and $d^*(z) = 2p+1$. Hence scope(Dual Degree)= $2p+1-(4p+1)/(2p+1) = 4p^2/(2p+1)$. Therefore scope(Dual Degree)$-\alpha(G) = (2p^2-3p-1)/2p+1)$ is positive and arbitrarily large, which disproves Conjecture 642.

The degree sequence of H_p is $2p+1, 2$ (2p times), 1. In the process of the determination of the residue, we get the 1-Residue at the first step (sequence of 2p times 1 and one 0). Therefore length of 1-residue= $\sqrt{2p} > 3 = \chi(G)$, which disproved Conjecture 625. Moreover, $R = p+1$, depth= $n - R = p+1$ and since p is odd, the number of components of Mid-Degree is equal to $n - (p+1)/2 = 3(p+1)/2$, which also disproved Conjecture 643.

Family $L_{p,q}$ Let $L_{p,q}$ be obtained from a complete split graph $K^*_{p,q}$, where the part A is complete of order $2q$ and the part B is an independent set of order $2p \geq 8$, by adding p independent edges in B. This graph satisfies $n = 2(p+q)$, $m = q(2q-1) + 4pq + p$, $\nu = n/2$, $\chi(L_{p,q}) = 2q+2$ and $\chi(\overline{L_{p,q}}) = p$. Hence $n - \nu = n/2 = p + q$ and $\chi(L_{p,q}) + \chi(\overline{L_{p,q}}) = p + 2q + 2$. Since $L_{p,q}$ has diameter 2, even$(x) = n - d(x) = 1$ for each vertex x in A and even$(y) = n - d(y) = 2p - 1$ for each vertex y in B. Moreover, sum(Odd)$\leq$sum(Even) if and only if $4m \leq n^2$, that is when $(p-q)(p+q-1) \geq 2pq$. In particular, if $q = p-2$, then sum(Even)$<$sum(Odd) since $p \geq 4$ and if $p = 3q$, then sum(Odd)$<$sum(Even).

Conjecture 667 Every graph G such that sum(Even) $\leq$ sum(Odd) satisfies

$$\text{mode(Even)} \leq n - \nu.$$

Conjecture 682 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

$$\max(\text{Dual Degree}) \leq \chi(G) + \chi(\overline{G}).$$

Conjecture 683 Every graph G such that sum(Odd) $\leq$ sum(Even) satisfies

mean(Dual Degree) $\leq$ number of components of Mid-Degree.

Counterexample to Conjecture 667

We saw that the graph $G = L_{p,p-2}$ with $p \geq 4$ is such that sum(Even) $<$ sum(Odd).
Since $|B| > |A|$, the vector Even has a unique mode which is equal to $2p - 1 > 2p - 2 = n - \nu(G)$. Therefore this graph disproves Conjecture 667.

Counterexamples to Conjectures 682 and 683

We saw that the graph $G = L_{3q,q}$ is such that sum(Odd)$<$sum(Even).

In G, $d^*(y) = ((2q+1) + 2q(8q-1))/(2q+1) = (16q^2+1)/(2q+1)$ for the $6q$ vertices of B and $d^*(x) = (6q(2q+1) + (2q-1)(8q-1))/(8q-1) = (28q^2 - 4q + 1)/(8q-1)$ for the $2q$ vertices of A. Since $d^*(y) > 5q + 2 = \chi(L_{3q,q}) + \chi(\overline{L_{3q,q}})$, this graph disproves Conjecture 682.

Moreover mean(Dual Degree)$= (6qd^*(y) + 2qd^*(x))/8q = 55q/8 + O(1)$ when $q \to +\infty$. On the other hand, the calculus of the residue leads to a sequence of $6q$ elements equal to 1. Hence $R = 3q$ and depth$= n - R = 5q$. If we choose q even, the number of components of Mid-Degree is $n - 5q/2 = 11q/2$ which is less than $55q/8$. Therefore this graph disproves Conjecture 683 for q sufficiently large.

4. Some results and problems on the Randić index

There exist interesting results and problems on the Randić index of a graph G among Graffiti Conjectures and in relation to the order of G, its size, the degree of its vertices, the distance parameters or the eigenvalues of its adjacency matrix. We survey here some of them.

Recall the respective values, easy to compute, of the radius r, the mean distance μ and the Randić index Rc of a path P_n and of a star $K_{1,n-1}$ of order n:

$$r(P_n) = \lfloor \tfrac{n}{2} \rfloor \qquad \mu(P_n) = \tfrac{n+1}{3} \qquad Rc(P_n) = \tfrac{n-3+2\sqrt{2}}{2}$$

$$r(K_{1,n-1}) = 1 \qquad \mu(K_{1,n-1}) = 2 - \tfrac{2}{n} \qquad Rc(K_{1,n-1}) = \sqrt{n-1}$$

4.a Randić index, order and size

It is well known that every graph of order n satisfies $Rc \leq n/2$ with equality if and only if $\delta \geq 1$ and every component of G is regular (see for instance the comment following Conjecture 67 in [9]). In [1], Bollobás and Erdős proved the following lower bounds on Rc in terms of the order or the size of G.

Theorem 4.1[1]: 1. In every graph G of order n with $\delta(G) \geq 1$, $Rc(G) \geq \sqrt{n-1}$ with equality if and only if G is a star $K_{1,n-1}$.
2. In every graph G of size m, $Rc(G) \geq \dfrac{\sqrt{8m+1}+1}{4}$ with equality if and only if G consists of a clique K_p and $n-p$ isolated vertices.

We can remark that $\sqrt{\dfrac{m}{2}} \leq \dfrac{\sqrt{8m+1}+1}{4} \leq \sqrt{\dfrac{m}{2}} + 1$. When the graph G has girth at least four or five, Favaron, Mahéo and Saclé got higher lower bounds for Rc. The first part of Theorem 4.2 (Corollary 2.12 of [10]) proved Conjecture 213 of [9]. The second part is a consequence of Corollaries 2.11 and 2.6 of [10].

Theorem 4.2 [10]: 1. In every triangle-free graph G of order n, $Rc \geq \sqrt{m}$ with equality if and only if G consists of a clique K_p and $n-p$ isolated vertices.
2. In every graph G of order n and size m with girth at least five, $Rc(G) \geq \dfrac{m}{\sqrt{n-1}}$.

In trees of order n, which are connected graphs of size $m = n-1$ and with infinite girth, the minimum value of the Randić index is attained for stars (particular case of Theorem 4.1) and its maximum value is attained by paths as shown by different authors (see for instance [2],

[16] or the research report [5]). This is conform to Randić's idea to take this parameter as a molecular branching index.

4.b Randić index and degrees

The lower bound $\sqrt{n-1}$ on $Rc(G)$ given in Theorem 4.1 holds for minimum degree at least one. In [5], Delorme, Favaron and Rautenbach found a larger bound under the stronger hypothesis that $\delta(G) \geq 2$ and gave a conjecture for the general case $\delta(G) \geq \delta$. The extremal graphs are the complete split graphs $K^*_{\delta,n-\delta}$ generalizing the stars and obtained from a complete bipartite graph $K_{\delta,n-\delta}$ by joining each pair of vertices in the part with δ vertices by a new edge.

Theorem 4.3 [5]: Let G be a graph of order n with $\delta(G) \geq 2$. Then

$$Rc(G) \geq \sqrt{2(n-1)} + \frac{1}{n-1} - \frac{\sqrt{2}}{\sqrt{n-1}}$$

with equality if and only if $G = K^*_{2,n-2}$.

Conjecture 4.4 [5]: Let G be a graph of order n with $\delta(G) \geq \delta$. Then

$$Rc(G) \geq \frac{\delta(n-\delta)}{\sqrt{\delta(n-1)}} + \binom{\delta}{2}\frac{1}{n-1}$$

with equality if and only if $G = K^*_{\delta,n-\delta}$.

If moreover the graph G is triangle-free, they also got the following bound:

Theorem 4.5 [5]: Let G be a triangle-free graph of order n with $\delta(G) \geq \delta \geq 1$. Then

$$Rc(G) \geq \sqrt{\delta(n-\delta)}$$

with equality if and only if $G = K_{\delta,n-\delta}$.

Note that the two lower bounds $\sqrt{m}$ and $\sqrt{\delta(n-\delta)}$ on the Randić index of triangle-free graphs respectively given in Theorems 4.2 and 4.5 are not comparable. For instance for n even > 2, if G is obtained from the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ by deleting the edges of a perfect matching, then $m < \delta(n-\delta)$, while if G is obtained from $K_{\frac{n}{2},\frac{n}{2}}$ by deleting at least two edges incident to a vertex v, then $m > \delta(n-\delta)$.

Let us cite two more conjectures of Graffiti related to the Randić index and the degrees and which remain open.

Conjecture 4.6 (27 of [9]): For every graph G, Deviation(Degree) $\leq Rc(G)$.

A partial result is that this property is true in triangle-free graphs (Corollary 2.29 of [10]).

Conjecture 4.7 (136 of [9]): For every graph G, Deviation(Temperature) $\leq Rc(G)$.

4.c Randić index and distances

Let us first remark that some conjectures of [9] related to distances in graphs appear in rather similar versions respectively involving the radius and the mean distance of the graph. Such conjectures are not easily comparable because the radius can be less or more than the mean distance (see [8]). For instance for a star, $r < \mu$ and for a path of order at least 5, $r > \mu$.

Conjecture 3 of [9] claims that in every connected graph the mean distance is at most the Randić index. This conjecture is still open and with the aid of their program AutographiX, Caporossi and Hansen refined it to be

Conjecture 4.8 (Conjecture 3' of [3]): Every connected graph of order n satisfies

$$\mu(G) + \sqrt{n-1} + \frac{2}{n} - 2 \leq Rc(G).$$

If true, Conjecture 4.8 would be sharp since equality holds for stars.

Another interesting Graffiti conjecture (12) is that for every connected graph of radius r, $r \leq 1 + Rc$. As above, this conjecture was strengthened in [3] to be

Conjecture 4.9 (Conjecture 12' of [3]): Every connected graph different from a path of even order satifies $r(G) \leq Rc(G)$ (for even paths, $Rc(P_{2k}) = k + \sqrt{2} - \frac{3}{2} < k = r(P_{2k})$).

Moreover Caporossi and Hansen proved their new conjecture for trees.

Theorem 4.10 [3]: For all trees except even paths, $r \leq Rc$.

4.d Randić index and eigenvalues of the adjacency matrix

The following two theorems of Favaron, Mahéo and Saclé were not conjectured under this form by Graffiti, but the authors established them with the aim of proving some conjectures of [9]. Recall that the eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n$ satisfy (3).

Theorem 4.11 (Corollary 2.11 of [10]): Every non-empty graph G satisfies $Rc(G) \geq m/\lambda_1$.

As already said above, Theorem 4.2 is a consequence of Theorem 4.11.

Theorem 4.12 (Corollary 2.16 of [10]): Every graph satisfies $Rc(G) \geq |\lambda_i|$ for $2 \leq i \leq n$.

Theorem 4.12 was used in [10] to prove Conjecture 19 (case $i = n$), Conjecture 556 (case $i = 2$), Conjecture 713 and Conjecture 200 (with some exceptions) of [9].

Let us cite to end an interesting conjecture of AutographiX related to another parameter, the chromatic number of G. If true, this conjecture is sharp since equality holds for K_n and $K_{1,n}$.

Conjecture 4.13 [3]: For any connected graph of order $n \geq 2$ with chromatic number $\chi(G)$, $Rc(G) \geq \frac{\chi(G)-2}{2} + \frac{1}{\sqrt{n-1}}(\sqrt{\chi(G)-1} + n - \chi(G))$.

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