Les Cahiers du GERAD ISSN: 0711–2440

Exhaustive and metaheuristic exploration of two new structural irregularity measures

P.O. Boaventura-Netto,
L. Silva de Lima, G. Caporossi

G–2016–16

March 2016

GERAD HEC Montréal
3000, chemin de la Côte-Sainte-Catherine
Montréal (Québec) Canada H3T 2A7

Tél. : 514 340-6053
Téléc. : 514 340-5665
info@gerad.ca
www.gerad.ca

Exhaustive and metaheuristic exploration of two new structural irregularity measures

Paulo Oswaldo Boaventura-Netto [a]
Leonardo Silva de Lima [b]
Gilles Caporossi [c]

[a] *Program of Production Engineering, COPPE/UFRJ, Brazil*

[b] *Program of Production and Systems Engineering, CEFET/RJ, Brazil*

[c] *GERAD & HEC Montréal, Montréal (Québec) Canada, H3T 2A7*

boaventu@po.coppe.ufrj.br
leonardo.lima@cefet-rj.br
gilles.caporossi@gerad.ca

March 2016

Les Cahiers du GERAD

G–2016–16

Abstract: This paper presents the results of two explorations: one, exhaustive, of the graph sets from 4 to 10 vertices, and other, using AGX-III program on graphs from 11 to 30 vertices, both looking for extremal graphs for two new irregularity measures. Some discussions on the obtained results are presented. The involved measures have polynomial complexity.

Key Words: Graphs, irregularity, irregularity measures, graph extensions.

Résumé : Cet article présente les résultats de deux explorations, une exhaustive, des graphes de 4 à 10 sommets, et l'autre utilisant le programme AGX-III, des graphes de 11 à 30 sommets, en cherchant dans les deux cas des graphes extrêmes pour deux nouvelles mesures d'irrégularité. Des discussions sur les résultats obtenus sont présentées. Les mesures proposées ont une complexité polynomiale.

1 Introduction

1.1 Objectives and content

The irregularity in graphs is a property of relatively recent study. It was initially motivated by applications in chemistry, where it is a consequence of the different valences of the chemical elements present in the graph structures associated with chemical formulas, [GHM05]. Despite this structural motivation, the literature has shown, with a single exception – the Albertson measure, [Al97], [HM05] – expressions aimed at measuring the irregularity based only on degree sequences, which leads to obtaining the same values for different graphs. The proposal discussed here, as in our previous work, [Bo13a], [Bo14], [Bo15], is based on Albertson measure.

This section contains a quick discussion of the nomenclature and the notation relevant for the work. Section 2 presents the proposed irregularity measures. Section 3 discusses the resources utilized in the graph search. Section 4 presents the results obtained. Section 5 aligns some conclusions and suggestions for future research.

1.2 Nomenclature and notation

We consider, in this text, simple graphs $G = (V, E)$ (non-oriented, without multiple edges and without loops) where $V = \{v_i, i = 1, \ldots, n\}$ is the *vertex set*, $E - \{(v_i, v_j), i, j = 1, \ldots, n, i \neq j\}$ is the *edge set* and $n = |V|$ is *G's order*. The theory includes other equivalent definitions. We call *G(n)* the set of all graphs G of order n. We can define a *degree vector* $d = [d_i]$ where d_i is the number of edges from which the vertex i participates. The content of d is also called the *degree sequence*, considered in the order of the vertex set numbering. A number sequence is *graphic* if and only if it corresponds to the degree sequence of some graph, [SH91] A graphic sequence has to show its term sum equal to *2m*, where m in the number of the corresponding graph edges. A degree sequence can be also ordered by value, frequently in non-increasing order, producing an *ordered degree sequence (ODS)*. A graph G is *regular* (*k-regular)* if every vertex in G has the same degree k. If there is no $k \in N$, such that G is k-regular, then G is *irregular*. A graph G on n vertices is *antiregular* if its degree sequence has $n-1$ different values. For every $n \geq 2$ there is a connected antiregular graph on n vertices, [Me03], which we denote by AR_n. For every n, the complement $(AR_n)^c$ of AR_n is also antiregular and no other graph matches these structures. There is only one graph for each order, the *complete graph* (K_n), which contains all possible edges. A *path* in a graph is a family of sequentially adjacent edges. A graph is *connected* if for every pair v_i, v_j of vertices there is a path joining v_i to v_j and is *not connected*, or *disconnected*, if this is not true. An *independent set* $S \subseteq V$ is a vertex set where no vertex pair defines an edge. Several matrices associated to a given graph can be defined. The most immediate is the *adjacency matrix* $A = [a_{ij}]$, where $a_{ij} = 1$ if $\exists (v_i, v_j) \in E$ and $a_{ij} = 0$ on the contrary. The *diversity* $\xi(G)$ of a graph is the number of (different) degree values of its sequence, $\xi(G) = 1$ if G is is k-regular, $\xi(G) = |\{d_i | d_i \neq d_j, i = 1, \ldots, n-1, j = i+1, \ldots, n\}|$, if G is irregular. The *multiplicity* $\mu(x)$ of a given value x in a sequence associated with a graph is the number of times x appears in the sequence. Here, we apply this concept to the degree sequence of a graph. The *complement* of a graph G is a graph $\bar{G}$ on the same vertices such that two distinct vertices of $\bar{G}$ are adjacent if and only if they are not adjacent in G. A *split graph* is a graph where the vertex set can be partitioned into a complete graph and an independent set. More details can be found in [Be71], [BM78] and [Bo12].

2 The proposed irregularity measures

An *irregularity measure (IM)* of a graph G is a real function $F : I(G) \to R$ of a G invariant set I, such that $F(G) = 0$ if and only if G is regular. The work on this subject involves not only the definition of new measures which better express the irregularity, but also concerns the search for extremal graphs associated with the existing measures – i.e., graphs that present maximum value for a given IM. These extremal graphs would then be the "most irregular" for the corresponding measure. This last topic proved to be quite difficult, without complete success until today. Details concerning the known extremal graph families for a number of IMs are in [Ol12] and [OOJA13].

[Al97] and [HM05] defined the *imbalance measure*,

$$irr(G) = \sum_{(i,j)\in E} |d_i - d_j|. \tag{1}$$

The module of the difference between i and j degrees is the *unbalancing* of the edge (i, j). This measure presents some zero values for disconnected graphs with regular components of different degrees. This violates the necessity condition to define an IM but, even with this drawback, it has been included in the IM literature, which can be understood by the fact that it was, among the existing polynomial IMs, the one in which the definition involves the edges and therefore properties of structure. We call a measure having this property a *structural IM*.

We propose two new measures (*division* and *multiplication measures*), which are also structural and take into account the degree multiplicities. Their expressions are based on that of Albertson measure and they should present the same drawback previously discussed concerning that measure, except for a new term, whose purpose is to avoid this problem.

The *division IM (IRRdiv)* is given by

$$IRRdiv(G) = \frac{(\xi - 1)}{n} + \sum_{(i,j)\in E} \left| \frac{d(i)}{\mu(d(i))} - \frac{d(j)}{\mu(d(j))} \right|, \tag{2}$$

where $\mu(d(k))$ is the degree multiplicity of k in the degree sequence. It is an IM, since for a r-regular graph G with n vertices, we have $\mu(r) = n$ and all difference modules are $|r/n - r/n| = 0$. In this case the first term, being itself a (nonstructural) IM, will be also null, then $IRRdiv(G) = 0$ for a regular graph. This term marks the presence of irregular graphs even when the second term is null.

The second term of *IRRdiv(G)* presents zeroes for P_6 and for graphs within a family given by the ODS (4,4,4,4,4,4,2,2,2) for $n = 9$, (4,4,4,4,4,4,4,4,2,2,2,2) for $n = 12$ and so on, provided the obtained sequences are graphic (like these examples).

The *multiplication IM (IRRmult)* is given by

$$IRRmult(G) = \frac{(\xi - 1)}{n} + \sum_{(i,j)\in E} \left| d(i)\mu(d(i)) - d(j)\mu(d(j)) \right|. \tag{3}$$

It is easy to see that $IRRmult(G) = 0$ for regular graphs. Here, once again, the first term acts as a correction for the case of disconnected graphs having regular components with different degrees and other possible zeroes.

The sum of all degree multiplicities is equal to n. For vertices of equal degree, the degree multiplicities being equal, the results will be null. On the other hand, the greater the diversity of the graph, the smaller the number of zero differences, but the final value depends both on degrees and multiplicities values.

The second term of this IM presents zeroes where multiplicities and degrees have concurrent values (e.g., $d(i) = k, \mu(i) = 1, d(j) = 1, \mu(j) = k$). Some examples are the path P_3, the 4-vertex star, and some graphs such as $C_5 + u$ (ODS = (3,3,2,2,2)). As with *IRRdiv*, some indeterminate analysis can be applied to look for other cases showing concurrent values.

3 Exhaustive exploration

3.1 The graphs dataset

The calculation involved all graphs (connected and non-connected) with orders from 4 to 10. Table 1, [RW98], below, presents the number of different graphs for each order. As it can be seen, the proportion of connected graphs grows very quickly with the order. More detailed investigations for small orders, as for

Table 1: Amount of graphs and connected graphs with orders from 4 to 10

Order	4	5	6	7	8	9	10
All graphs	11	34	156	1,044	12,346	274,668	12,005,168
Connected graphs	6	21	112	853	11,117	261,080	11,716,571
% connected graphs	54.5	61,8	71,8	81,7	90,0	95,0	97,6
Maximum of $(\xi - 1)/n$	0.500	0.600	0.667	0.714	0.750	0.778	0.800

instance, determining non-connected extremal graphs, can be easily done. The obtained extremals are chiefly connected, which in some sense confirm that connectivity constraints are not so important to the general computations here.

We can observe that $0 \leq (\xi - 1)/n \leq (n-2)/n$, [Bo15]. Table 1 shows the maximum values of this term as a function of graph order. Given the low values obtained, its calculation was limited to the second term.

It is easily seen that second-term *IRRmult* values are always integer. Unless we need a more detailed investigation of the final values, the sum of the first term is not needed for an extremality study. For the extremal second-term values, vastly outnumbered, the final verification can be done separately, looking for different diversities.

Regarding to *IRRdiv*, some doubts about the extremality may appear for smaller orders; however, it turns out that their second-term values are integer and, for these graphs, it is worth the same argument of the previous case.

Some additional discussion is presented together with the results (Section 4).

3.2 Some details on the associated programming

We used the well-known *GENG* procedure from ***nauty*** routines, [MP13], in order to generate all non-isomorphic graphs of orders from 4 to 10. For each order n, *GENG* generates a text file containing the adjacency matrices of all graphs. We also implemented a function *irregularity (G,IrrFunc)* that, given a graph G and the IM, *IrrFunc*, computes the sequence degree of G and its multiplicities and return the value of the chosen IM. The pseudocode of the implemented algorithm is presented below.

Algorithm 1: *ComputeIrregularity (IrrFunc, n)*

```
ObjFunc* ⟵0
File = GENG(n);
while not EndOfFile(File)
        G ⟵ ReadAdjMatrix(File);
        ObjFunc ⟵ irregularity (G,IrrFunc);
        if Objfunc* < Objfunc
                G* ⟵ G;
                ObjFunc* ⟵ ObjFunc
        end_if
end_while
return G*, ObjFunc*
```

The experiments were performed in Matlab R2014b on 2.5 GHz Intel Core i5 processor (Mac OS X 10.9.4) and 8 GB of RAM. The extremal graphs for the two IMs, within each order, were shown graphically. The results are as follows.

3.3 Results

3.3.1 Extremal graphs for IRRdiv and their values

Figure 1 displays the extremal graphs and Table 2 shows the IM values and a note about the intersection with the split graph family.

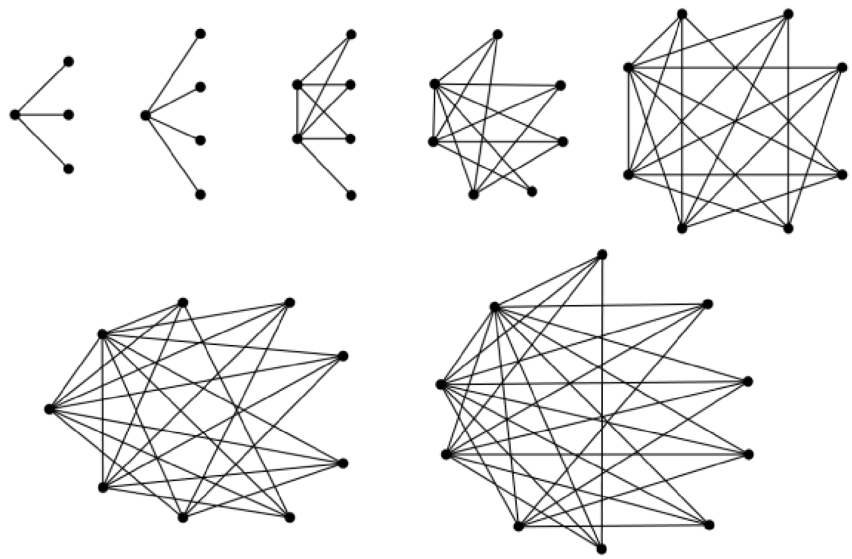

Figure 1: Extremal graphs for *IRRdiv* ($4 \leq n \leq 10$)

Table 2: *IRRdiv* values and possible split structure for extremal graphs, $4 \leq n \leq 10$

Order	4	5	6	7	8	9	10
Second term	8	15	28	46	76.80	113.6	161.333
$(\xi - 1)/n$	0.250	0.200	0.500	0.571	0.375	0.444	0.400
IRRdiv value	8.250	15.200	28.500	46.571	77.175	114.044	161.733
Split ($\|K\|$, $\|I\|$)	1,3	1,4	2,4	2,5	no	no	no

We found extremals presenting both low and high diversity values. The most interesting is the presence of a $G(8)$ extremal with $\xi = 2$, the same value shown by the $G(4)$ and $G(5)$ extremals. On the other hand, $G(6)$ and $G(7)$ extremals have $\xi = 4$ while $G(9)$ and $G(10)$ extremals have $\xi = 5$. Other interesting observation, for the extremals from 4 to 7 vertices, is that they are all split graphs, while for $G(8)$ through $G(10)$ extremals it is not true.

3.3.2 Extremal graphs and their IRRmult values

We also calculated separately the second term values. Figure 2 displays the extremal graphs. Table 3 gives the extremal *IRRmult* values for these datasets.

Table 3: *IRRmult* values for extremal graphs, $4 \leq n \leq 10$

Order	4	5	6	7	8	9	10
Second term	8	36	96	200	380	660	1056
$(\xi - 1)/n$	0.250	0.200	0.167	0.142	0.250	0.222	0.333
IRRmult value	8.250	36.200	96.167	200.142	380.250	660.222	1056.333

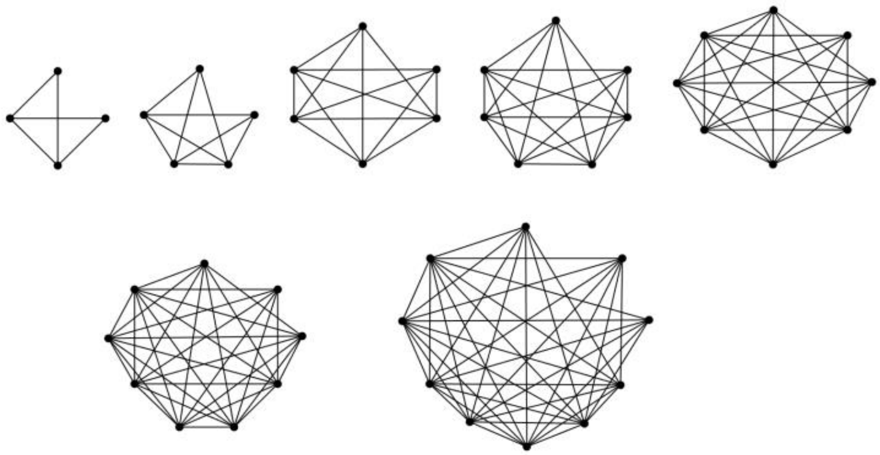

Figure 2: Extremal graphs for *IRRmult* ($4 \leq n \leq 10$)

Unlike that observed with *IRRdiv*, here all the extremals have low diversity, 2 for $G(4)$ to $G(7)$, 3 for $G(8)$ and $G(9)$ and 4 for $G(10)$. Their general structure is near to that of K_n, with one or two less edges.

4 Metaheuristic exploration with AGX-III

4.1 Exploring IRRdiv landscape

A systematic exploring of *IRRdiv* and *IRRmult* landscapes, from orders 11 to 30, was done with the aid of AGX-III, [Ca15], Version 3.1.6. This software applies the Variable Neighborhood Search (VNS) [MH97, CH00, HM01] metaheuristic to a universe of graphs automatically added in order to look, in our case, for maximum *IRRdiv* and *IRRmult* values. Depending on the problem, the optimization may fail when no better solution is found in the neighborhood of the current one. Diversification of the search is then needed. If the perturbation phase of VNS aims at handling this difficulty, we used the new multi-objective capability of AGX-III to help the search. Indeed, a secondary criterion based on a very discriminant invariant to be minimized and maximized was added to the problem. A solution then becomes a tentative Pareto front, which yields a large number of graphs with rather good quality. The neighborhood of this set of graphs being larger, the chances to find a better solution are increased. The Balaban index [Ba82], which is known to be very discriminative was used, which clearly improved the efficiency of the search.

For *IRRdiv*, and chiefly for *IRRmult*, the results were strongly consistent with the structures obtained by the initial exhaustive exploration. The *IRRdiv* landscape showed to be more complex.

Through that exploration we can see that the vertex set V of a *IRRdiv* extremal graph can be, since $n = 4$, partitioned according to their multiplicity values, into two subsets, which we call A and B (Table 4).

We can observe that for $n = 6$ and 7 the set A presented one degree value lesser than that of set B, which is an exception, as long as it is shown by the results obtained with greater orders, both with exhaustive research and metaheuristic application.

Table 4: Partitioning of vertex sets according to degrees ($n = 4$ to 10)

Order	A	B	Divers.	Order	A	B	Divers.
4	3	1^3	2	8	7,6,5	4^5	4
5	4	1^4	2	9	8,7,6,5	4^5	5
6	5,4,1	2^3	4	10	9,8,7,6	4^6	5
7	6,5,2	3^3	4				

Table 5 below gives the best *IRRdiv* values found and the degree sequences corresponding to the associated graphs. A continuously descending degree subsequence is indicated by $a \to b$, where a and b are its maximum and minimum values.

Table 5: Maximum *IRRdiv* values found by AGX-III and their degree sequences

		Degree seq. subsets							
n	*IRRdiv*	A	B	**m**	Diversity	$\|A\|$	Mult. d_B	Mult. $d_B = d_k$	$d_k - d_B$
8	77.175	$7 \to 5$	4^5	19	4	3	5	S	1
9	114.044	$8 \to 5$	4^5	23	5	4	5	S	1
10	161.733	$9 \to 6$	4^6	27	5	4	6	S	2
11	219.121	$10 \to 6$	5^6	35	6	5	6	S	1
12	291.845	$11 \to 7$	5^7	40	6	5	7	S	2
13	374.635	$12 \to 8$	5^8	45	6	5	8	S	3
14	467.468	$13 \to 9$	5^9	50	6	5	9	S	4
15	579.333	$14 \to 9$	7^9	66	7	6	9	S	2
16	713.104	$15 \to 9$	8^9	78	8	7	9	S	1
17	847.804	$16 \to 9$	8^9	86	9	8	9	S	1
18	1033.64	$17 \to 10$	8^{10}	94	9	8	10	S	2
19	1195.88	$18 \to 11$	10^{11}	113	9	8	11	S	1
20	1379.43	$19 \to 13$	8^{13}	108	8	7	13	S	5
21	1640.07	$20 \to 13$	8^{13}	113	9	8	13	S	5
22	1875.18	$21 \to 13$	11^{13}	148	10	9	13	S	2
23	2178.68	$22 \to 14$	10^{14}	151	10	9	14	S	4
24	2477.98	$23 \to 15$	9^{15}	153	10	9	15	S	6
25	2846.02	$24 \to 13$	12^{13}	189	13	12	13	S	1
26	3192.96	$25 \to 15$	14^{15}	215	12	11	16	S	1
27	3537.90	$26 \to 17$	11^{17}	201	11	10	17	S	6
28	3956.16	$27 \to 17$	1^{217}	223	12	11	17	S	5
29	4477.00	$28 \to 17$	14^{17}	254	13	12	17	S	3
30	4809.73	$29 \to 18$	15^{18}	276	13	12	18	S	3

4.1.1 Some discussion based on the obtained results

Table 5 allows us to observe some interesting points in what concerns the structure of (presumably) *IRRdiv*-extremal graphs. In what follows, we call $|A| = k$, then $d_{\min(A)} = d_k$, $\mu(d_B) = n - k$.

First of all, the majority of orders between 8 and 30 presents a set A formed by descending consecutive degree values. All results but those of $n = 25$ were presented by AGX-III. We managed the exception through building a graph with the same characteristics found in every other order from 11 to 30, using the same reasoning discussed in this same item for an upper bound calculation.

Another point of interest is the comparison between d_k and $\mu(d_B)$: in all cases, they were equal.

A number of cases present $d_k - d_B > 1$, which allows us to explore similar structures based on different d_B values. For instance, the difference $d_k - d_B$ is 5 for $n = 20$ and 31 and 6 for $n = 24$ and 27.

These points were used as a basis for a conjecture.

Conjecture 1 *For any order, an IRRdiv-extremal graph $G = (V, E)$ has a partition $V = \{A, B\}$, such that the vertex degrees in A can be ordered by consecutively decreasing from $n - 1$ to d_k and the vertex degrees in B are all equal and lesser than d_k. Besides that, we have $|B| = \mu(d_B) = d_k$.*

Figure 3 shows extremal graphs with orders 10 and 17, where the (A, B) partition can be observed. Both graphs follow the equality $|B| = d_k$. The difference $d_k - d_B$ is 2 for the graph on the left and 1 for that on the right.

Discussion: The edge set E can be partitioned into three subsets:

$$(A, A) = \{(u, v)|u \in A, v \in A\}; (A, B) = \{(u, v)|u \in A, v \in B\}; (B, B) = \{(u, v)|u \in B, v \in B\}.$$

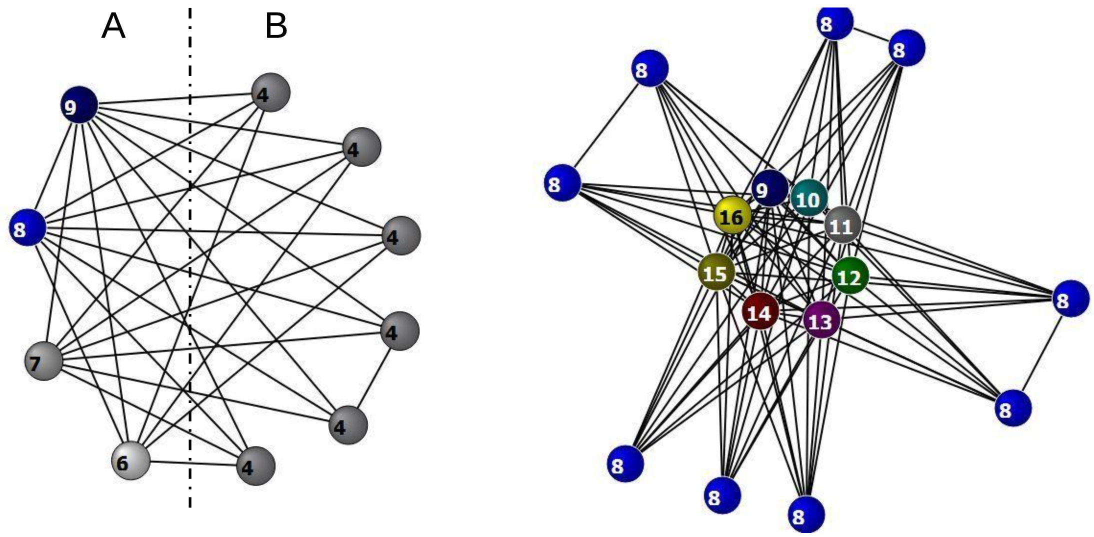

Figure 3: *IRRdiv*-extremal graphs of orders 10 and 17

From *IRRdiv* definition, we conclude that the edges giving the greater contribution for its value should be the (A, B) ones, because every degree in A has multiplicity *1* and the single degree in B has multiplicity $|B|$. The lesser contribution of (A, B) edges is $d_k - d_B/(n-k)$, while the (A, A) edges contribute with values between 1 and $d_1 - d_k = k - 1$.

Then, for an (A, B) construction to contribute for an upper bound of *IRRdiv*, we should have

$$d_1 - d_k \leq d_k - d_B/(n-k), \tag{4}$$

from which, with $d_1 = n - 1$, we have

$$3n - 4k + 1 \geq \sqrt{(n-1)^2 - 8d_B} \tag{5}$$

We can use (5) to verify the feasibility of different d_B values, if they are available.

When building an (A, B) set, for each new added edge $(a, b), a \in A, b \in B$, we will discount a unity of d_a and another for d_b. After the process is finished, every vertex will have a *residual degree value*. Let's consider the set A and the *residual degree sequence* S_A.

Looking for an upper bound for *IRRdiv*, we can add (A, A) edges and sum their contribution to the current (A, B)-obtained value. This can be done, even if S_A is not graphic – in that case, there will be at least one degree value not completely fulfilled. Let's call ω_P this provisional value.

If S_A is graphic, the (A, A) and (A, B) edge contributions will be added to give the *IRRdiv* value (the eventually present (B, B) edges give no contribution). Otherwise, we will have to eliminate (A, B) edges in order to modify S_A. This can result in the addition of new (B, B) edges to compensate the degree changes.

Let $S_{A'}$ be the graphic sequence obtained as described. We had already a provisional *IRRdiv* value, which is not correct as discussed before. To obtain $S_{A'}$ we had to trade (the cheaper) (A, B) edges for (A, A) ones – and (5) guarantees the result of this trade as being a value loss. Then ω_P is an upper bound for *IRRdiv*.

When building the (A, B) set, one should always work with the current higher degrees in A, in order to guarantee the greater contributions.

We defined a *percent slack, Slack%* $= 100(\omega_P - IRRdiv)/IRRdiv$. Table 6 shows ω_P values for n between 8 and 30, with the respective percent slacks.

Table 6: Better *IRRdiv* values and corresponding upper bounds

n	*IRRdiv*	ω_P	Slack %
8	77.175	79.375	2.851
9	114.044	117.444	2.982
10	161.733	167.400	3.504
11	219.121	222.455	1.521
12	291.845	297.417	1.909
13	374.635	382.385	2.069
14	467.468	477.357	2.116
15	579.333	592.400	2.256
16	713.104	722.437	1.309
17	847.804	870.470	2.673
18	1033.64	1050.44	1.626
19	1195.88	1230.42	2.888
20	1379.43	1422.35	3.112
21	1640.07	1686.38	2.824
22	1875.18	1940.41	3.478
23	2178.68	2228.39	2.282
24	2477.98	2534.37	2.276
25	2846.02	2867.48	0.754
26	3192.96	3241.42	1.518
27	3537.90	3615.38	2.190
28	3956.16	4077.40	3.065
29	4374.38	4547.42	1.573
30	4809.73	5021.40	4.401

4.2 Exploring IRRmult landscape

We can divide the degree sequences in a way similar to that used with *IRRdiv*. Here, we call A the set of greater degrees with their multiplicity values and B the set of the remaining, and value-non-increasing, degrees. Preliminary results for small graphs are given in Table 7, where we can notice some facts: for $n = 4$ to 10 the diversity is a non-decreasing sequence; the set A has only one element and it is equal to $n - 1$; the minimum degree of the set B is equals to $\mu(d_A)$.

Table 7: Partitioning of vertex sets according to degrees ($n = 4$ to 9)

Order	A	B	Divers.	Order	A	B	Divers.
4	3^2	2^2	2	8	7^5	6^2,5	3
5	4^3	3^2	2	9	8^6	7^2,6	3
6	5^4	4^2	2	10	9^6	8,7^2,6	4
7	6^5	5^2	2				

Table 8 below gives the best *IRRmult* values found and the degree sequences corresponding to the associated graphs. A continuously descending degree subsequence is indicated by $a \to b$, where a and b are their maximum and minimum values.

4.2.1 Some discussion based on the obtained results

From the results obtained in Table 8, we observe some interesting points on the structure of (presumably) *IRRmult*-extremal graphs: all of them are supergraphs of a complete split graph where the set A induces a clique, say of size $|A| = n - t$ and the set B induces the complement of an antiregular graph of size $|B| = t$, that is, G is isomorphic to K_{n-t} join $(AR_t)^c$; the degree sequence of B decreases from $n - 2$ to $n - t$ and the vertex of degree $n - [t/2] - 1$ has multiplicity 2 and the others multiplicity one, where $[x]$ is the floor of a real number x.

These points were used as a basis for Conjecture 2.

Table 8: Maximum *IRRmult* values found by AGX-III and their degree sequences

		Degree seq. subsets			
n	*IRRmult*	A	B	m	*Diversity*
10	1056.30	9^6	$8, 7^2, 6$	41	4
11	1638.27	10^7	$9, 8^2, 7$	51	4
12	2286.33	11^8	$10, 9^2, 8$	62	4
13	3366.23	12^9	$11, 10^2, 9$	74	4
14	4612.29	13^9	$12, 11^2 \rightarrow 9$	85	5
15	6204.27	14^{10}	$13, 12^2 \rightarrow 10$	99	5
16	8122.25	15^{10}	$14, 13^2, 12, 11$	114	5
17	10522.30	16^{11}	$15 \rightarrow 13^2, 12, 11$	127	6
18	13398.30	17^{12}	$16 \rightarrow 14^2 \rightarrow 12$	144	6
19	16750.30	18^{13}	$17 \rightarrow 15^2 \rightarrow 13$	162	6
20	20712.30	19^{13}	$18 \rightarrow 16^2 \rightarrow 13$	178	7
21	25412.30	20^{14}	$19 \rightarrow 17^2 \rightarrow 14$	198	7
22	30776.30	21^{15}	$20 \rightarrow 18^2 \rightarrow 15$	219	7
23	36816.30	22^{16}	$21 \rightarrow 19^2 \rightarrow 16$	241	7
24	44182.30	23^{16}	$22 \rightarrow 19^2 \rightarrow 16$	260	8
25	52212.30	24^{17}	$23 \rightarrow 20^2 \rightarrow 17$	284	8
26	61150.30	25^{18}	$24 \rightarrow 21^2 \rightarrow 18$	309	8
27	71680.30	26^{18}	$25 \rightarrow 22^2 \rightarrow 18$	331	9
28	83146.30	27^{19}	$26 \rightarrow 23^2 \rightarrow 19$	358	9
29	95760.30	28^{20}	$27 \rightarrow 24^2 \rightarrow 20$	386	9
30	110452.0	29^{20}	$28 \rightarrow 24^2 \rightarrow 20$	410	10

Conjecture 2 *For any order, an IRRmult-extremal graph* $G = (V, E)$ *is a join of a clique of size* $n - t$ *and a complement of an antiregular graph with size* t*. Besides, the degree sequence of* G *is given by*

$$d_G = (n-1)^{n-t}, n-2, n-3, \ldots, (n - [t/2] - 1)^2, \ldots, n-t.$$

Figure 4 shows extremal graphs with orders 12 and 18, where the (A, B) partition, the antiregular structure and the degree sequence can be observed.

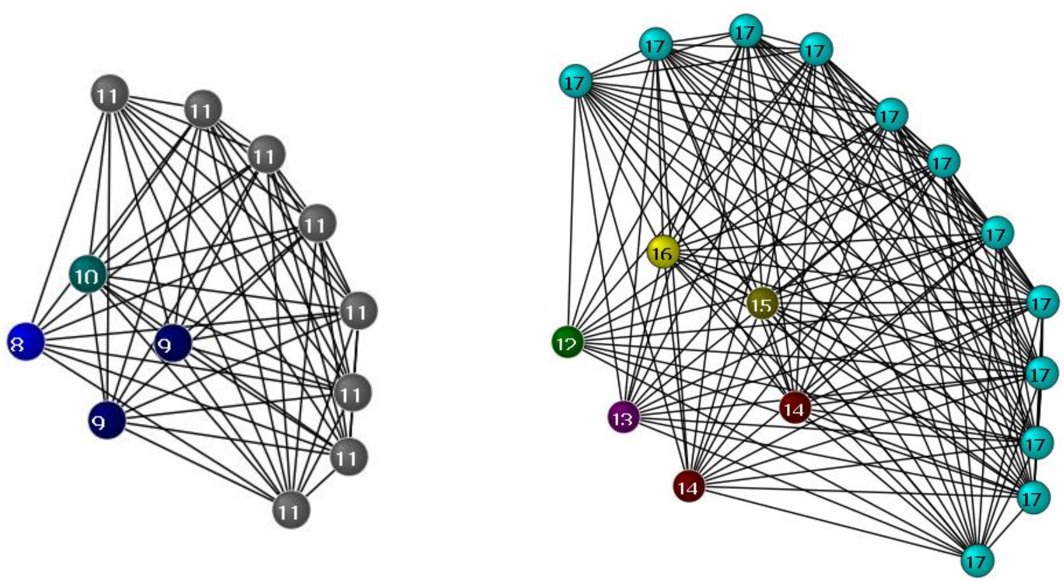

Figure 4: *IRRmult*-extremal graphs of orders 12 and 18

Discussion: The edge set E can be partitioned into three subsets:

$$(A, A) = \{(u, v) | u \in A, v \in A\}; (A, B) = \{(u, v) | u \in A, v \in B\}; (B, B) = \{(u, v) | u \in B, v \in B\}.$$

In what follows, let $d_{\min(B)}$ and $d_{\max(B)}$ respectively be the minimum and maximum degrees of B. From the results, the following equalities hold: $\mu(d_A) = d_{\min(B)} = n - t$, which implies that the diversity is given by t, and $d_{\max(B)} = n - 2$. Also, $d_A = n - 1$.

From *IRRmult* definition, the edges (A, A) do not contribute to the summation. The edge in (A, B) that contributes the most to the irregularity is the one connecting the vertices of degrees d_A and $d_{\min(B)}$ and its contribution is equal to $(n-t)(n-2)$. The lesser contribution is $(n-1)(n-t-1)+1$, given by connecting the vertices of degrees d_A and $d_{\max(B)}$. The edges of the set (B, B) contribute with values between 0 and $t - 2$.

It is interesting to note that the degree sequence of an *IRRmult*-extremal graph is unigraphic, i.e., there is no other graph with the same degree sequence. This fact occurs for the following reasons: the $n-t$ vertices of degree $n-1$ should be connected to every vertex which generates a complete split graph; the residual degrees are $0, 1, 2, \ldots, t-1$, and the remaining edges should only connect vertices in B. Since both (complementary) antiregular sequences are unigraphic, and the residual degrees correspond to the sequence of a disconnected antiregular graph, the whole degree sequence is unigraphic. It means that there is no other graph with the same degree sequence of the extremal ones with better *IRRmult* values.

5 Conclusions and suggestions for future research

1. An interesting feature of *IRRdiv*-extremal graphs is the existence of a two-subset partition, $V = \{A, B\}$, according to their degree values. Particularly appealing is the fact that the cardinality $|B|$ is always equal to the lesser degree in A. We conjecture that these structural properties should be valid for every graph order.

From this conjecture we were able to derive an upper bound for *IRRdiv*.

Some of these graphs have parameters that point to the possibility of generating graphs with similar structures and high *IRRdiv* values; nevertheless, among these, AGX-III was always able to present graphs with the highest value for this measure, with the only exception of $n = 25$.

We observed that *IRRdiv* landscape is generally complex, presenting a number of local optima. The case $n = 25$ is particularly difficult, as we can see, initially, for the low slack it presents with respect to the upper bound. When using AGX-III it finished always at a local optimum of value 2839.58 with structure $A = \{24 \to 15, 13\}$ and $B = \{12^{14}\}$, only 0.21% far from the optimum, which we know as $A = \{24 \to 13\}$ and $B = \{12^{13}\}$.

2. In what concerns *IRRmult*, it seems that the sequence degree of the extremal graphs follows some sort of a pattern where the vertex set can be partitioned into two sets A and B, $V = \{A, B\}$, where A is a clique of size $n - t$ and B is isomorphic to $(AR_t)^c$. The complementary graph $\bar{G}$ of the extremal one has even clearer structure since it is a union of an independent set of size $n - t$ union to AR_t. We conjecture that the same structural properties hold for any graph and that the degree sequences of the extremal ones are unigraphic.

3. Both from the graph-theoretical and the numerical comparison point of view, we think there are multiple interesting points to explore in what concerns these two measures. They can certainly allow for the research of still better measures, since their maximum values do not correspond to antiregular graphs, which, from a numerical point of view, are the most irregular among all graphs.

References

[Al97] Albertson, P.(1997). The irregularity of a graph. Ars Combinatoria, 46, 219–225.

[Ba82] Balaban, A. (1982). Distance connectivity index. Chemical Physics Letters, 89, 399–404.

[Be71] Berge, C. (1971). Graphes et hypergraphes. Dunod, Paris.

[Bo08] Boaventura-Netto, P.O.(2008). P-antiregular graphs. Advances and Applications in Discrete Mathematics, 1(2), 133–148.

[Bo13a] Boaventura-Netto, P.O. (2013). Medidas polinomiais de irregularidade em grafos: discussão e proposta (in Portuguese). Presented to Optima2013, Concepción, Chile, October 2013.

[Bo13b] Boaventura-Netto, P.O. (2013). QAPV: A polynomial invariant for graph isomorphism testing. Pesquisa Operacional, 33(2), 163–184.

[Bo14] Boaventura-Netto, P.O. (2014) Structural versus nonstructural irregularity measures. Proceedings of the ALIO-EURO 2014, Montevideo, Uruguay.

[Bo12] Boaventura-Netto, P.O. (2012). Grafos: Teoria, modelos, algoritmos, 5e ed. Blucher, São Paulo.

[Bo15] Boaventura-Netto, P.O. (2015). Graph irregularity: Discussion, graph extensions and new proposals. Revista de Matemática: Teoría y Aplicaciones, 22(2), 293–310. Universidad de Costa Rica, Costa Rica.

[BM78] Bondy, J.A. and Murty, U.S.R. (1978). Graph Theory and Applications. Macmillan.

[Ca15] Caporossi, G. (2015). Variable neighborhood search for extremal vertices: The system AGX-III. Les Cahiers du GERAD, G–2015–09.

[CH00] Caporossi, G. and Hansen, P. (2000). Variable neighborhood search for extremal graphs: 1. The Auto-GraphiX system. Discrete Mathematics, 212(2), 29–44.

[GHM05] Gutman, P. Hansen, and H. Mélot (2005). Variable neighborhood search for extremal graphs. 10. Comparison of Irregularity Indices for Chemical Trees. J. Chem. Inf. Model. 45, 222–230.

[HM01] Hansen, P. and Mladenović, N. (2001). Variable neighborhood search: Principles and applications. European Journal of Operational Research, 130(3), 449–467.

[Ha87] Harary, F. (1987). Graph Theory. Addison-Wesley.

[HM05] Hansen, P. and Mélot, H. (2005). Variable neighborhood search for extremal graphs. 9. Bounding the irregularity of a graph. In S. Fajtlowicz (Eds.), Graphs and Discovery, DIMACS Series in Discrete Mathematics and Theoretical Computer Science, Providence, American Mathematical Society, 69, 253–264.

[Me03] Merris, R. (2003). Antiregular graphs are universal for trees. Univ. Beograd. Publ. Elektrotehn. Fak. Ser. Mat. 14, 1–3.

[MH97] Mladenović, N. and Hansen, P. (1997). Variable neighborhood search. Computers and Operations Research, 24, 1097–1100.

[MP13] McKay, B.D. and Piperno, A. (2013). Practical Graph Isomorphism, II. J. Symbolic Computation, 60, 94–112.

[Ol12] Oliveira, J.A. (2012). Medidas de irregularidade em grafos (in Portuguese). D.Sc. Thesis, COPPE/UFRJ.

[OOJA13] Oliveira, J.A., Oliveira, C.S., Justel, C. and Abreu, N.M.M. (2013). Measures of irregularity of graphs. Pesquisa Operacional, 33(3), 383–398.

[Po11] Porumbel, D.C. (2011). Isomorphism testing via polynomial-time graph extensions. Journal of Mathematical Modelling and Algorithms, 10(2), 119–143.

[RW98] Read, R.C. and Wilson, R.J. (1998). An Atlas of Graphs. Clarendon, Oxford.

[SH91] Sierksma, G. and Hoogeven, H. (1991). Seven criteria for integer sequences being graphic. J. Graph Theory, 15(2), 223–231.