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 him 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 unbalance, 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 unbalance index called the Trinajstić index. We present results about the maximum peripherality and the minimum and maximum unbalance 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 be traversed to get from u to v, and it is denoted d(u, v). To ensure that this quantity is all defined, all graphs discussed are assumed to be connected, meaning that it is possible to traverse between any pair of vertices. Define \( n_u(v) \) to be the number of vertices of G such that d(u, v) < d(v, v). In other words, it is the number of vertices that are closer to u than to v. Naturally, a vertex u for which \( n_u(v) \) tends to be relatively small can be considered peripheral, and a vertex v for which \( n_u(v) \) tends to be relatively large can be considered to be central.

Peripherality Index
The peripherality index of a vertex, denoted by \( p(v) \), is the number of vertices u such that \( n_u(v) > n_v(u) \). The peripherality index of a graph is defined as \( P(G) = \sum_v p(v) \).

The exact maximum possible value of \( P(G) \) over n-vertex graphs and over n-vertex trees was previously known to be equal to \( \binom{n-1}{2} \) for all n ≥ 2. We complete this result by computing these maxima for all n ≤ 8. The main technique used to identify the cases in which \( P(G) \) is not achievable is the observation that G has vertices u and v and a nontrivial automorphism which maps u to v, then \( n_u(v) = n_v(u) \), preventing \( P(G) \) from achieving \( \binom{n-1}{2} \).

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

Tinajstić Index
The Trinajstić index of a pair of vertices is defined as \( N_T(u, v) = n_u(v) - n_v(u) \). 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 \( N_T(G) = \sum_v N_T(u, v) \). 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 pendant vertex to each vertex of the subgraph. This graph has a Trinajstić index of \( \left[ \binom{n}{2} (1 + o(1)) \right] \). We disprove the conjecture by proving that the spider graph \( S_{n, 1} \) with a leg of b vertices each achieves a greater Trinajstić index when a and b both go to infinity. In fact, \( N_T(S_{n, b}) = \left[ \frac{b}{4} (1 - o(1)) \right] \), which achieves the greatest possible leading term. Examples of both graphs are shown below.

The spider graph \( S_{n, 1} \)

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 N-T-balancedness. For any integer a, define \( n_a(v) \) to be the number of vertices, x, such that \( d(x, v) < d(x, w) \). Then call a graph ultra N-T-balanced if every pair of vertices satisfies \( n_a(v) = n_a(u) \). Since \( n_0 \) and \( n_a \) are equivalent, we have that every ultra N-T-balanced graph is also ultra N-T-balanced. It turns out that \( K_n, C_n, C_4 \), and the graphs of the rhombic dodecahedron and the rhombic triacontahedron are also ultra N-T-balanced. The critical observation is that the Cartesian product of two ultra N-T-balanced graphs is itself ultra N-T-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 \( e_p(u, v) = n_u(v) + n_v(u) \). The edge sum peripherality index of a graph is defined as \( E_p(G) = \sum_{u \neq v} e_p(u, v) \).

The maximum possible value of \( E_p(G) \) over n-vertex graphs was previously known to lie in the interval \( \frac{\binom{n}{2}}{2} - O(1), n^2 \). The construction that achieves the improved lower bound is shown below. We also determine the leading terms of the maximum over n-vertex graphs of diameter 2 and n-vertex bipartite graphs of diameter at most 3, namely \( \frac{3}{8} n^2 \) and \( \frac{1}{8} n^2 \), respectively.

References

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