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Research Article

Extremal bounds on peripherality measures

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Abstract

Several measures of peripherality for vertices and edges in networks are investigated. Asymptotic bounds are improved on the maximum value achieved by the (i) edge peripherality over connected n-vertex graphs, (ii) edge sum peripherality over connected n-vertex graphs, (iii) edge sum peripherality over n-vertex graphs with diameter at most 2, (iv) edge sum peripherality over bipartite n-vertex graphs with diameter at most 3, and (v) Trinajstić index over n-vertex graphs. The maximum value achieved by the peripherality index over connected n-vertex graphs and n-vertex trees is also computed for all $1 \le n \le 8$. Two conjectures of Furtula are refuted; the first one is on necessary conditions for minimizing the Trinajstić index and the second one is about maximizing the Trinajstić index. Finally, an asymptotic expression for the expected value of the irregularity of the random graph $G_{n,p}$ is found for arbitrary p satisfying $0 < p < 1$.

Keywords: peripherality; sum peripherality; centrality; Trinajstić index; irregularity; Mostar index.

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1. Introduction

A centrality measure is an approximate descriptor of the importance or influence of a vertex in a graph. Central vertices are often ones with large degrees and are critical in the structure of the graph. Peripherality measures are the opposite; peripheral vertices are the least important in a graph. Centrality and peripherality measures can also be defined on edges of a graph.

Geneson and Tsai [9] defined three measures called peripherality, edge peripherality, and edge sum peripherality. They proved extremal results about the minimum and maximum values taken by these measures over connected graphs G of order n. Došlić et al. [5] defined the Mostar index of a graph G. A related index, defined by Miklavič and Šparl [16], is the total Mostar index, or distance-unbalancedness. The Mostar index has been the subject of dozens of papers. Deng and Li [4] proved extremal results about the Mostar index of chemical trees (trees where every vertex has degree at most 4) and general trees of any fixed diameter. In [3], the same authors determined the trees of any fixed degree sequence that maximize the Mostar index. In [10], Ghorbani et al. determined a sufficient condition for the Mostar index of a graph to equal 0. In [14, 15], Miklavič et al. proved bounds on the maximum Mostar index over connected graphs, split graphs, and bipartite graphs. In [11, 12], Kramer and Rautenbach established bounds on the maximum and minimum distance-unbalancedness of trees.

Furtula [7] defined the Trinajstić index of a graph, denoted by $NT(G)$. Furtula [7] ran statistical tests to find the correlation between the Trinajstić index and several other measures, finding a loose correlation with the total Mostar index. Few extremal results about the Trinajstić index have been proven, but computer searches led Furtula to three conjectures on trees that minimize $NT(G)$, graphs that maximize $NT(G)$, and graphs that minimize $NT(G)$.

For an edge $\{u, v\}$ of a graph, Albertson [1] defined its irregularity, denoted by $\mathrm{irr}(\{u, v\})$. Albertson also defined the irregularity of a graph G, denoted by $\mathrm{irr}(G)$. Gao et al. [8] determined the maximum difference $\mathrm{Mo}(T) - \mathrm{irr}(T)$ over n-vertex trees T for all $n \le 22$. Geneson and Tsai [9] proved an asymptotic bound of $n^2(1 - o(1))$.

In Section 3, we improve the extremal bounds on the maximum value attained by $\mathrm{eperi}(G)$ over n-vertex graphs. Whereas Geneson and Tsai proved in [9] that this value was between $\frac{2}{125}n^3$ and $\frac{1}{2}n^3$, we narrow these bounds to $\frac{\sqrt{3}}{24}n^3(1-o(1))$ and $\frac{1}{6}n^3$. In Section 4, we improve the analogous bounds on $\mathrm{espr}(G)$ from $\frac{1}{8}n^4 - O(n^2)$ and n^4 to $\frac{5}{32}n^4 - O(n^3)$ and $\frac{1}{4}n^4$, respectively. Additionally, in Section 4, we prove that the maximum value of $\mathrm{espr}(G)$ over n-vertex graphs G with diameter 2 is $\frac{4}{27}n^4 - O(n^3)$. We also prove that the maximum value of $\mathrm{espr}(G)$ over bipartite n-vertex graphs G with diameter 3 is $\frac{1}{8}n^4 - O(n^2)$. In Section 5, we detail computations that establish the maximum value of the peripherality

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index over n-vertex graphs and over n-vertex trees, $n \leq 8$. In Section 6, we disprove two conjectures from Furtula [7] about the Trinajstić index. One conjecture suggests that every graph with a Trinajstić index of 0 must be regular. We provide several infinite classes of counterexamples to this conjecture. The other conjecture guesses that a certain family of graphs achieves the maximum possible value of the Trinajstić index of an n-vertex graph. We show that this conjecture has infinitely many counterexamples by determining that the maximum value achieved by the Trinajstić index of an n-vertex graph is $(0.5 - o(1))n^4$ and proving that the family described does not achieve this asymptotic maximum.

2. Preliminaries

All graphs discussed are simple finite undirected graphs unless otherwise specified. The set of vertices and the set of edges of a graph G will be denoted by V and E, respectively. For vertices u, v of graph G, $d(u, v)$ is defined to be the graph theoretic distance between u and v. For vertices u, v of graph G, $n_G(u, v)$ is defined to be the number of vertices x of G such that $d(x, u) < d(x, v)$. In other words, it is the number of vertices that are closer to u than to v. Naturally, a vertex u for which $n_G(u, v)$ tends to be relatively small can be considered to be peripheral, and a vertex u for which $n_G(u, v)$ tends to be relatively large can be considered to be central. The peripherality of a vertex, denoted by $\mathrm{peri}(v)$, is the number of vertices u such that $n_G(u, v) > n_G(v, u)$. The peripherality of a graph is defined as $\mathrm{peri}(G) = \sum_{v \in V} \mathrm{peri}(v)$.

The edge peripherality of an edge, denoted by $\mathrm{eperi}(\{u, v\})$, is the number of vertices x such that $n_G(x, u) > n_G(u, x)$ and $n_G(x, v) > n_G(v, x)$. In other words, the vertices x counted are the ones for which more vertices are closer to x than to u and more vertices are closer to x than to v. The edge peripherality of a graph is defined as $\mathrm{eperi}(G) = \sum_{\{u,v\} \in E} \mathrm{eperi}(\{u, v\})$. The edge sum peripherality of an edge is defined as $\mathrm{espr}(\{u, v\}) = \sum_{x \in V - \{u,v\}} (n_G(x, u) + n_G(x, v))$. As with edge peripherality, the edge sum peripherality of a graph is defined as $\mathrm{espr}(G) = \sum_{\{u,v\} \in E} \mathrm{espr}(\{u, v\})$.

The Mostar index of a pair of vertices is defined as $\mathrm{Mo}(\{u, v\}) = |n_G(u, v) - n_G(v, u)|$. Note that the order of u and v does not matter. The Mostar index of a graph is the sum of this quantity over all of its edges, $\mathrm{Mo}(G) = \sum_{\{u,v\} \in E} \mathrm{Mo}(\{u, v\})$. The total Mostar index sums over all pairs of vertices, $\mathrm{Mo}^*(G) = \sum_{\{u,v\} \subset V} \mathrm{Mo}(\{u, v\})$.

The Trinajstić index of a pair of vertices is defined as $NT(\{u, v\}) = (n_G(u, v) - n_G(v, u))^2$. Note that $\{u, v\}$ need not be an edge and that the order of u and v does not matter. This is similar to the definition of the total Mostar index, except that a square, not an absolute value, is taken. As with the total Mostar index, the Trinajstić index of a graph is given by $NT(G) = \sum_{\{u,v\} \subset V} NT(\{u, v\})$.

The irregularity of an edge is defined as $\mathrm{irr}(\{u, v\}) = |\deg(u) - \deg(v)|$. Note that the order of u and v does not matter. As with $\mathrm{Mo}(G)$, the irregularity of a graph is given by $\mathrm{irr}(G) = \sum_{\{u,v\} \in E} \mathrm{irr}(\{u, v\})$. The definition of irregularity is similar to the definition of the Mostar index, except that each n_G has been replaced with the degree of a vertex.

3. Edge peripherality index

In this section, we prove extremal results about the edge peripherality index. We first define a family of graphs that achieves $\mathrm{eperi}(G) \geq \frac{\sqrt{3}}{24} n^3(1 - o(1))$, up from the $\frac{2}{125} n^3$ achieved by the construction in [9]. We also improve the upper bound on $\mathrm{eperi}(G)$ from the $\frac{1}{2} n^3$ given in [9] to $\frac{1}{6} n^3$.

Definition 3.1. *In a graph G, an ordered pair $(\{u, v\}, x)$ consisting of an edge $\{u, v\}$ and a vertex x is said to be* dominant *if $n_G(x, u) > n_G(u, x)$ and $n_G(x, v) > n_G(v, x)$.*

Thus, $\mathrm{eperi}(G)$ is equal to the number of dominant pairs.

Theorem 3.1. *The maximum possible value of* $\mathrm{eperi}(G)$ *among all connected graphs of order n is at least $\frac{\sqrt{3}}{24} n^3(1 - o(1))$.*

Proof. Define the constant $\alpha = \frac{\sqrt{3}-1}{2}$. For each positive integer s, construct the graph G_s as follows.

Start with the following complete graphs:

- $K_{\lfloor \frac{s}{1-\alpha} \rfloor}$ with vertices $a_{-1,1}, a_{-1,2}, \ldots, a_{-1,\lfloor \frac{s}{1-\alpha} \rfloor}$
- $K_{\lfloor s\alpha^i \rfloor}$ with vertices $a_{i,1}, a_{i,2}, \ldots, a_{i,\lfloor s\alpha^i \rfloor}$ for each $i \geq 0$ for which $s\alpha^i \geq 1$. Let $i_{\max}$ be the maximum such i.

Next, connect each complete graph to the same central vertex w through chains of vertices such that larger connected components have longer chains. In particular, for each $-1 \leq i \leq i_{\max}$, construct vertices $b_{i,1}, b_{i,2}, \ldots b_{i,2i_{\max}+1-2i}$. Add an edge between $b_{i,j}$ and $b_{i,j+1}$ for each $1 \leq j \leq 2i_{\max} - 2i$. Then add an edge between $a_{i,1}$ and $b_{i,1}$ and an edge between $b_{i,2i_{\max}+1-2i}$ and w.

We now approximate $\frac{\mathrm{eperi}(G)}{n^3}$. Note that $n = (\frac{s}{1-\alpha} + s + s\alpha + s\alpha^2 + \cdots)(1 \pm o(1)) = \frac{2s}{1-\alpha}(1 \pm o(1))$, neglecting the vertices w and $b_{i,j}$ because they make up only $O(i_{\max}^2) = O((\log s)^2)$ of the $\Theta(s)$ total vertices. Also, vertex w is placed in such a central position that $d(x, w) < d(y, w) \to n_{G_s}(x, y) > n_{G_s}(y, x)$ for all vertices x, y, provided that the largest "arm" extending from

w (the one containing the vertices $a_{-1,j}$) has less than half of the total vertices in the graph. This is true for all $s > \alpha^{-3}$, as shown below.

We want to show that $\left\lfloor \frac{s}{1-\alpha} \right\rfloor + 2i_{\max} + 2$ (the number of vertices in the largest arm) is less than $\sum_{i=0}^{i_{\max}} \lfloor s\alpha^i \rfloor + 2i_{\max} - 2i$ (the total number of vertices in all other arms). Indeed,

$$\begin{aligned}\sum_{i=0}^{i_{\max}} \lfloor s\alpha^i \rfloor + 2i_{\max} - 2i \geq -i_{\max} - 1 + \sum_{i=0}^{i_{\max}} s\alpha^i + 2i_{\max} - 2i = i_{\max}^2 - 1 + \sum_{i=0}^{i_{\max}} s\alpha^i = i_{\max}^2 - 1 + \frac{s}{1-\alpha} - \frac{s\alpha^{i_{\max}+1}}{1-\alpha} \\ > i_{\max}^2 - 1 + \frac{s}{1-\alpha} - \frac{1}{1-\alpha} > \left\lfloor \frac{s}{1-\alpha} \right\rfloor + 2i_{\max} + 2. \qquad (1)\end{aligned}$$

The second-last inequality in (1) follows from the definition of $i_{\max}$ as the greatest i such that $s\alpha^i \geq 1$. The last inequality in (1) holds because $s > \alpha^{-3}$ and so $i_{\max} \geq 4$, and hence $i_{\max}^2 - 2i_{\max} - 3 \geq 5 > \frac{1}{1-\alpha}$.

Having established that the largest arm extending frrom w contains less than half of the total vertices in the graph, it follows that $d(x,w) < d(v,w) \to n_{G_s}(x,v) > n_{G_s}(v,x)$ for all vertices x, y. For every edge $\{u,v\}$ in the complete subgraph consisting of $a_{i,j}$ and for every vertex $x = a_{I,j}$ for $I > i$, we have that $(\{u,v\},x)$ is dominant because x is closer to w than both u and v. When $i = -1$, the edge-vertex pairs described above contribute $\frac{1}{16}n^3(1 \pm o(1))$ dominant pairs. This is because the edge must be chosen from a complete subgraph with $\left\lfloor \frac{s}{1-\alpha} \right\rfloor = \frac{n}{2}(1 \pm o(1))$ vertices, and the vertex must be chosen from a set of $\frac{n}{2}(1 \pm o(1))$ other vertices.

When $i \geq 0$, the edge-vertex pairs described above contribute $\frac{1}{2}(\lfloor s\alpha^i \rfloor)^2 \lfloor s\alpha^I \rfloor$ dominant pairs. We now sum over i and I. In our first step, we remove floor functions and append a factor of $(1 - o(1))$, a step that is justified later.

$$\begin{aligned}\sum_{i=0}^{i_{\max}} \sum_{I=i+1}^{i_{\max}} \frac{1}{2}(\lfloor s\alpha^i \rfloor)^2 \lfloor s\alpha^I \rfloor &= \left[\sum_{i=0}^{\infty} \sum_{I=i+1}^{\infty} \frac{1}{2}(s\alpha^i)^2(s\alpha^I)\right](1-o(1)) = \left[\frac{1}{2}s^3 \sum_{i=0}^{\infty}\sum_{j=1}^{\infty} \alpha^{3i+j}\right](1-o(1)) = \left[\frac{1}{2}s^3 \sum_{i=0}^{\infty} \frac{\alpha^{3i+1}}{1-\alpha}\right](1-o(1)) \\ &= \left[\frac{1}{2}s^3 \frac{\alpha}{(1-\alpha)(1-\alpha^3)}\right](1-o(1)) = \left[\left(\frac{\sqrt{3}}{24} - \frac{1}{16}\right)n^3\right](1-o(1)).\end{aligned}$$

Note that α was chosen to maximize $\frac{\alpha}{(1-\alpha)(1-\alpha)^3}$. We now demonstrate why ignoring the floor functions can be corrected by appending a factor of $(1 - o(1))$, as was done in the first line of the above computation. The difference between the expressions with and without the floor functions is

$$\begin{aligned}-\sum_{i=0}^{i_{\max}} \sum_{I=i+1}^{i_{\max}} \frac{1}{2}(\lfloor s\alpha^i \rfloor)^2 \lfloor s\alpha^I \rfloor + \sum_{i=0}^{\infty} \sum_{I=i+1}^{\infty} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) &= \sum_{i=0}^{i_{\max}} \sum_{I=i+1}^{i_{\max}} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) - \frac{1}{2}(\lfloor s\alpha^i \rfloor)^2 \lfloor s\alpha^I \rfloor + \sum_{i=i_{\max}+1}^{\infty} \sum_{I=i+1}^{\infty} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) \\ &\leq \sum_{i=0}^{i_{\max}} \sum_{I=i+1}^{i_{\max}} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) - \frac{1}{2}(s\alpha^i - 1)^2(s\alpha^I - 1) + \sum_{i=i_{\max}+1}^{\infty} \sum_{I=i+1}^{\infty} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) \\ &\leq \sum_{i=0}^{i_{\max}} \sum_{I=i+1}^{i_{\max}} \frac{1}{2}(2s^2\alpha^{i+I} + s^2\alpha^{2i} + 1) + \sum_{i=i_{\max}+1}^{\infty} \sum_{I=i+1}^{\infty} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) = O(s^2) + \sum_{i=i_{\max}+1}^{\infty} \sum_{I=i+1}^{\infty} \frac{1}{2}(s\alpha^i)^2(s\alpha^I) \\ &= O(s^2) + \frac{1}{2}s^3 \sum_{i=i_{\max}+1}^{\infty} \sum_{I=i+1}^{\infty} \alpha^{2i+I} = O(s^2) + O(s^3\alpha^{3i_{\max}}) = O(s^2). \qquad (2)\end{aligned}$$

The last equality in (2) holds because $s\alpha^{i_{\max}} = O(1)$. The discrepancy caused by ignoring the floor functions is $O(s^2)$ in a $\Theta(s^3)$ expression, so it can be addressed by tacking on a factor of $(1 - o(1))$.

Adding $\left[\left(\frac{\sqrt{3}}{24} - \frac{1}{16}\right)n^3\right](1 - o(1))$ to the previous $\frac{1}{16}n^3(1 \pm o(1))$, we have $\operatorname{eperi}(G) \geq \frac{\sqrt{3}}{24}n^3(1 - o(1))$, as desired. □

Theorem 3.1 is an improvement from the family of graphs provided in Theorem 8.11 of [9] that achieved $\operatorname{eperi}(G) = \frac{2}{125}n^3$. Next, we improve the upper bound on $\operatorname{eperi}(G)$.

Theorem 3.2. *The maximum possible value of* $\operatorname{eperi}(G)$ *among all connected graphs of order* G *is at most* $\frac{1}{6}n^3$.

Proof. Let G be a connected graph with n vertices. For any triple (v_1, v_2, v_3) of vertices, at most one of the following is a dominant pair: $(\{v_1,v_2\},v_3)$, $(\{v_2,v_3\},v_1)$, $(\{v_3,v_1\},v_2)$. For example, if the first two are both dominant pairs, then $n_G(v_1,v_3) > n_G(v_3,v_1) > n_G(v_1,v_3)$, a contradiction. Since there are only $\binom{n}{3} < \frac{1}{6}n^3$ triples of vertices, it follows that the number of dominant pairs is $\operatorname{eperi}(G) < \frac{1}{6}n^3$. □

Theorem 3.2 is an improvement from the $\frac{1}{2}n^3$ upper bound proven in Theorem 8.11 of [9].

4. Edge sum peripherality index

In this section, we first define a family of graphs that achieves $\mathrm{espr}(G) \geq \frac{5}{32}n^4 - O(n^3)$, up from the $\frac{1}{8}n^4 - O(n^2)$ achieved by the construction in [9]. We also improve the upper bound on $\mathrm{espr}(G)$ from n^4 to $\frac{1}{4}n^4$. Furthermore, we prove that the maximum value of $\mathrm{espr}(G)$ over graphs G of diameter 2 is $\frac{4}{27}n^4 - O(n^3)$. Additionally, we find that the maximum value of $\mathrm{espr}(G)$ over bipartite graphs G of diameter at most 3 is $\frac{1}{8}n^4 - O(n^2)$.

Bounds on maximum edge sum peripherality over n-vertex graphs

In Corollary 6.6 of [9], the authors supplied a family of graphs achieving $\mathrm{espr}(G) = \frac{1}{8}n^4 - O(n^2)$. We improve this lower bound through a family of graphs achieving $\mathrm{espr}(G) = \frac{5}{32}n^4 - O(n^3)$. We begin with a helpful lemma.

Lemma 4.1. *We have* $\mathrm{espr}(G) = \sum_{u\in V} \deg(u) \sum_{x\in V} n_G(x,u) - O(n^3)$.

Proof. The lemma follows from the following computation:

$$\begin{aligned}\mathrm{espr}(G) &= \sum_{\{u,v\}\in E}\ \sum_{x\in V-\{u,v\}} n_G(x,u) + n_G(x,v) = \sum_{\{u,v\}\in E}\ \sum_{x\in V} n_G(x,u) + n_G(x,v) - O(n^3)\\ &= 2\sum_{\{u,v\}\in E}\ \sum_{x\in V} n_G(x,u) - O(n^3) = \sum_{u\in V}\deg(u)\sum_{x\in V} n_G(x,u) - O(n^3),\end{aligned}$$

where the factor of 2 is eliminated in the last step to account for double-counting edges. □

Theorem 4.1. *The maximum possible value of* $\mathrm{espr}(G)$ *among all connected graphs of order* G *is at least* $\frac{5}{32}n^4 - O(n^3)$.

Proof. Let $n = 4s+1$. Define vertices a_i, b_i, c_i, d_i for each $1 \leq i \leq s$. Also, define vertex v. Add an edge between a_i and a_j for each $i \neq j$; do the same for b, c, and d. Add an edge between a_i and b_j for each i and j. Add an edge between c_i and d_j for each i and j. Add an edge between v and b_i for each i; do the same for c. We now proceed to compute $\mathrm{espr}(G)$. By Lemma 4.1, we want to compute $\sum_{u\in E}\deg(u)\sum_{x\in V} n_G(x,u)$. For any $1 \leq i,j \leq s$: if $u = a_i$ and $x = b_j$, $x = c_j$, or $x = d_j$, then $\deg(u) \geq 2s-1$ and $n_G(x,u) \geq 2s$; if $u = b_i$ and $x = c_j$ or $x = d_j$, then $\deg(u) \geq 2s$ and $n_G(x,u) \geq 2s$; if $u = c_i$ and $x = a_j$ or $x = b_j$, then $\deg(u) \geq 2s$ and $n_G(x,u) \geq 2s$; if $u = d_i$ and $x = a_j$, $x = b_j$, or $x = c_j$, then $\deg(u) \geq 2s-1$ and $n_G(x,u) \geq 2s$. Summing over all the mentioned four cases, we have $\mathrm{espr}(G) \geq 40s^4 - O(n^3) = \frac{5}{32}n^4 - O(n^3)$, proving the theorem. Note that we are free to ignore the $u = v$ case because we are proving a lower bound. In fact, including the $u = v$ case does not give a better bound because its contribution is $\deg(v)\sum_{x\in V} n_G(x,v) = O(n^3)$. □

This construction is an improvement from the one given in Theorem 6.6 of [9], which achieved $\mathrm{espr}(G) = \frac{1}{8}n^4 - O(n^2)$. We now turn to improve the upper bound.

Theorem 4.2. *The maximum possible value of* $\mathrm{espr}(G)$ *among all connected graphs of order* G *is at most* $\frac{1}{4}n^4$.

Proof. Let G be any connected graph with n vertices. Again by Lemma 4.1,

$$\begin{aligned}\mathrm{espr}(G) &= \sum_{u\in V}\deg(u)\sum_{x\in V} n_G(x,u) - O(n^3) \leq \sum_{u\in V}\deg(u)\sum_{x\in V}(n-\deg(u)) - O(n^3)\\ &= \sum_{u\in V}\deg(u)(n)(n-\deg(u)) - O(n^3) \leq \sum_{u\in V}\frac{1}{4}n^3 - O(n^3) = \frac{1}{4}n^4 - O(n^3).\end{aligned}$$ □

Theorem 4.2 is an improvement from the n^4 upper bound on $\mathrm{espr}(G)$ given in Corollary 6.7 of [9].

Diameter-specific extremal results

Theorem 4.3. *The maximum value of* $\mathrm{espr}(G)$ *over all* n*-vertex graphs* G *of diameter* 2 *is* $\frac{4}{27}n^4 - O(n^3)$.

Proof. Note that $2\sum_{\{u,x\}\in E}\deg(u)\deg(x)$ is the number of walks of length 3, where the direction matters and vertices can be repeated, counted by casework on the two middle vertices. It is known that the number of such walks of length k is at least $\frac{(2|E|)^k}{n^{k-1}}$, a fact which is proven in various forms in [2, 13, 17, 18] and referenced in [6, 19]. The $k = 3$ case tells us that $2\sum_{\{u,x\}\in E}\deg(u)\deg(x) \geq \frac{8|E|^3}{n^2}$, which is used in the following computation.

Let G be a graph with diameter less than or equal to 2. We first prove the upper bound.

$$\mathrm{espr}(G) = \sum_{u\in V}\deg(u)\sum_{w\in V} n_G(w,u) - O(n^3) = \sum_{u\in V}\deg(u)\sum_{w\in V}\sum_{x\in V}\mathbb{1}[d(x,w) < d(x,u)] - O(n^3)$$

$$= \sum_{u\in V}\deg(u)\sum_{x\in V}\begin{cases}0 & \{u,x\}\in E\\ \deg(x) & \text{else}\end{cases} - O(n^3) = \sum_{u\in V}\sum_{x\in V}\begin{cases}0 & \{u,x\}\in E\\ \deg(u)\deg(x) & \text{else}\end{cases} - O(n^3)$$
$$= \sum_{u\in V}\sum_{x\in V}\deg(u)\deg(x) - 2\sum_{\{u,v\}\in E}\deg(u)\deg(x) - O(n^3) \le \sum_{u\in V}\sum_{x\in V}\deg(u)\deg(x) - \frac{8|E|^3}{n^2} - O(n^3)$$
$$= \left(\sum_{u\in V}\deg(u)\right)\left(\sum_{x\in V}\deg(x)\right) - \frac{8|E|^3}{n^2} - O(n^3) = 4|E|^2 - \frac{8|E|^3}{n^2} - O(n^3) \le \frac{4}{27}n^4 - O(n^3).$$

We now prove the lower bound of $\frac{4}{27}n^4 - O(n^3)$. Consider any graph, G, with n vertices such that $\deg(v) = \frac{2}{3}n \pm O(1)$ for each vertex v. We will show that $\mathrm{espr}(G) = \frac{4}{27}n^4 - O(n^3)$. Each $O(n^3)$ below is outside all summations.

$$\mathrm{espr}(G) = \sum_{u\in V}\deg(u)\sum_{x\in V}n_G(x,u) - O(n^3) = \sum_{u\in V}\deg(u)\sum_{x\in V}\begin{cases}0 & \{u,x\}\in E\\ \deg(x) & \text{else}\end{cases} - O(n^3) = \frac{4}{27}n^4 - O(n^3).$$

Thus, the upper and lower bounds have been proven, and the maximum value of $\mathrm{espr}(G)$ over all n-vertex graphs G of diameter 2 is indeed $\frac{4}{27}n^4 - O(n^3)$. □

Theorem 4.4. *The maximum value of* $\mathrm{espr}(G)$ *over all bipartite n-vertex graphs G of diameter at most 3 is* $\frac{1}{8}n^4 - O(n^2)$.

Proof. The lower bound is given by the complete bipartite graph with the maximum number of edges (which has diameter 2). By Corollary 6.6 of [9], this graph has $\mathrm{espr}(G) = \left\lfloor \frac{n^2}{4}\right\rfloor\left(2\left\lfloor\frac{n^2}{4}\right\rfloor - 2\right)$, which is $\frac{1}{8}n^4 - O(n^2)$.

Now, the following computation proves an upper bound on $\mathrm{espr}(G)$ over bipartite graphs G with diameter at most 3. Below, V_u denotes the (vertex set of the) side of the bipartite graph containing u, and V'_u denotes the other side.

$$\mathrm{espr}(G) \le \sum_{u\in V}\deg(u)\sum_{x\in V}n_G(x,u) = \sum_{u\in V}\deg(u)\sum_{x\in V}\sum_{y\in V}\mathbb{1}[d(y,x)<d(y,u)] \le \sum_{u\in V}\deg(u)[|E| + (|V'_u| - \deg(u))n]$$
$$= |E|\sum_{u\in V}\deg(u) + n\sum_{u\in V}\deg(u)(|V'_u| - \deg(u)) = 2|E|^2 + n\left[\sum_{u\in V_1}\deg(u)(|V_2|-\deg(u)) + \sum_{u\in V_2}\deg(u)(|V_1|-\deg(u))\right]$$
$$\le 2|E|^2 + n\left[\sum_{u\in V_1}\frac{|E|}{|V_1|}\left(|V_2| - \frac{|E|}{|V_1|}\right) + \sum_{u\in V_2}\frac{|E|}{|V_2|}\left(|V_1| - \frac{|E|}{|V_2|}\right)\right] = 2|E|^2 + n\left[|V_1|\cdot\frac{|E|}{|V_1|}\left(|V_2| - \frac{|E|}{|V_1|}\right) + |V_2|\cdot\frac{|E|}{|V_2|}\left(|V_1| - \frac{|E|}{|V_2|}\right)\right]$$
$$= 2|E|^2 + n|E|\left(|V_2| - \frac{|E|}{|V_1|} + |V_1| - \frac{|E|}{|V_2|}\right) = 2|E|^2 + n|E|\left(n - \frac{n|E|}{|V_1||V_2|}\right) \le 2|E|^2 + n|E|\left(n - \frac{n|E|}{n^2/4}\right) = |E|(n^2 - 2|E|) \le \frac{n^4}{8},$$

where we have used Lemma 4.1, Jensen's inequality, and the following work.
To upper bound the quantity $\sum_{x\in V}\sum_{y\in V}\mathbb{1}[d(y,x)<d(y,u)]$, we swap the summations and do casework on y.

Case 1: $d(y,u) = 2$. Then $d(y,x) = 1$. Since y must be in V_u, every edge $\{x,y\}$ is counted at most once. Thus, this case contributes at most $|E|$ to the summation.

Case 2: $d(y,u) = 3$. Then y is in V'_u but is not a neighbor of u. After choosing y, there are at most n choices for x. Thus, this case contributes at most $(|V'_u| - \deg(u))n$.
This justifies the following inequality used in the above computation: $\sum_{x\in V}\sum_{y\in V}\mathbb{1}[d(y,x)<d(y,u)] \le |E| + (|V'_u| - \deg(u))n$. □

Although the proof of Theorem 4.4 is specific to bipartite graphs of diameter at most 3, we conjecture that the bound holds for all bipartite graphs.

Conjecture 4.1. *The maximum value of* $\mathrm{espr}(G)$ *over all bipartite n-vertex graphs G is* $\frac{1}{8}n^4 - O(n^2)$.

5. Peripherality index

We compute the exact value of the maximum peripherality index over connected n-vertex graphs and over n-vertex trees for $n \le 8$. The authors of [9] prove that this maximum is given by $\binom{n}{2}$ for $n \ge 9$ (for both trees an connected graphs).

We first establish the following lemma.

Lemma 5.1. *Any n-vertex graph G with a nontrivial automorphism has* $\mathrm{peri}(G) < \binom{n}{2}$.

Proof. Let u be a vertex mapped to a vertex $v \notin \{u\}$ by some nontrivial automorphism on $\mathrm{spr}(G)$. Then $n_G(u,v) = n_G(v,u)$. It follows that $\mathrm{peri}(G) = \sum_{u\neq v}\mathbb{1}[n_G(u,v) \neq n_G(v,u)] < \binom{n}{2}$, proving the lemma. □

Theorem 5.1. *The maximum value of the peripherality index over connected n-vertex graphs and over n-vertex trees for $n \le 8$ is given in Table 1.*

n	1	2	3	4	5	6	7	8
$\max \mathrm{peri}(T)$	0	0	2	4	9	13	21	27
$\max \mathrm{peri}(G)$	0	0	2	5	9	15	21	28

Table 1: The maximum value of $\mathrm{peri}(T)$ and $\mathrm{peri}(G)$ over n-vertex trees T and connected n-vertex graphs, G, for $1 \leq n \leq 8$.

Proof. For $n \leq 4$, an exhaustive search of all trees and graphs is feasible, and the results are given as follows. For $n = 4$, the maximum over trees is achieved by the 4-vertex path, and the maximum over connected graphs is given by a triangle with a pendent vertex. For some of the values $n \geq 5$, we make claims about how few n-vertex trees or n-vertex graphs there are that lack nontrivial automorphisms. These claims can be verified by drawing a vertex and three neighbors, then exhausting the ways to add the remaining edges in the graph in a way that eliminates nontrivial automorphisms. The only connected graphs that do not have any vertices with at least three neighbors are path and cycle graphs, which have nontrivial automorphisms for all $n \geq 2$. For $n = 5$, note that any 5-vertex graph, G, has a nontrivial automorphism. Thus, by Lemma 5.1, $\mathrm{peri}(G) \leq \binom{5}{2} - 1 = 9$. Equality is achieved by the spider with legs of lengths 1, 1, and 2. For $n = 6$ over connected graphs, $\mathrm{peri}(G) = \binom{6}{2} = 15$ is achieved by the graph with vertices $1, 2, \ldots, 6$ and edges $\{\{1,2\},\{2,3\},\{3,4\},\{4,5\},\{5,6\},\{3,5\}\}$. For $n = 6$ over trees, every tree has a nontrivial automorphism. Of these trees, if some automorphism maps u_1 to v_1 and u_2 to v_2 for distinct u_1, u_2, v_1, v_2, then we have $n_G(u_1, v_1) = n_G(v_1, u_1)$ and $n_G(u_2, v_2) = n_G(v_2, u_2)$, so by similar reasoning to that used to prove Lemma 5.1, $\mathrm{peri}(T) \leq \binom{6}{2} - 2 = 13$. The only tree that is not taken into account by the above argument is the spider with legs of length 1, 1, and 3, which has an index of 12. $\mathrm{spr}(T) = 13$ is achieved by the spider with legs of lengths 1, 2, and 2. For $n = 7$, the balanced spider with legs of length 1, 2, and 3 achieves $\mathrm{peri}(G) = \binom{7}{2} = 21$. For $n = 8$ over connected graphs, $\mathrm{peri}(G) = \binom{8}{2} = 28$ is achieved by the graph with vertices $1, 2, \ldots, 8$ and edges $\{\{1,2\},\{2,3\},\{3,4\},\{4,5\},\{5,6\},\{6,7\},\{7,8\},\{4,6\}\}$. For $n = 8$ over trees, the spider with legs of length 1, 1, 2, and 3 achieves $\mathrm{peri}(T) = 27$. To see why $\mathrm{peri}(T) = \binom{8}{2} = 28$ is not achievable, by Lemma 5.1, it suffices to check trees with no nontrivial automorphism. The only such tree is the spider with legs of length 1, 2, and 4, which has $\mathrm{peri}(T) < 28$. □

6. Trinajstić index

Conjecture 3.2 of [7] suggests that every graph with a Trinajstić index of 0 must be regular. Conjecture 3.3 of [7] suggests that the maximal value of the Trinajstić index among all n-vertex graphs G is achieved by "a complete subgraph $K_{\lceil n/2 \rceil}$, on whose vertices are attached $\lfloor n/2 \rfloor$ pendent vertices." Both conjectures were based on a computer search of all graphs with 5 to 10 vertices. In this section, we prove that the conjecture is false for infinitely many values of n. To do so, we first show that the maximum value of $NT(G)$ over all graphs G is $(0.5 - o(1))n^4$. Additionally, we present a class of counterexamples to Conjecture 3.2 of [7].

Conjecture 3.3 of [7] states the following:

Conjecture 6.1 (see [7])**.** *The graph with the maximal value of the Trinajstić index is unique. It consists of a complete subgraph $K_{\lceil n/2 \rceil}$, on whose vertices are attached $\lfloor n/2 \rfloor$ pendent vertices. One pendent vertex is allowed per vertex that belongs to the complete subgraph.*

Conjecture 6.1 is false because the graph that it describes does not achieve the asymptotic maximum of $(0.5 - o(1))n^4$ which is proven below.

Theorem 6.1. *The maximum value of $NT(G)$ over all connected graphs G is $(0.5 - o(1))n^4$.*

Proof. We first show the upper bound. Each of the $\binom{n}{2}$ pairs of vertices contributes at most $(n-2)^2$ to $NT(G)$, giving an upper bound of $\binom{n}{2}(n-2)^2 = (0.5 - o(1))n^4$. To show the lower bound, we consider the Trinajstić index of balanced spider graphs. As in [9], let $S_{a,b}$ denote the balanced spider graph with a legs of length b, each attached to a central vertex (for a total of $ab + 1$ vertices). For any vertices u, v with $d(u, c) \neq d(v, c)$ (where vertex c is the center of $S_{a,b}$), we have $(n_G(u, v) - n_G(v, u))^2 \geq (n - 2b)^2$. There are at least $\frac{n(n-a)}{2}$ such pairs u, v, so

$$NT(S_{a,b}) \geq \frac{n(n-a)}{2}(n-2b)^2 \geq \frac{n^2(1-\frac{1}{b})}{2} n^2 \left(1 - \frac{2}{a}\right)^2 \geq n^4(0.5)\left(1 - \frac{1}{b} - \frac{4}{a}\right);$$

the second inequality uses the fact that $n = ab + 1$, and the third uses the inequality $(1-x)(1-y)(1-z) \geq 1 - x - y - z$ with $x = \frac{1}{b}$ and $y = z = \frac{2}{a}$, which holds for all $0 \leq x, y, z, \leq 1$.

Choosing a and b to be arbitrarily large, we have that $NT(S_{a,b}) = (0.5 - o(1))n^4$, proving the lower bound. □

Theorem 6.2. *Conjecture 6.1 is false for infinitely many n.*

Proof. Consider the graph, G, described in the conjecture, "a complete subgraph $K_{\lceil n/2 \rceil}$, on whose vertices are attached $\lfloor n/2 \rfloor$ pendent vertices. One pendent vertex is allowed per vertex that belongs to the complete subgraph." Choosing u from the complete subgraph and v from the set of pendent vertices makes $(n_G(u,v) - n_G(v,u))^2$ at most n^2. All other choices of $\{u,v\}$ contribute negligibly, if at all, to $NT(G)$. Thus, $NT(G) = 0.25n^4(1 \pm o(1))$ for the graph G described in the conjecture. By Theorem 6.1, there exist arbitrarily large graphs that have a greater Trinajstić index than the graph given by Conjecture 6.1. □

Conjecture 3.2 of [7] suggests the following:

Conjecture 6.2 (see [7]). *The minimum value of the Trinajstić index is equal to 0. The necessary but not sufficient condition for a graph to reach the minimum of the Trinajstić index is to be a regular graph.*

In the proof of the following theorem, we provide a class of counterexamples to Conjecture 6.2.

Theorem 6.3. *There exist arbitrarily large connected graphs that are not regular but that achieve the minimum Trinajstić index of 0.*

Proof. For any integer a, let $n_a(u,v)$ be the number of vertices, x, such that $d(x,u) < a + d(x,v)$. Let $N_a(u,v) = n_a(u,v) - n_a(v,u)$. Note that $NT(G) = 0$ if $N_0(u,v) = 0$ for all pairs u, v of vertices. We will call such a graph NT-balanced. Call a graph ultra NT-balanced if $N_a(u,v) = 0$ for all integers a and vertices u, v.

Obviously, every ultra NT-balanced graph is also NT-balanced. Furthermore, the graphs of the rhombic dodecahedron and rhombic triacontahedron (shown in Figure 1) are both ultra NT-balanced. Neither graph is regular. To generate arbitrarily large counterexamples, we prove the next claim.

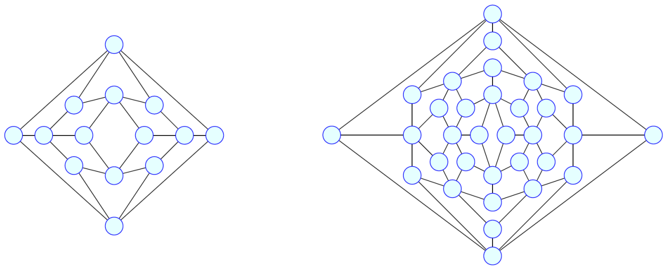

Figure 1: The graphs of the rhombic dodecahedron (left) and rhombic triacontahedron (right).

Claim 6.1. *If G and H are ultra NT-balanced, then their Cartesian product $G \Box H$ is as well.*

Proof. Let $\{x_1, x_2, \ldots, x_m\}$ be the vertex set of G and $\{y_1, y_2, \ldots, y_n\}$ be the vertex set of H. Let $z_{i,j}$ denote the vertex of $G \Box H$ that corresponds to vertex x_i in graph G and vertex y_j in graph H. Fix integer a' and vertices $u = z_{i_1,j_1}$ and $v = z_{i_2,j_2}$. We aim to show that $n_{a'}(u,v) = n_{a'}(v,u)$. For $(a,b) \in \{1,2,\ldots,m\}^2$, let $s(a,b) = d(x_a, x_b)$ in G. For $(c,d) \in \{1,2,\ldots,n\}^2$, let $t(c,d) = d(y_c, y_d)$ in H. We have $d(z_{a,c}, z_{b,d}) = s(a,b) + t(c,d)$ in $G \Box H$. Since G is ultra NT-balanced, it follows that there exists an involution X on $\{1,2,\ldots,m\}$ such that $s(i,i_1) - s(i,i_2) = -s(X(i),i_1) + s(X(i),i_2)$ holds for all $i \in \{1,2,\ldots,m\}$. In other words, this involution pairs vertices that are counted in $n_{a''}(x_{i_1}, x_{i_2})$ with vertices that are counted in $n_{a''}(x_{i_2}, x_{i_1})$ for each integer a'', and such an involution is guaranteed to exist because each counts the same number of vertices by ultra NT-balancedness of G. Define an analogous involution Y on $\{1,2,\ldots,n\}$. Then $Z((i,j)) = (X(i), Y(j))$ is an involution on $\{1,2,\ldots,m\} \times \{1,2,\ldots,n\}$ with the property that

$$
\begin{aligned}
&d(z_{i,j}, z_{i_1,j_1}) - d(z_{i,j}, z_{i_2,j_2}) = (s(i,i_1) + t(j,j_1)) - (s(i,i_2) + t(j,j_2)) = (s(i,i_1) - s(i,i_2)) + (t(j,j_1) - t(j,j_2)) \\
&= (-s(X(i),i_1) + s(X(i),i_2)) + (-t(Y(j),j_1) + t(Y(j),j_2)) \\
&= -(s(X(i),i_1) + t(Y(j),j_1)) + (s(X(i),i_2) + t(Y(j),j_2)) = -d(z_{X(i),Y(j)}, z_{i_1,j_1}) + d(z_{X(i),Y(j)}, z_{i_2,j_2}).
\end{aligned}
$$

Therefore, this involution Z pairs vertices $z_{i,j}$ that are counted in $n_{a'}(u,v)$ with vertices $z_{X(i),Y(j)}$ that are counted in $n_{a'}(v,u)$, proving that $n_{a'}(u,v) = n_{a'}(v,u)$. Thus, $G \Box H$ is ultra NT-balanced, as claimed. □

The desired arbitrarily large counterexamples follow easily from Claim 6.1; for example, by crossing the rhombic dodecahedron graph with K_n or C_n for arbitrary n. □

Remark 6.1. *Every NT-balanced graph whose existence is implied by the proof of Theorem 6.3 is also Ultra NT-balanced. Thus, we set forth the following conjecture.*

Conjecture 6.3. *Every NT-balanced graph is also Ultra NT-balanced.*

7. Discussion and future directions

In this paper, we improved the bounds on the maximum value achieved by eperi and espr over n-vertex graphs and over other classes of graphs. We computed the maximum of peri over n-vertex trees and graphs for $n \le 8$, completing a result from [9] that does the same for $n \ge 9$. We disproved two conjectures from [7] about graphs that maximize and minimize the Trinajstić index.

One direction for future research is to continue improving bounds on the maxima of $\mathrm{eperi}, \mathrm{espr}$, and NT over connected graphs. The corresponding maxima of these measures over bipartite graphs also remain open. Another is the investigation of the expected value of peripherality indices of random graphs. For example, [9] proves the following result:

Theorem 7.1. *The expected value of* $\mathrm{irr}(G_{n,\frac{1}{2}})$ *is* $\frac{n^{5/2}(1-o(1))}{4\sqrt{\pi}}$.

This result can be generalized to any probability $0 < p < 1$ in place of $\frac{1}{2}$.

Theorem 7.2. *For any fixed* $0 < p < 1$*, the expected value of irr*$(G_{n,p})$ *is* $= p\sqrt{\frac{p(1-p)}{\pi}}n^{5/2}(1 \pm o(1))$

Proof. By linearity of expectation, it suffices to find the contribution from each unordered pair (u, v) and multiply it by $\binom{n}{2}$. Let u and v be the two vertices. The probability that they are connected by an edge is p. For all vertices $w \notin \{u, v\}$, let $X_w = \mathbb{1}[\{u, w\} \in E] - \mathbb{1}[\{v, w\} \in E]$. Thus, X_w is 1 with probability $p(1-p)$, -1 with probability $p(1-p)$, and 0 otherwise. It follows that the distribution X_w has standard deviation $\sqrt{2p(1-p)}$, and all $n-2$ of them are independent. By the Central Limit Theorem, the limit of the distribution $\frac{\deg(u)-\deg(v)}{\sigma} = \frac{\sum_{w \notin \{u,v\}} X_w}{\sigma}$ as $n \to \infty$ is the normal distribution with mean 0 and standard deviation 1, where $\sigma = \sqrt{2p(1-p)(n-2)}$. Let k be the mean absolute deviation of this distribution. The limit of the expected value of $\frac{|\deg(u)-\deg(v)|}{\sigma}$ as $n \to \infty$ is k. Thus, the expected value of $|\mathrm{irr}(G_{n,p})|$ is $\binom{n}{2}k\sigma = (1 \pm o(1))pk\sqrt{\frac{p(1-p)}{2}}n^{2.5}$. We now compute k, the mean absolute deviation of a normal distribution with standard deviation 1.

$$k = \int_{-\infty}^{\infty} |x| \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} \mathrm{d}x = 2 \cdot \frac{1}{\sqrt{2\pi}} \int_0^{\infty} x e^{-\frac{1}{2}x^2} \mathrm{d}x = -\sqrt{\frac{2}{\pi}} \left[e^{-\frac{1}{2}x^2}\right]_0^{\infty} = \sqrt{\frac{2}{\pi}}.$$

Plugging in this value of k, we now have that the expected value of $|\mathrm{irr}(G_{n,p})|$ is

$$(1 \pm o(1))pk\sqrt{\frac{p(1-p)}{2}}n^{2.5} = (1 \pm o(1))p\sqrt{\frac{p(1-p)}{\pi}}n^{2.5}.$$ □

Another direction for future research is to attempt to define peripherality measures that harness the full structure of chemical networks. Chemical networks, such as MOZART-4 and SuperFast, consist not of undirected edges, but rather of chemical reactions with several reactants and several products. However, most existing measures, including all of the measures studied in this paper, are specific to undirected graphs.

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