Extremal Bounds on Peripherality Measures

Introduction

Graphs are mathematical structures, consisting of vertices and connections between them, called edges. These structures have been used to study many real-world phenomena, such as an infection spreading through a population. For example, a person who maintains a lot of social connections during an epidemic tends to be especially likely to spread a contagious disease; in the context of graph theory, such a person is considered to be central to the social network. Conversely, someone whose lack of social connections makes them unlikely to spread a contagious disease would be considered peripheral to the social network. There are several numerical measures of centrality and peripherality in the literature, which quantify the extent to which vertices or edges in a graph are central or peripheral and can be computed based on the structure of the graph. Centrality and peripherality also have applications in chemical reaction systems and neural networks. In chemical reaction systems, centrality measures can be used to determine the most important chemicals. In neural networks, peripheral vertices are slower to affect the flow of information, so peripherality measures can be used to analyze the efficiency of neural networks. Besides centrality and peripherality measures, there are also measures of graph unbalancedness, which quantify the extent to which graphs contain both central and peripheral vertices. We investigate measures of peripherality called the peripherality index, edge peripherality, and edge sum peripherality, and an unbalancedness index called the Trinajstić index. We present results about the maximum peripherality and the minimum and maximum unbalancedness of n-vertex graphs.

Preliminaries

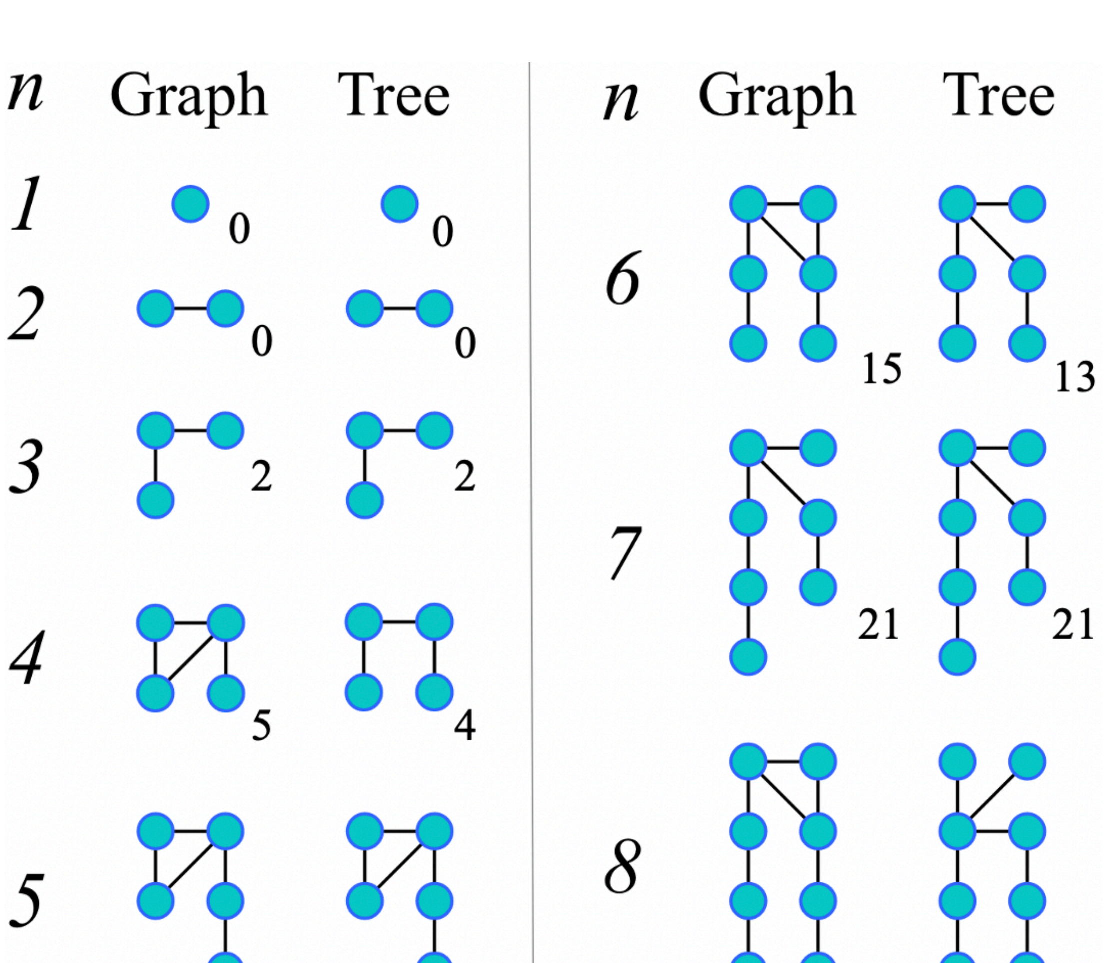
The distance between two vertices, u and v, of a graph G is the minimum number of edges that can traversed to get from u to v, and it is denoted $d(u, v)$. To ensure that this quantity is always defined, all graphs discussed are assumed to be connected, meaning that it is possible to traverse between any pair of vertices. Define $n_G(u, v)$ 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.

Peripherality Index

The peripherality index of a vertex, denoted by $\text{peri}(v)$, is the number of vertices u such that $n_G(u, v) > n_G(v, u)$. The peripherality index of a graph is defined as $\text{peri}(G) = \sum_{v \in V} \text{peri}(v)$.

The exact maximum possible value of $\text{peri}(G)$ over n-vertex graphs and over n-vertex trees was previously known to be equal to $\binom{n}{2}$ for all $n \geq 9$. We complete this result by computing these maxima for all $n \leq 8$. The main technique used to identify the cases in which $\binom{n}{2}$ is not achievable is the observation that if G has vertices u, v and a nontrivial automorphism that maps u to v, then $n_G(u, v) = n_G(v, u)$, preventing $\text{peri}(G)$ from achieving $\binom{n}{2}$.

One graph that achieves each maximum is shown below, along with its peripherality index.

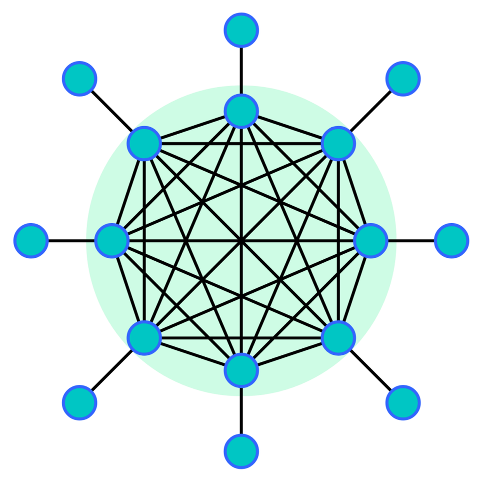


Trinajstić Index

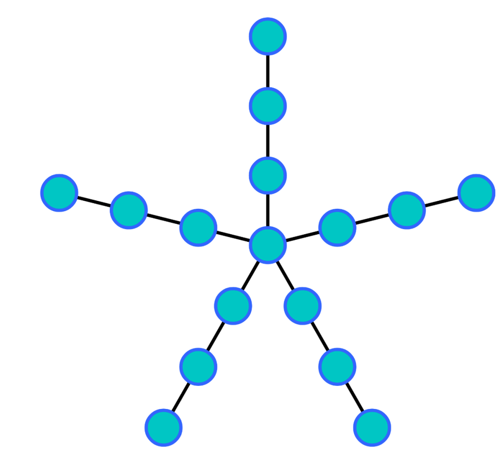
The Trinajstić index of a pair of vertices is defined as $NT(\{u, v\}) = (n_G(u, v) - n_G(v, u))^2$. Note that $\{u, v\}$ need not be an edge and that the order of u and v does not matter. The Trinajstić index of a graph is given by $NT(G) = \sum_{\{u,v\} \subset V} NT(\{u, v\})$.

We refute two conjectures about graphs that minimize and maximize the Trinajstić index.

The first of these conjectures is that the Trinajstić index of an n-vertex graph is maximized by taking a complete subgraph with half of the vertices and attaching a pendent vertex to each vertex of the subgraph. This graph has a Trinajstić index of $\frac{1}{4}n^4(1 \pm o(1))$. We disprove the conjecture by proving that the spider graph $S_{a,b}$ with a legs of b vertices each achieves a greater Trinajstić index when a and b both go to infinity. In fact, $NT(S_{a,b}) = \frac{1}{2}n^4(1 - o(1))$, which achieves the greatest possible leading term. Examples of both graphs are shown below.

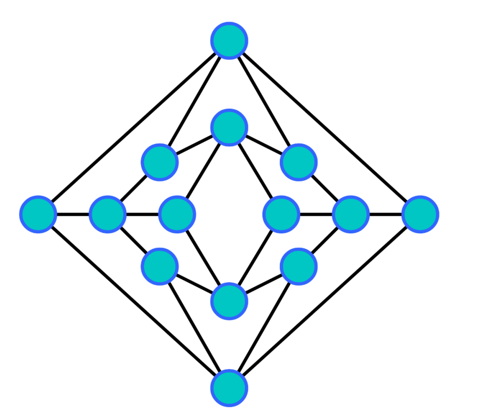


Example of the graph described by the refuted conjecture on maximizing $NT(G)$, with $n = 16$ vertices.

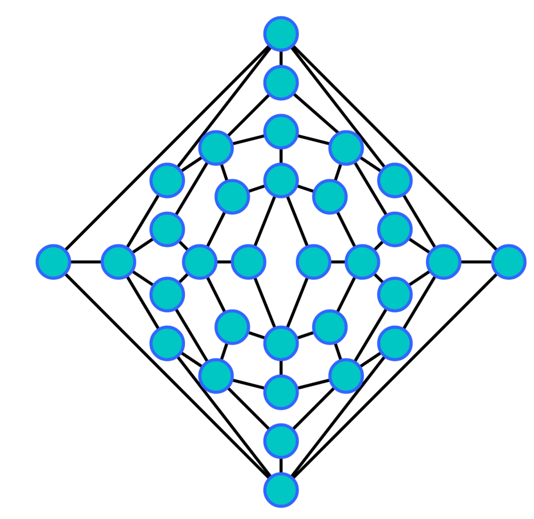


The spider graph $S_{5,3}$

The second conjecture is that every graph with a Trinajstić index of 0 is a regular graph (meaning that every vertex has equally many neighbors). Examples of such graphs include the complete graph K_n, the complete bipartite graph $K_{n,n}$, and the cycle C_n. Note that the condition $NT(G) = 0$ is equivalent to the condition that all pairs u, v of vertices satisfy $n_G(u, v) = n_G(v, u)$. Call a graph *NT-balanced* if it satisfies this condition. We first disprove the conjecture by supplying two NT-balanced graphs that are not regular, namely the graphs of the rhombic dodecahedron and the rhombic triacontahedron (which have 14 and 32 vertices, respectively). Due to the symmetries of these graphs, only two pairs of vertices of the rhombic dodecahedron and three pairs of vertices of the rhombic triacontahedron need to be checked manually for the condition that $n_G(u, v) = n_G(v, u)$ to confirm their NT-balancedness.



The graph of the rhombic dodecahedron



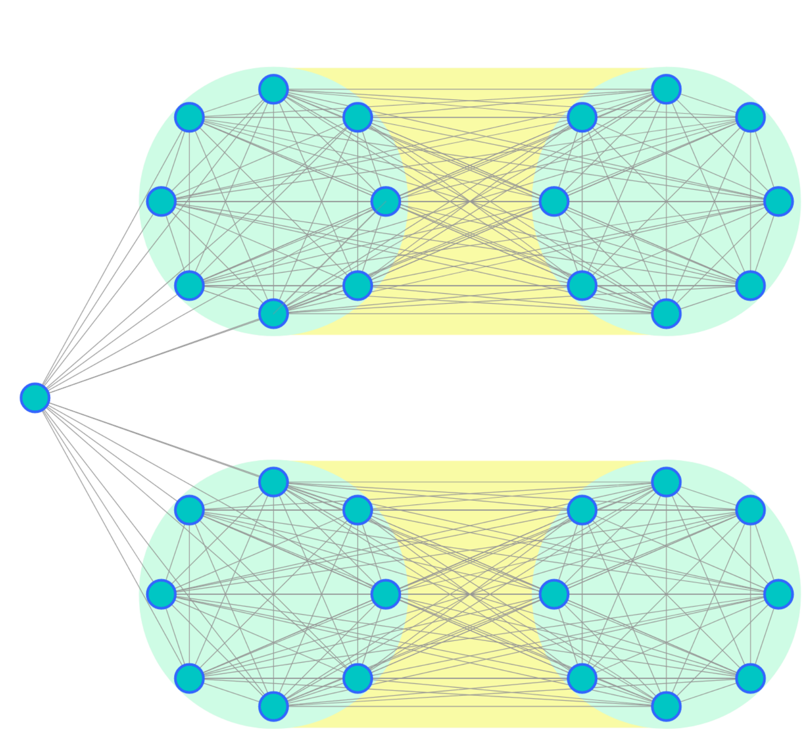
The graph of the rhombic triacontahedron

It turns out that there are not just two, but infinitely many counterexamples to the second conjecture. To generate these counterexamples, we first strengthen the condition of NT-balancedness. For any integer a, define $n_a(u, v)$ to be the number of vertices, x, such that $d(x, u) < a + d(x, v)$. Then call a graph *ultra NT-balanced* if every pair u, v of vertices satisfies $n_a(u, v) = n_a(v, u)$. Since n_0 and n_G are equivalent, we have that every ultra NT-balanced graph is also NT-balanced. It turns out that K_n, $K_{n,n}$, C_n, and the graphs of the rhombic dodecahedron and the rhombic triacontahedron are also ultra NT-balanced. The critical observation is that the Cartesian product of two ultra NT-balanced graphs is, itself ultra NT-balanced. From this observation, there are many ways to generate infinitely many irregular graphs with Trinajstić index 0, such as taking the product of the rhombic dodecahedron graph with K_n for arbitrary n.

Edge Sum Peripherality

The edge sum peripherality of an edge is defined as $\text{espr}(\{u, v\}) = \sum_{x \in V - \{u,v\}} (n_G(x, u) + n_G(x, v))$. The edge sum peripherality of a graph is defined as $\text{espr}(G) = \sum_{\{u,v\} \in E} \text{espr}(\{u, v\})$.

The maximum possible value of $\text{espr}(G)$ over n-vertex graphs G was previously known to lie in the interval $[\frac{1}{8}n^4 - O(n^2), n^4]$. We improve these bounds to $[\frac{5}{32}n^4 - O(n^3), \frac{1}{4}n^4]$. The construction that achieves the improved lower bound is shown below. We also determine the leading terms of the maximums over n-vertex graphs of diameter 2 and n-vertex bipartite graphs of diameter at most 3, namely $\frac{4}{27}n^4$ and $\frac{1}{8}n^4$, respectively.

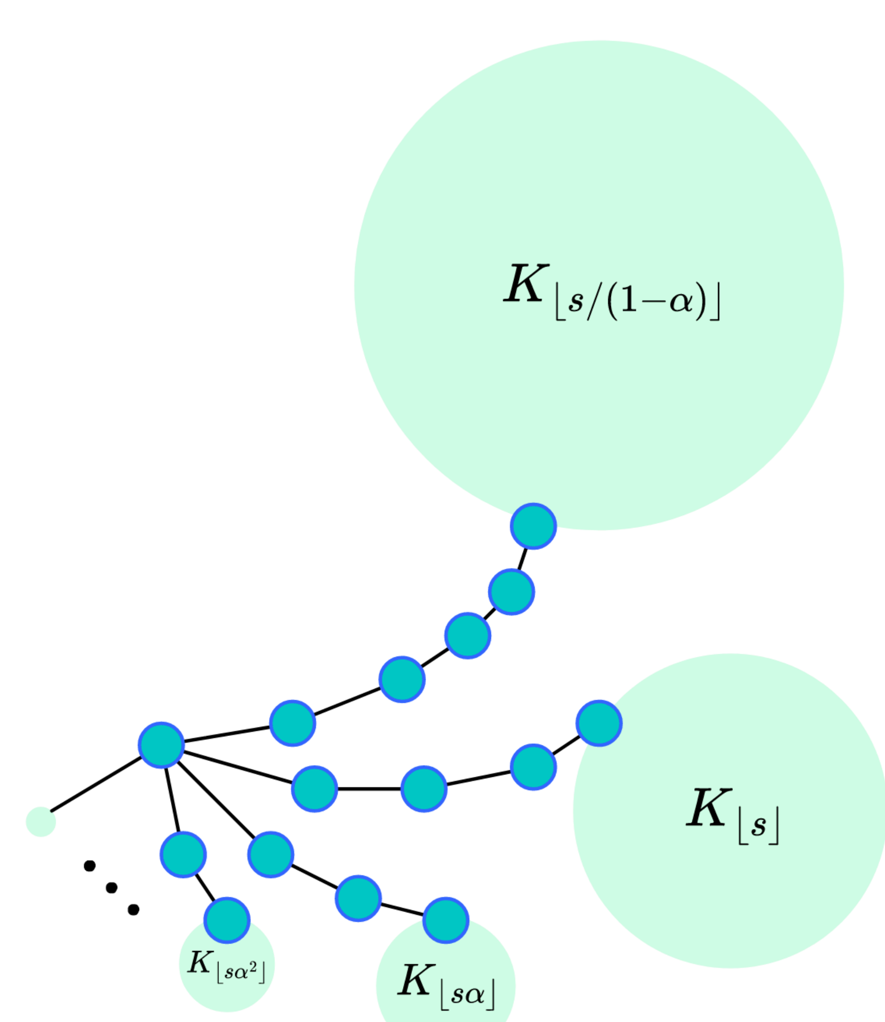


Increasing the number of vertices in each complete subgraph together, espr(G) achieves $\frac{5}{32}n^4 - O(n^3)$.

Edge Peripherality

The edge peripherality of an edge, denoted by $\text{eperi}(\{u, v\})$, 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 $\text{eperi}(G) = \sum_{\{u,v\} \in E} (\{u, v\})$.

The maximum possible value of $\text{eperi}(G)$ over n-vertex graphs G was previously known to lie in the interval $[\frac{2}{125}n^3, \frac{1}{2}n^3]$. We improve these bounds to $[\frac{\sqrt{3}}{24}n^3(1 - o(1)), \frac{1}{6}n^3]$. The construction that achieves the improved lower bound is shown below. Here, K_r denotes a complete subgraph with r vertices.



As s increases, eperi(G) achieves $\frac{\sqrt{3}}{24}n^3(1 - o(1))$.

References

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