

GRAPH IRREGULARITY: DISCUSSION, GRAPH
EXTENSIONS AND NEW PROPOSALS

IRREGULARIDAD DE GRAFOS: DISCUSIÓN,
EXTENSIONES DE GRAFOS Y NUEVAS
PROPUESTAS

PAULO OSWALDO BOAVENTURA-NETTO*

Received: 30/May/2014; Revised: 7/Apr/2015; Accepted: 21/May/2015

*Programa de Engenharia de Produção, COPPE, Federal University of Rio de Janeiro, Brazil.
E-Mail: boaventu@po.coppe.ufrj.br

Abstract

This paper presents some measures of graph irregularity found in the literature. From their discussion two important points appear: first, the absence of relationship between all of them, but a single exception, with the structures of the corresponding graphs and, moreover, their known extremal values correspond to graphs having degree sequences with few different values. Two new measures are proposed, seeking to meet these points. Their values are calculated for extremal graphs associated with other measures and for antiregular graphs. Finally, we calculate the boxplots of all these measures for some sets of graphs taken from the literature and also for four sets where the ordered degree sequences are constant. All measures involved have polynomial complexity.

Keywords: Graphs; irregularity; irregularity measures; graph extensions.

Resumen

Este artículo presenta un análisis de las medidas de irregularidad de grafos que se encuentran en la literatura. Desde su discusión dos puntos importantes aparecen: primero, la ausencia de relación entre todos ellos, sino una sola excepción - con las estructuras de los grafos correspondientes y, además, sus valores extremales conocidos corresponden a grafos que tienen secuencias de grados con pocos valores diferentes. Se proponen dos nuevas medidas, tratando de cumplir con estos puntos. Sus valores se calculan para grafos extremales asociados con otras medidas y para grafos antiregulares. Por último, se determinan los gráficos de cuartiles o boxplots de todas estas medidas, para algunos conjuntos de grafos de la literatura y para cuatro conjuntos donde las secuencias ordenadas de grados son constantes. Todas las medidas estudiadas tienen complejidad polinómica.

Palabras clave: grafos; irregularidad; medidas de irregularidad; extensiones de grafos.

Mathematics Subject Classification: 05C07, 05C35, 05C99.

1 Introduction

1.1 The purpose of the discussion

The irregularity in graphs is a topic of interest for the analysis of models based on them, as exemplified by the study of acyclic molecules [15]. Over the recent years, the literature has shown a significant number of works devoted to the subject, usually dealing, with a single exception, with measures calculated using

only the degree sequences. We try to go a little further by considering the graph edge set as the basis for the measure calculation, looking to obtain more accurate information, by engaging the influence of the graph structure in the calculation. This work proposes new features for determining undirected graph irregularity. Section 2 deals with a brief discussion of the polynomial measures in the literature. Section 3 discusses the expressions for these measures when applied to antiregular graphs. Section 4 is dedicated to the proposal of two new measures. Section 5 presents a series of comparison tests using extremal graphs of some irregularity measures (IMs) from the literature and a collection of graphs with maximum or near-maximum values for them. Section 6 presents a statistical analysis of the results given by all IMs when applied to 100-graph collections from the literature [25]. The proposed IMs were also tested with collections generated from given graphs by successive blocks of edge exchanges. All results were submitted to a statistical analysis by using boxplots, in order to evaluate the sensitivity of the IMs. We consider an IM to be more sensible to structure differences if their results concerning a collection of differently-structured graphs are more dispersed, which can be easily seen with boxplot graphics. To distinguish among graphs with the same number of vertices and edges, but different in terms of their structures, we apply to the determination of all measures some auxiliary resources already used in the study of graph isomorphism, such as powers of graphs and extensions, [7], [23]. In particular, the results are examined with the square and the squared extension of the adjacency matrix, respectively A^2 and $A \cup A^2$.

1.2 Nomenclature and notation

We consider, in this text, simple graphs $G = (V, E)$ (non-oriented, without multiple edges and without loops) where $V = \{v_i, i = 1, \dots, n\}$ is the vertex set, $E = \{(v_i, v_j), i, j = 1, \dots, n, i \neq j\}$ is the edge set and $n = |V|$ is G order. The theory includes other equivalent definitions. We call $G(n)$ the set of all graphs G of order n and $G(n, m)$ the set of all graphs with n vertices and m edges. The *degree* d_i of a vertex v_i is the number of edges from which it participates and we can define the *degree sequence*, $d = \{d_i, i = 1, \dots, n\}$, considered in the order of the vertex set numbering. This sequence can be also ordered by value, frequently in non-increasing order, producing an *ordered degree sequence* (ODS). A graph G is *k-regular* if every vertex in G has the same degree k . If there is no $k \in \mathbb{N}$, such that G is k -regular, then G is *irregular*. 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 with 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 k -regular, $\xi(G) = |\{d_i, d_i \neq d_j, i = 1, \dots, n-1, j = i+1, \dots, n\}|$, if G is irregular. The *multiplicity* $\mu(x)$ of a given value x in a sequence 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 \overline{G} on the same vertices such that two distinct vertices of \overline{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 [6], [11] and [9].

1.3 Presenting the problem

The concept of irregularity has been treated in the literature following two trends: (i) structural irregularity, defining “more irregular” graphs according to given criteria; (ii) definition of numeric values that somehow express this property. An example of the first approach is [12]. Here, various structural criteria are considered, the most important of which corresponds to *locally* (or *highly*) irregular (HI) graphs. A graph $G = (V, E)$ is HI if, for every $v \in V$, all neighbors of v have different degrees, [2], [18]. [4] and [19] discuss the *antiregular graphs* (AR), which are split graphs having maximum diversity equal to $(n-1)$. A single degree repetition is allowed and it has to concern the value $\lfloor n/2 \rfloor$. We can observe that HI graphs do not reach this diversity, a fact which shows that diversity does not cover all irregularity aspects. These graph classes are quite restricted. In the first case, there is not a HI graph for every order and, in addition, in [2] it is proved that the number of HI graphs decreases exponentially with the order n . In the second case, there are exactly two AR graphs for each order, one of them connected and the other disconnected and complementary to the first. Such restrictions probably influenced the later approaches on the subject, including because there was, in the work cited above, no proposal for measuring irregularity.

2 Irregularity measures

An *irregularity measure* (IM) of a graph G is a real function $F : I(G) \rightarrow R$ of a G invariant set I , such that $F(G) = 0$ if and only if G is regular. The research has focused not only on the definition of new measures which better express the irregularity, but also towards the search for extremal graphs associated with the existing measures, i.e. graphs that present maximum value for a given IM. We can observe that these initiatives, when applied to some polynomial IMs, have resulted in extremal graphs with diversity equal to 2 - or, in another case, not larger than 4, for every order n , which seems contradictory in relation to the notion of irregularity, when considering its opposite - the regularity: regular graphs G have a single degree value, then $\xi(G) = 1$ for them. Details concerning the known extremal graph families for IMs are in [22].

- i) [5] defined the *variance measure*, based on the variance of the vertex degree set,

$$\nu(G) = (1/n) \sum_i d_i^2 - (1/n^2) (\sum_i d_i)^2. \tag{1}$$

- ii) [3] and [16] defined the *imbalance measure*, $irr(G) = \sum_{(i,j) \in E} |d_i - d_j|$. The module of the difference between i and j degrees is the *unbalancing* of the edge (i, j) . This measure presents null values for disconnected graphs with regular components of different degrees, a fact which violates the necessity condition to define an IM. Nevertheless, it has been included in the literature in the set of these measures, a fact that can be understood because that it is, among the existing polynomial IMs, the only one in which the definition consider the edges and therefore involves structure properties. A similar measure covering all vertex pairs is the *total irregularity*, $irr_t(G)$, [1]. We can observe that $irr_t(G) = irr(G) + irr(\overline{G})$.

- iii) [20] defined the *deviation degree measure*, $s(G) = \sum_i |d_i - \bar{d}|$, that is, the sum of the absolute values of the degree deviations relative to their average.

- iv) [13], [14] defined a *heterogeneity index*,

$$\rho(G) = \sum_{i,j} ((d_i)^{(-1/2)} - (d_j)^{(-1/2)})^2 \tag{2}$$

- v) Aside from Albertson (AHM) IM, the other polynomial measures are uniquely characterized by the degree sequences. When one attempts to interpret the meaning of their values, it should be noted that a given degree

sequence may correspond to more than one graph. Therefore, the set of graphs associated with a given degree sequence presents the same values for these IMs, regardless of structural differences. We will use for them, where appropriate, the general designation of nonstructural IMs. Unigraphic sequences, which represent but one graph - e.g, these from antiregular graphs [19] do not, naturally, have this drawback.

3 Some IM applied to antiregular graphs

The ODS of an AR graph is $d = (n-1, \dots, \lfloor (n-r)/2 \rfloor, \lfloor (n-r)/2 \rfloor, \dots, 2, 1)$. From there, the determination of expressions for Bell, Albertson and Nikiforov IMs is immediate, [10].

3.1 The Bell measure

$$\nu(G) = \frac{1}{n} \left(\frac{n(n-1)(2n-1)}{6} + \frac{(n-r)^2}{4} \right) - \frac{1}{n^2} \left(\frac{n^2-r}{2} \right)^2 \quad (3)$$

Here we have $r = 0$, for n even and $r = 1$, for n odd.

3.2 The Albertson measure

Here, we need a characterization of sequences known as *graphic*. A finite sequence of n integers is *graphic* if and only if it is the degree sequence of some simple graph. A necessary condition for a sequences to be *graphic* is the sum of their terms equals $2m$. Moreover, there are many equivalent theorems [26], which establish necessary and sufficient conditions for a sequence to be *graphic*. We use here the following:

Theorem 1, [6], [26]: A non-increasing ordered number sequence is *graphic*, if and only if

$$\sum_{i=1}^k d_i \leq \sum_{i=1}^k \delta_i, \quad \forall k = 1, \dots, n, \quad (4)$$

where the first member is the row sum and the second, the column sum, of an order n matrix $B(G)$, where the main diagonal is zero and the first d_i other elements of each row have value 1.

Proof. [6].

Let then be matrices $B(G)$ of antiregular graphs of even and odd order and let us consider the degree differences in each row as required by the measure, for the existing edges (Figure 1):

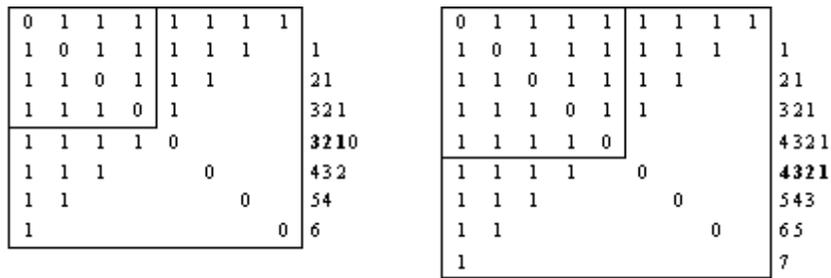


Figure 1: Matrices $B(G)$ from antiregular graphs.

It can be seen that the sums of the degree differences for each vertex are triangular numbers $(1, 3, 6, \dots)$. In the following expression, the first term takes into account the repetitions (shown above in bold).

$$irr(A_n) = \sum_{k=1}^{\lfloor n/2 \rfloor - p} k + \sum_{r \in \mathbb{N}, 2r+q < n} \sum_{k=1}^{2r+q} k \tag{5}$$

with $p = 1, q = 0, n$ even, $p = 0, q = 1$ (n odd)

3.3 The Abdo-Dimitrov measure

Alongside the possibility of this measure calculation by the aforementioned relationship, $irr_t(G) = irr(G) + irr(\overline{G})$, it can be done directly, considering on one hand the differences of successive degrees and in the other hand the differences related to the repetition of the degree. The result is

$$irr_t(G) = C_{n,3} + 2 \left\{ \sum_{k=1}^{\lfloor (n-2)/2 \rfloor} k + p \lfloor n/2 \rfloor \right\} \tag{6}$$

3.4 The Nikiforov measure

For AR graphs we have, [7],

$$m = 1/2 \{ \lceil n/2 \rceil (\lceil n/2 \rceil - 1) + \lfloor n/2 \rfloor (\lfloor n/2 \rfloor + 1) \} \tag{7}$$

from which we can derive

$$s(A_n) = \left\{ \sum_{k=1}^n |d_i - (n^2 - r)/2n| \right\} \tag{8}$$

where $r = 0$ (n even) and $r = 1$ (n odd).

4 The proposed measures

Looking for an expression involving sequence information related to degree diversities, we propose two new measures (division and multiplicity measures). Their expressions are based on that of AHM measure and they would present the same drawback previously discussed concerning that measure (see 2.3). We avoid it by introducing the term $(\xi - 1)/n$, which can be seen as a non-structural IM, since $\xi = 1$ corresponds to the definition of a regular graph. This addition covers the already mentioned drawback. On the other hand, we have $0 \leq (\xi - 1)/n \leq (n - 2)/n$ for finite graphs, its greater values being found among AR graphs, a value range normally much lower than those normally given by the second terms. This addition does not overshadow, therefore, the meaning of the final results. The division IM (*IRRdiv*) is given by

$$IRRdiv(G) = \frac{\xi - 1}{n} + \sum_{(i,j) \in E} |(d_i/\mu(d_i) - (d_j/\mu(d_j)))| \quad (9)$$

where $\mu(d_k)$ is the degree multiplicity of a vertex with degree 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 every difference $|r/n - r/n| = 0$. The first term being itself an IM, it will be also null, then $IRRdiv(G) = 0$. This calculation shows, for AR graphs, $n - 1$ fractions equal to the corresponding degrees and one fraction whose value is half the degree value (which is $\lceil n/2 \rceil$). For less irregular graphs (greater $\mu(k)$ values), the fractions $d(k)/\mu(d(k))$ present lesser values and the same could be observed with the modules of their differences. Then $IRRdiv(G)$ will, very probably, have its extremal value among AR or near-AR graphs. We can look for connected irregular graphs presenting null value for the edge-difference term. For instance, paths $P_k (k > 3)$ present null differences for the internal edges and positive or null ones, $|2/(k-2) - (1/2)|$ for the external ones. Among the path graphs, only P_6 nullifies this expression. A similar analysis could be applied to find other particular structures presenting differences between equivalent fractions. The cases $n = 9$ with ODS = (4,4,4,4,4,4,2,2,2) and $n = 12$ with ODS = (4,4,4,4,4,4,4,4,2,2,2,2) show connected graphs with null sum parcel. It is not difficult to go further, provided the sequences obtained are graphic, like these examples.

The multiplicity IM (*IRRmult*) is given by

$$IRRmult(G) = \frac{\xi - 1}{n} + \sum_{(i,j) \in E} |(d_i\mu(d_i) - (d_j\mu(d_j)))|. \quad (10)$$

From similar considerations, it can be concluded 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. In this case, degree multiplicities will have a different influence. The sum of all multiplicities is evidently equal to n . If the difference modules are calculated within vertices of equal degree, the degree multiplicities will also be equal and the differences will be null. On the other hand, the greater the diversity of the graph, the smaller the number of zero differences. Then $IRRmult(G)$ will also show greater values for graphs having greater irregularity. For antiregular graphs, its value will be greater than that of the AHM IM, since there will be $\lceil n/2 \rceil$ differences with different degree multiplicities. Null parcels can be found where multiplicities and degrees have concurrent values (e.g., $d(i) = k$, $\mu(i) = l$, $d(j) = l$, $\mu(j) = k$). 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. The tests involving graph families, described in this work, included a second term value-checking for $IRRdiv$ and $IRRmult$ and it didn't show any null value.

5 Some tests with chosen graphs

This item involves tests of polynomial IMs, both from the literature and those here proposed, with some extremal graphs described above and also antiregular and HI graphs. Figure 2 shows three graphs related to the HI-graph literature and used in the tests. The first graph, from $G(12, 19)$, is not HI, although shown as such in the reference (each 5-degree vertex is connected to a pair of 5-degree vertices). The second one, from $G(14, 22)$, built by starting with the first, is HI. The third one, from $G(26, 25)$, is an HI tree [12], [2].

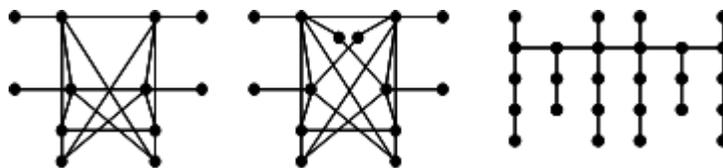


Figure 2: Some examples of HI and HI-related graphs.

Figure 2 shows the results of these tests. In this table, QS and QC graphs are extremal for the Bell measure; SC and SCF graphs, for the AHM measure; and AD graphs, for the Abdo-Dimitrov measure. The literature does not present extremals for Nikiforov and Estrada IMs. The AR and near-AR graphs are denoted as $A_{\kappa c}(n, m)$, where κ is the vertex-connectivity [7].

Note 1. Where the results allow for comparison within $G(n, m)$, the highest values obtained for each measure are in bold italic.

Note 2. Extremals are indicated by the bold shorthands: (B) for Bell, (A) for AHM, (AD) for Abdo-Dimitrov. Some SC (split-complete) graphs are extremal for AHM (Aa), [21].

Notes for Figure 4 (see Appendix 1):

- (*) The graphs $SC(6, 2)$ ($= AD(6, 2)$) and $AD(8, 2)a$ (Lines 4 and 15), indicated as being extremal for Abdo-Dimitrov measure, present lesser values than $A1c(6, 9)$ and $qA1c(8, 15)$ (Lines 6 and 18), respectively, for this measure.
- (**) These graphs are shown in Figure 2. Figure 5 (see Appendix 1) shows antiregular and almost antiregular graphs used in the tests [7].

6 Application to some graph families

6.1 Databases utilized

We tested the IM sensibilities to structure changes by using graph families of same order and with similar properties. Ten 100-graph sets from the database of [25] were used to test the case of different ODS. The orders went from 20 to 100 vertices. The families were identified by the denomination $r01_0klm_A00_99$ and $r001_0klm_A00_99$ where $klm \in \{020, 040, 060, 080, 100\}$, performing a total of 1,000 graphs.

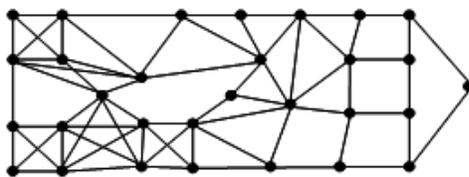


Figure 3: The graph G_{4K4_K5} .

In these families, the edge density corresponds approximately to 10% and 1% respectively. We also built a graph G_{4K4_K5} (Figure 3) with 30 vertices, containing complete graphs K_4 and K_5 as local irregularities and, from it, we generated four sets of 100 graphs, with two, three, five and seven random 2-exchanges. These sets were called $Col100_{4K4K5_rt}$, where r is the number

of 2-exchanges. Remember that in a 2-exchange, we take 2 vertex pairs, $\{a, b\}$ and $\{c, d\}$ having the same adjacency relations and exchange presence and absence of 2 edges between them (e.g., substituting $\{a, c\}$ and $\{b, d\}$ for $\{a, b\}$ and $\{c, d\}$), which does not change their degrees, hence allows no ODS change.

6.2 Tests with the described graph families

The tests were run with some graph families, using their adjacency matrices $A(G)$, their squares $A^2(G)$ and their squared extensions $A(G) \cup A^2(G)$, trying to identify irregularities in neighborhoods larger than the adjacency one. We call these three matrices the *basic test matrices*. The ODS constancies of *Col100_4K4K5_rt* are not kept with the second and the third matrices, then even the non-structural IMs can show non-zero values for these cases. For sake of avoiding an excessive mass of results, this is not included in the paper. The efficiency of the IMs in distinguishing the irregularity within graph collections can be easily evaluated by looking at the boxplots, (see Appendix 2) [24], of their values in each case. They are default R graphics with box width equal to the interquartile range (IQR). The boxplot whiskers are indicated at $(Q3 + 1.58IQR)$ and $(Q1 - 1.58IQR)$ limited to zero. To allow for comparison, we used the percent normalized values, $100 * x/avg(x|x \in X)$, where X is the set of values for each IM. All boxplots are in Appendix 2, Figures 6 to 8. From left to right, they correspond respectively to the three basic matrices. Inside, the presentation order in Figure 6 is 1. *AHM*; 2. *IRRdiv*; 3. *IRRmult*. Figures 7 and 8 present the following internal order: 1. Bell; 2. *AHM*; 3. Abdo-Dimitrov; 4. Nikiforov; 5. Estrada; 6. *IRRdiv*; 7. *IRRmult*.

7 Conclusions

7.1 Tests with individual graphs

Figure 4 allows for some interesting observations. To begin with, we can see that Graph 3 ($(qA1c(6, 8))$) is extremal for the Bell IM. We observed, as already indicated, two discrepancies concerning the extremals for Abdo-Dimitrov measure. Graphs 6, 9 and 16 are Bell-extremal and not connected: they belong to the exception set for *AHM* IM, which is null for everyone of them, even if they are not regular. Graphs 4, 13, 20 and 28 are split-complete, [16]: they are extremal for the *AHM* measure and, since their complements have no edge between vertices with different degrees, their Abdo-Dimitrov IM values are equal to their *AHM* values. We can observe that the family $(q)AR\kappa c(n, m)$ presents frequently the higher values within the given $G(n, m)$ examples. On the other hand, we cannot

guarantee $IRRdiv$ and $IRRmult$ as presenting extremal values for antiregular graphs, that is, $AR1c(n, m)$ graphs: Graph 25, $A2c(10, 25)b$ is 2-connected-AR and presents higher values for these two IMs, than $A1c(10, 25)$. The examples from Figure 4 (Graphs 30 to 32) were included to call the reader attention to the possible influences of the weird HI structure in what concerns quantitative irregularity.

7.2 Tests with graph families

The boxplots obtained from $Col100_4K4K5_rt(r \in \{2, 3, 5, 7\})$ show the influence, on the structures, of a progressively higher number of 2-exchanges. By working with $A(G)$, while the 2-exchange family is seen by the three structural IMs with the same sensitivity, $IRRdiv$ appears more sensitive for the other three families (3-, 5- and 7-exchanges). All cases show outliers, chiefly the last one. The use of $A^2(G)$ enhances $IRRdiv$ sensitivity, the boxes and the whisker extensions being significantly greater than those shown by $A(G)$. The same can be observed with $IRRmult$, although it shows itself less sensible, at least within these families. A similar view is observed when $A(G) \cup A^2(G)$ is used. The families from [25] showed a very different behavior of $IRRdiv$ when compared with every other IM tested, both in what concerns the 1st - 3rd quartiles amplitude and the occurrence of outliers. The same behavior, although less pronounced, can be observed for $IRRmult$. The three basic matrices presented similar pictures for both proposed IMs. Here we can observe that the second and the third basic matrices enhanced the sensibility of $IRRdiv$ and $IRRmult$. Both $r01$ and $r001$ families produce related graphs where these IMs are more sensible, in a way reproducing their irregularity, but with a greater density.

7.3 Proposals for future research

We think it would be interesting to extend this study by defining structural counterparts for Bell, Nikiforov and Estrada measures and compare these counterparts with the traditional and the new measures. To add the term $(\xi - 1)/n$ to AHM measure would produce a full IM, covering the cases of disconnected graphs with regular components of different degrees. Tests with specific irregular graph families, such as planar graphs, would also be enlightening.

References

- [1] Abdo, H. ; Dimitrov, D. (2012) “The total irregularity of a graph”, in: <http://arXiv.org:1207.5267v1> [cs.DM] consulted 10-10-13.
- [2] Alavi, Y.; Chartrand, G.; Chung, F.R.K.; Graham, R.L; Oellermann, O.R.(1987). “Highly irregular graphs”, *Journal of Graph Theory* **11**(2):235–249.
- [3] Albertson, P.(1997) “The irregularity of a graph”, *Ars Combinatoria* **46** 219–225.
- [4] Behzad, M.; Chartrand, G. (1967) “No graph is perfect”, *American Mathematical Monthly* **74**: 962–963.
- [5] Bell, F.K. (1992) “A note on the irregularity of graphs”, *Linear Algebra and its Applications* **161**: 45–54.
- [6] Berge, C. (1971) *Graphes et Hypergraphes*. Dunod, Paris.
- [7] Boaventura-Netto, P.O. (2008) “P-antiregular graphs”, *Advances and Applications in Discrete Mathematics* **1**(2): 133-148.
- [8] Boaventura-Netto, P.O. (2012) *Grafos: Teoria, Modelos, Algoritmos*. 5th ed. Blucher, São Paulo.
- [9] Boaventura-Netto, P.O. (2013a) “Medidas polinomiais de irregularidade em grafos: discussão e proposta”, *Optima2013*, Concepción, Chile, October 2013.
- [10] Boaventura-Netto, P.O. (2013b) “QAPV: a polynomial invariant for graph isomorphism testing”, *Pesquisa Operacional* **33**(2): 163–184.
- [11] Bondy, J.A.; Murty, U.S.R. (1978) *Graph Theory and Applications*. Macmillan, London.
- [12] Chartrand, G.; Erdos, P.; Oellermann, O.R. (1988) “How to define an irregular graph”, *The College Mathematical Journal* **19**(1): 36–42.
- [13] Estrada, E. (2010a) “Quantifying network heterogeneity”, *Physical Review E* **82**: 66102.
- [14] Estrada, E. (2010b) “Randić index, irregularity and complex biomolecular networks”, *Acta Chimica Slovenica* **57**: 597-603.

- [15] Gutman, I.; Hansen, P.; Mélot, H. (2005) “Variable neighborhood search for extremal graphs. 10. Comparison of irregularity indices for chemical trees”, *J. Chem. Inf. Model.* **45**: 222–230.
- [16] Hansen, P.; 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, **69**. American Mathematical Society, Providence RI: 253–264.
- [17] Harary, F. (1987) *Graph Theory* Addison-Wesley, Reading MA.
- [18] Majcher, Z.; Michael, J. (1997) “Degree sequences of highly irregular graphs”, *Discrete Mathematics* **164**: 225–236.
- [19] Merris, R. (2003) “Antiregular graphs are universal for trees”, *Publ. Elektrotehn. Fak. Univ. Beograd Ser. Mat* **14**: 1–3.
- [20] Nikiforov, V. (2006) “Eigenvalues and degree deviation in graphs”, *Linear Algebra and its Applications* **414**: 347–360.
- [21] Oliveira, J.A. (2012) *Medidas de Irregularidade em Grafos*. D.Sc. Thesis (in Portuguese) COPPE/Federal University of Rio de Janeiro.
- [22] Oliveira, J.A.; Oliveira, C.S.; Justel, C.; Abreu, N.M.M. (2013) “Measures of irregularity of graphs”, *Pesquisa Operacional* **33**(3): 383–398.
- [23] Porumbel, D.C. (2011) “Isomorphism testing via polynomial-time graph extensions”, *Journal of Mathematical Modelling and Algorithms* **10**(2): 119–143.
- [24] R Core Team (2014) “R: A language and environment for statistical computing”, *R Foundation for Statistical Computing*, Vienna, Austria, in: <http://www.R-project.org/>.
- [25] Santo, M. De; Foggia, P.; Sansone, C.; Vento, M. (2003) “A large database of graphs and its use for benchmarking graph isomorphism algorithms”, *Pattern Recognition Letters* **24**: 1067–1079.
- [26] Sierksma, G.; Hoogeveen, H. (1991) “Seven criteria for integer sequences being graphic”, *J. Graph Theory* **15**(2): 223–231.

Appendix 1: Particular graphs

	Graph	n	m	$\xi - 1$	Bell	AHM	AD	Nikiforov	Estrada	IRRdiv	IRRMuK
1	QC(6,8) (B)	6	8	3	1.89	8	26	6.67	0.98	2.50	26.50
2	QS(6,8) (B)	6	8	3	1.89	20	26	7.33	3.38	28.50	18.50
3	qA1c(6,8)	6	8	3	1.89	20	26	7.33	3.38	28.50	18.50
4	SC(6,2) (Aa)	6	9	1	2.00	24	(24*)	8.00	2.08	16.17	26.17
5	A1c(6,9)	6	9	4	1.67	16	26	6.00	3.38	22.67	32.67
6	QC(6,10) (B)	6	10	1	2.22	0	20	6.67	0.00	0.17	0.17
7	SCF(6,2,1) (A)	6	10	2	1.56	20	24	6.67	2.08	10.33	40.33
8	qA2c(6,10)	6	10	3	1.22	16	22	6.00	2.00	20.50	32.50
9	QC(7,10) (B)	7	10	1	3.26	0	40	11.43	0.00	0.14	0.14
10	qA1c(7,10)	7	10	4	2.69	26	44	9.14	5.81	33.57	52.57
11	qA1c(7,13)	7	13	4	2.49	22	42	8.86	4.59	38.57	66.57
12	A2c(7,13)	7	13	4	1.63	26	34	7.71	2.47	42.57	160.57
13	SC(7,3) (Aa)	7	15	1	2.20	36	36	10.29	2.03	15.14	90.14
14	qA3c(7,15)	7	15	4	1.63	22	34	7.71	2.42	32.57	184.57
15	AD(8,2)a (AD)	8	15	4	3.94	54	(66)*	13.50	4.57	31.50	35.50
16	QC(8,15)	8	15	1	4.69	0	80	15.00	0.00	0.12	0.12
17	qA1c(8,15)	8	15	4	3.69	40	68	12.50	6.47	60.50	120.50
18	AD(9,3)a (AD)	9	22	2	4.99	84	92	18.67	4.18	27.22	168.22
19	A3c(9,22)	9	22	6	3.65	58	88	15.11	4.88	73.67	61.67
20	SC(9,4) (Aa)	9	26	1	3.95	80	80	17.78	2.93	24.11	288.11
21	qA3c(9,26)	9	26	5	3.06	62	80	14.22	3.30	36.55	62.55
22	QC(10,25) (B)	10	25	3	7.00	24	130	22.00	1.13	12.30	72.30
23	A1c(10,25)	10	25	8	6.00	80	140	20.00	9.75	100.80	160.80
24	A2c(10,25)a	10	25	7	5.20	88	128	20.00	6.49	106.70	88.70
25	A2c(10,25)b	10	25	6	5.80	82	136	20.00	7.76	170.60	164.60
26	A2c(10,25)c	10	25	7	5.40	88	132	20.00	7.16	107.70	69.70
27	A2c(10,26)	10	26	7	4.76	79	124	18.40	6.20	107.70	276.70
28	SC(10,4) (Aa)	10	30	1	6.00	120	120	24.00	4.00	38.10	396.10
29	qA3c(10,30)	10	30	5	4.40	88	116	20.00	4.46	97.83	576.50
30	G(12,19)nHI**	12	19	3	2.81	30	132	18.00	18.00	9.25	60.25
31	G(14,22)HI**	14	22	5	3.26	52	200	22.29	24.71	27.36	104.36
32	G(26,25)arvHI**	26	25	3	0.84	26	328	18.46	66.15	14.12	260.12

Figure 4: Some comparisons among polynomial irregularity measures.

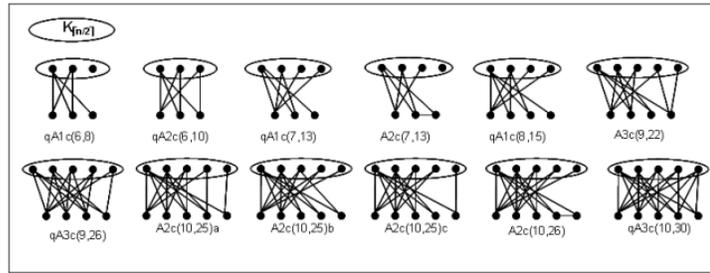


Figure 5: Some antiregular and quasi-antiregular graphs.

Appendix 2: Boxplots

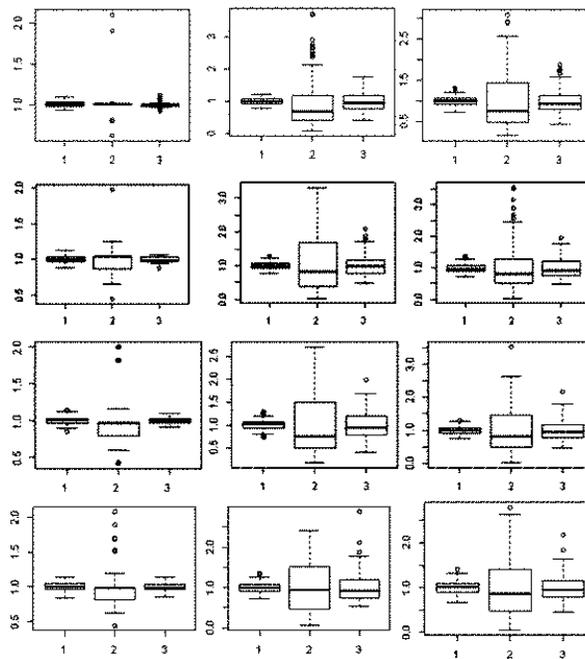


Figure 6: Boxplots, collections from G_{4K4_K5} : 2, 3, 5 and 7 two-exchanges.

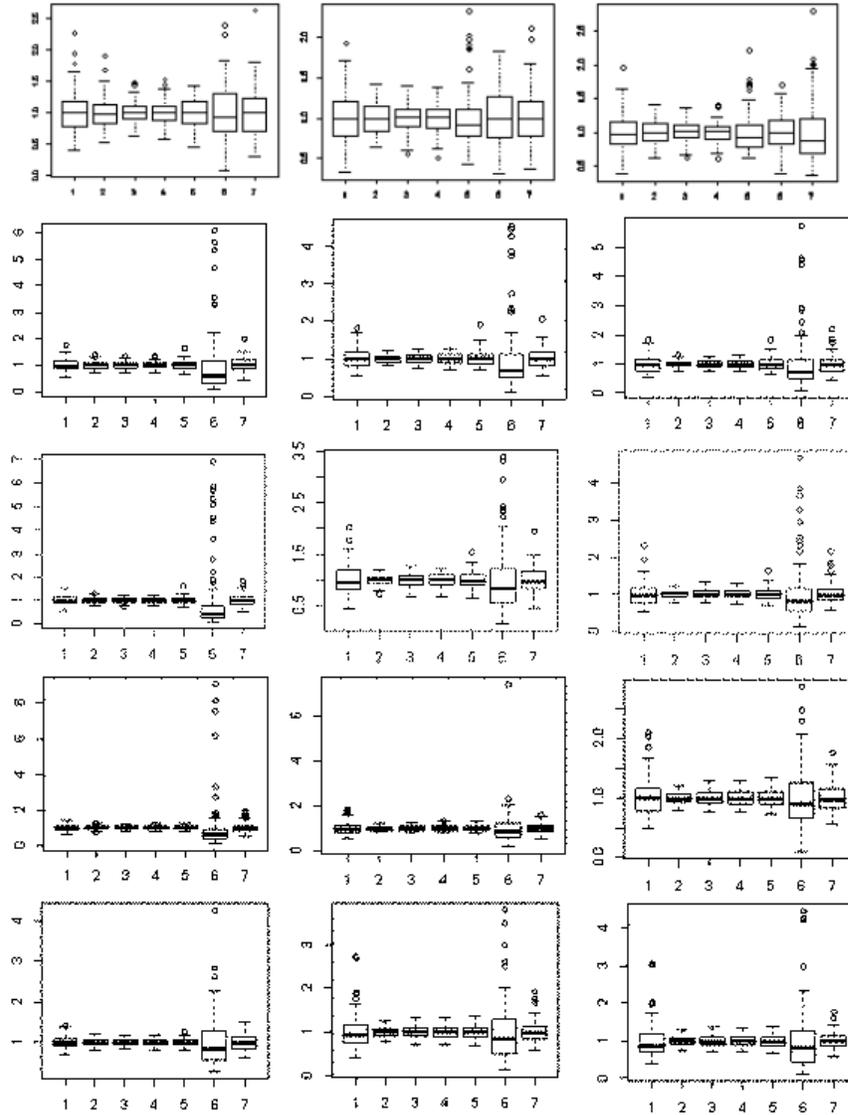


Figure 7: Boxplots from collections r01: 20, 40, 60, 80 and 100 vertices.

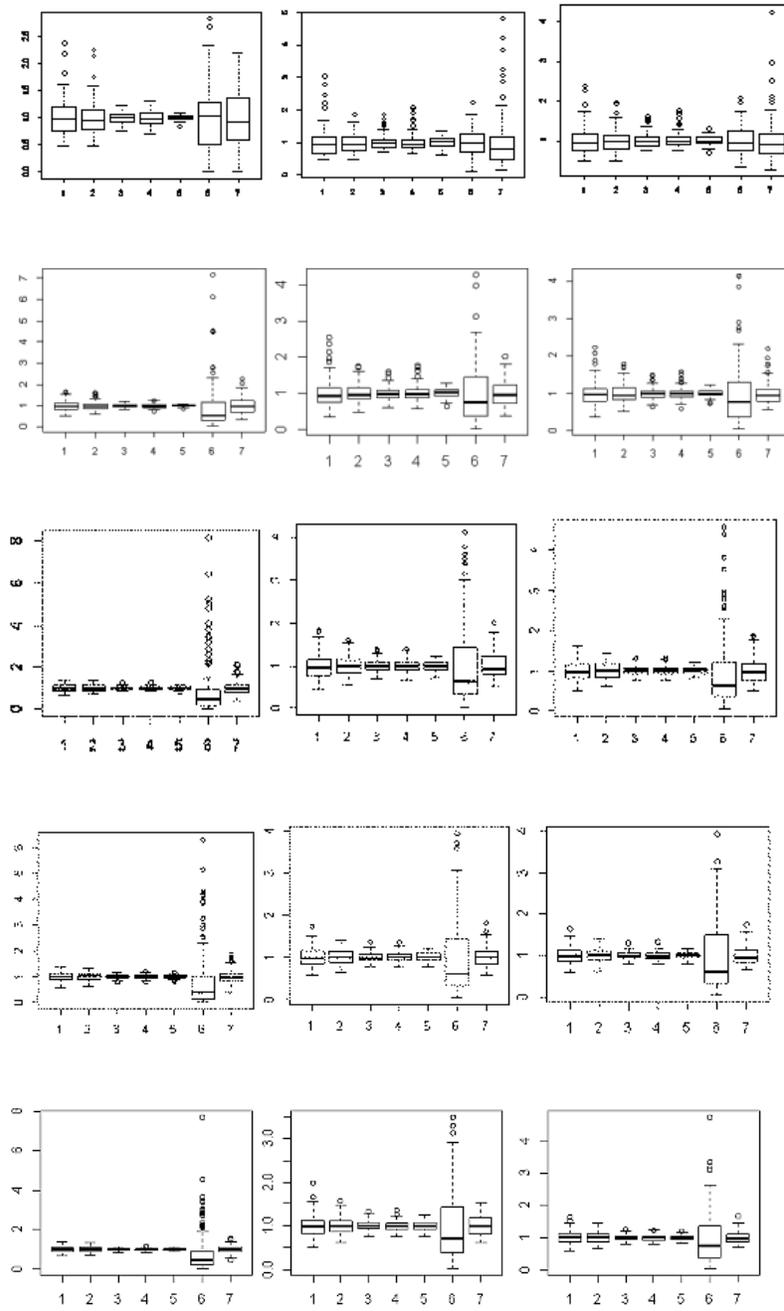


Figure 8: Boxplots from collections r001: 20, 40, 60, 80 and 100 vertices.