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Extremal problems for degree-based topological indices

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ABSTRACT

For a graph G, let $\sigma(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$; this defines the *sum-connectivity index* $\sigma(G)$. More generally, given a positive function t, the *edge-weight t-index* $t(G)$ is given by $t(G) = \sum_{uv\in E(G)} t(\omega(uv))$, where $\omega(uv) = d_G(u) + d_G(v)$. We consider extremal problems for the t-index over various families of graphs. The sum-connectivity index satisfies the conditions imposed on t in each extremal problem, with a small exception.

Minimization: When t is decreasing, and $(z-1)t(z)$ is increasing and subadditive, the star is the unique graph minimizing the t-index over n-vertex graphs with no isolated vertices. When also t has positive second derivative and negative third derivative, and $(z-1)t(z)$ is strictly concave, the connected n-vertex non-tree with least t-index is obtained from the star by adding one edge.

Maximization: When t is decreasing, convex, and satisfies $t(3) - t(4) < t(4) - t(6)$, the path and cycle are the unique n-vertex tree and unicyclic graph with largest t-index. When also $t(4) - t(5) \le 2[t(6) - t(7)]$, and $t(k+1) - t(k+2) - t(k+j)$ increases with k for $j \le 3$, we determine the n-vertex quasi-trees with largest t-index, where a *quasi-tree* is a graph yielding a tree by deleting one vertex. The maximizing quasi-trees consist of an n-cycle plus chords from one vertex to some number c of consecutive vertices (for the sum-connectivity index, $c = \min\{30, n-3\}$). Finally, we show that whenever t is decreasing and $zt(z)$ is strictly increasing, an n-vertex graph with maximum degree k has t-index at most $\frac{1}{2}nkt(2k)$, with equality only for k-regular graphs.

1. Introduction

We consider a class of degree-based invariants of connected simple graphs, special cases of which have been studied in chemical graph theory due to their predictive capabilities for physical and chemical properties of molecules. We use $d_G(u)$ for the degree of a vertex u in a graph G with vertex set $V(G)$ and edge set $E(G)$.

In chemical graph theory, graph invariants are called *topological indices*, intended as numerical values reflecting structural properties. Among the most successful of these is the *Randić index* $R(G)$ of a graph G. Proposed by Randić [9] in 1975, it is defined by

$$R(G) = \sum_{uv\in E(G)} (d_G(u)d_G(v))^{-1/2}.$$

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In his survey "Degree-based topological indices", Gutman [5] noted that hundreds of papers and several books have been written about the Randić index (see for example the survey by Randić [10]). This popularity results from the success of $R(G)$ in correlating with physical invariants of molecules.

In Gutman's treatment, a graph invariant ϕ having the form $\phi(G) = \sum_{uv\in E(G)} f(d_G(u), d_G(v))$ for some symmetric function f is a degree-based topological index. In recent decades, many such indices have been studied. As Gutman [5] observed, most of them are nowhere near as successful as $R(G)$ in correlating with physical parameters of molecules.

Nevertheless, many papers have been written on the extremal values of these indices over classes such as trees. Attention to the values on trees and other elementary graphs arises partly from the applications: "molecular graphs" describing the bonds in actual molecules tend to have very simple graph-theoretic structure such as trees or unicyclic graphs.

Many papers on this topic study just one topological index, finding its extremal values (and perhaps several near-extreme values) over n-vertex trees or other simple classes. We propose studying such problems in terms of general properties of the symmetric function f. Requiring only the properties needed for the argument yields a more general extremal result simultaneously for various symmetric indices. We consider such classes of indices.

Definition 1.1. The *weight* $\omega(uv)$ of an edge uv in a graph G is $d_G(u) + d_G(v)$. Given a positive real-valued function t, the *edge-weight index* $t(G)$ for a graph G is defined by $t(G) = \sum_{e\in E(G)} t(\omega(e))$; we also call $t(G)$ the *t-index* of G.

When t is decreasing, maximizing the t-index seeks edges with low weight, and minimizing it seeks edges with high weight. Among trees, it is then natural to expect stars to have the lowest t-index and paths to have the highest. With some additional conditions on t, we will make this precise and extend the optimization to larger families.

Our study was motivated by the *sum-connectivity index* $\sigma(G)$, introduced by Zhou and Trinajstić in [15], defined by

$$\sigma(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v))^{-1/2}.$$

Chemical applications of the sum-connectivity index were studied in [6,7], mathematical properties in [1,2,11,12,15]. The term "sum-connectivity index" is unrelated to graph connectivity, just as "topological index" is unrelated to surfaces; these are just terms from chemistry. For n-vertex trees, [15] showed $\frac{n-1}{\sqrt{n}} \le \sigma(G) \le \frac{n-3}{2} + \frac{2}{\sqrt{3}}$; the unique extremal trees are the star and the path.

For the sum-connectivity index, [15] also solved the minimization problem over n-vertex graphs without isolated vertices, proving for $n \ge 5$ that the n-vertex star still achieves the minimum. When the minimum degree is increased to at least 2, the star is no longer allowed. Wang, Zhou, and Trinajstić [11] solved the minimization problem over this class, showing that when $n \ge 11$ the minimum is achieved by the graph $K^*_{2,n-2}$ obtained from the complete bipartite graph $K_{2,n-2}$ by adding one edge joining the two vertices of high degree. For triangle-free graphs with minimum degree at least 2, they showed that $K_{2,n-2}$ achieves the minimum. Note that $\sigma(K^*_{2,n-2}) < \sigma(K_{2,n-2})$, so adding an edge can decrease the value.

It is natural to ask which of these results extend to more general indices. Zhou and Trinajstić [16] studied edge-weight indices generated by t of the form $t(z) = z^{-\alpha}$ for real α under the name *general sum-connectivity index*, obtaining upper and lower bounds in terms of other graph invariants and proving that the path and star are the unique extremal n-vertex trees (for positive α), but which maximizes and which minimizes depends on the value of α. In [3], the graphs minimizing the t-index of this form over n-vertex unicyclic graphs (for $\alpha \le 1$) were determined. In [4], the maximizing n-vertex trees were determined (for $\alpha > 4.36$). These papers actually write z^{α} for the function; we have changed the sign for consistency with our treatment.

Many decreasing functions of interest (such as $z^{-\alpha}$ for positive α) are convex. However, requiring that t be decreasing and convex is not sufficient to make the path achieve the maximum over n-vertex trees. Let P_n, C_n, and S_n denote the path, cycle, and star with n vertices, respectively.

Example 1.2. Let G_m be the tree with $2m + 1$ vertices obtained from a star with m edges by subdividing each edge. Note that $t(G_m) = mt(3) + mt(m + 2)$, while $t(P_{2m+1}) = 2t(3) + (2m - 2)t(4)$. Thus $t(P_{2m+1}) > t(G_m)$ if and only if $(m - 2)[t(3) - t(4)] < m[t(4) - t(m + 2)]$.

Reversing this inequality yields a decreasing convex t such that G_m maximizes the t-index among trees with $2m + 1$ vertices. For example, choose $t(3)$ and $t(m + 2)$ with $t(m + 2) < t(3)$, let $t(4)$ be slightly less than $\frac{(m-2)t(3)+mt(m+2)}{2m-2}$, and complete t to a decreasing convex function.

When $m = 3$, the condition for $t(P_7) > t(G_3)$ reduces to $t(3) - t(4) < 3[t(4) - t(5)]$. We will show that the similar but somewhat stronger inequality $t(3) - t(4) < t(4) - t(6)$ suffices to make the path the unique maximizing tree of each order. Example 1.2 shows not only that some condition similar to our sufficiency condition is necessary, but also that when the condition fails the maximizing tree can suddenly be much different from the path. It seems that as the number of vertices grows, weaker conditions suffice, but we will not address this.

With two conditions on t in addition to $t(3) - t(4) < t(4) - t(6)$, we will be able to solve the maximization on a larger family containing all trees.