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.

Keywords: sum-connectivity index; quasi-tree; topological index

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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

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

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 is a degree-based topological index if it has the form $\phi(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v))$ for some symmetric function f. 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 [7, 8], 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 are 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.

Definition 1.3. A *gradual function* is a positive real-valued function t on the positive real numbers that is decreasing, strictly convex, and has the following three properties:

(1) $t(3)-t(4)\le t(4)-t(6)$.
(2) $t(4)-t(5)\le 2[t(6)-t(7)]$.
(3) $t(k+1)-t(k+2)-t(k+j)$ is nondecreasing in k (over $k\ge 3$) for $j\le 3$.

A *gradual index* is the edge-weight index given by a gradual function t.

Convexity requires $t(j)-t(j+1)$ to decrease with increasing j, but the conditions (1) and (2) prevent t from decreasing too rapidly. This is the reason for the term "gradual". Note also that if t tends to 0, then convexity prevents $t(k+1)-t(k+2)-t(k+j)$ from being an increasing function of k when j is sufficiently large.

The sum-connectivity index is the gradual index defined using $t(z)=1/\sqrt{z}$; one easily computes $\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{4}}<\frac{1}{\sqrt{4}}-\frac{1}{\sqrt{6}}$ and $\frac{1}{\sqrt{4}}-\frac{1}{\sqrt{5}}<\frac{2}{\sqrt{6}}-\frac{2}{\sqrt{7}}$, and differentiating $t(x+1)-t(x+2)-t(x+j)$ for $t(z)=1/\sqrt{z}$ when $j\in\{1,2,3\}$ confirms (3). Indeed, $z^{-\alpha}$ is a gradual function when $0<\alpha<.869$ (condition (1) holds for $0<\alpha\le 1$). Unfortunately, when $t(z)=1/z$, condition (2) needed for our proof does not hold, although the conclusion still could hold. The value $\alpha=1$ corresponds to the *harmonic index*, which is the edge-weight index given by $t(z)=2/z$, studied in chemical graph theory by Zhong [13, 14].

Since the sum-connectivity index is the t-index for a gradual function t, our proofs apply to it. It is possible that the same conclusions hold under weaker restrictions than those we specify for gradual functions. In order to show that the path is the unique maximizing n-vertex tree (and that the cycle is the unique maximizing n-vertex unicyclic graph), we only need t to be decreasing, convex, and satisfy (1) (Theorem 3.3). After that, we maximize over a larger class of graphs using the stronger restriction to gradual functions.

Definition 1.4. A *quasi-tree* is a graph obtained from a tree T by adding one vertex u and edges joining u to some positive number of vertices in T. Such a vertex u is a *focal vertex* of the resulting quasi-tree. A quasi-tree is *nontrivial* if it is not a tree, meaning that a focal vertex has degree greater than 1.

Lu and Gao [6] found sharp upper and lower bounds for the Randić index of an n-vertex quasi-tree. In this paper, we describe the nontrivial n-vertex quasi-trees with largest t-index when t is a gradual function. Our most difficult result, proved in Section 4, is the following.

Theorem 1.5. *Over n-vertex quasi-trees, any gradual index is maximized by a graph consisting of a cycle plus chords from one vertex to a set of consecutive vertices on the cycle.*

For the sum-connectivity index, the maximizing quasi-tree uses $n-3$ consecutive chords (all possible chords) when $n \le 32$, and it uses exactly 30 chords when $n \ge 33$.

Let $\mathbf{Q}_n$ be the family of n-vertex quasi-trees, and let $\mathbf{Q}'_n$ be the subfamily consisting of those that are not trees. When $3t(4) > 2t(3)$, we have $t(C_n) > t(P_n)$; this condition holds for $t(z) = 1/z^\alpha$ with $0 < \alpha < 1.4$. Since $C_n \in \mathbf{Q}'_n$, maximizing over $\mathbf{Q}'_n$ also solves the maximization problem over $\mathbf{Q}_n$.

The minimization problem is somewhat different; to study it we place different restrictions on the decreasing function t. If also $(z-1)t(z)$ is increasing and subadditive, then the n-vertex star S_n is the unique n-vertex graph with least t-index among all n-vertex graphs having no isolated vertices. We prove this as a straightforward generalization of a result of [15] mentioned earlier, which proved the same statement for the sum-connectivity index. In essence, we just list the properties of $1/\sqrt{z}$ that are used in their proof; the same proof works for all t satisfying these conditions.

When we consider graphs with cycles, the star is excluded. The star S_n has smaller t-index than any member of $\mathbf{Q}'_n$. To study the minimization problem over non-trees, we restrict to connected non-trees. The minimum is still attained by a quasi-tree, in fact by the graph $\hat{S}_n$ with one cycle obtained by adding one edge joining two leaves of S_n. Hence this simultaneously solves the minimization problem among connected n-vertex non-trees for those with one cycle, for those that are quasi-trees, and over all such graphs. The conditions we need are that t be decreasing, with positive second derivative and negative third derivative, and that $(z-1)t(z)$ be increasing and strictly concave.

Again the sum-connectivity index satisfies these conditions. Also, our minimization result is close to showing that $\hat{S}_n$ is the connected graph with second-smallest t-index. It seems that for $n \ge 43$ no tree other than S_n has sum-connectivity index less than $\hat{S}_n$.

Finally, in Section 5 we show that when t is decreasing and $zt(z)$ is strictly increasing, the maximum of $t(G)$ over n-vertex graphs with $\Delta(G) \le k$ is $\frac{1}{2}nkt(2k)$, with equality precisely for k-regular graphs. This generalizes in a straightforward way the proof of [15], which proved the statement for the sum-connectivity index ($t(z) = 1/\sqrt{z}$).

2 Minimization Results

Over graphs without isolated vertices, we follow the approach used in [15] for sum-connectivity; the arguments remain valid for more general edge-weight indices. A function f is *subadditive* if always $f(a+b) \le f(a) + f(b)$.

Theorem 2.1. *Let t be an edge-weight index. If the function t is decreasing, and $(z-1)t(z)$ is an increasing function of z, then the star is the unique connected n-vertex graph with* *least t-index. If also $(z-1)t(z)$ is subadditive (for arguments at least 2), then the star also minimizes the t-index over n-vertex graphs with no isolated vertex.*

Proof. Let G be a graph with m edges. The weight of an edge uv exceeds the number of edges incident to uv by 2. Since at most $m-1$ edges are incident to uv, we have $\omega(uv) \le m+1$. Since t is decreasing, we thus have $t(G) \ge mt(m+1)$. Since $mt(m+1)$ increases with m, we have $t(G) \ge (n-1)t(n)$ when G is an n-vertex connected graph.

Equality holds for the star S_n. Equality requires having exactly $n-1$ edges and having each edge incident to all others. The only such connected graph is the star.

For the extension to graphs with no isolated vertices, we use induction on the number of vertices, with trivial basis. In the induction step with n vertices, the case of connected graphs was considered above, so suppose that G is disconnected, with every component having at least two vertices. Let j be the order of the smallest component, and let k be the remaining number of vertices. By the induction hypothesis, $t(G) \ge (j-1)t(j) + (k-1)t(k)$. By the subadditivity of $(z-1)t(z)$, we thus have $t(G) \ge (j+k-1)t(j+k) = t(S_n)$. □

Consider the sum-connectivity index σ, using $t(z) = 1/\sqrt{z}$. Here the function f defined by $f(z) = (z-1)t(z)$ is increasing, and it is almost subadditive. We have $f(j)+f(k) > f(j+k)$ when $j,k \ge 2$ and $j+k \ge 5$, but $f(2)+f(2) < f(4)$. Since $f(n) = \sigma(K_{1,n-1})$, the induction hypothesis and argument of the induction step are valid in the proof of Theorem 2.1 except when $j=2$ and $k=4$ (since j is the order of the smallest component, we need not worry about $k=4$ when $j>2$). In the only case not covered by the argument, we compare $\sigma(3K_2)$ with $\sigma(K_{1,5})$ and find that $\sigma(K_{1,5})$ is smaller.

Next we consider a more restricted family that excludes the star and also all trees and disconnected graphs. The graph achieving the minimum is still very much like the star. Let $\hat{\mathbf{Q}}_n$ be the set of connected n-vertex graphs containing cycles. Let $\hat{S}_n$ be the graph obtained by adding an edge joining two leaves of the star S_n. We prove that $\hat{S}_n$ is the unique graph in $\hat{\mathbf{Q}}_n$ that minimizes the edge-weight index t, for appropriate constraints on the function t.

For sum-connectivity, this conclusion does not extend to non-forests without isolated vertices, since $\sigma(C_3+K_2) < \sigma(\hat{S}_5)$, where $G+H$ denotes the disjoint union of G and H. There may be larger exceptions for other edge-weight indices having the specified properties, so we require connectedness.

The t-index of $\hat{S}_n$ is of particular interest; let $h(n) = t(\hat{S}_n) = (n-3)t(n)+2t(n+1)+t(4)$.

Lemma 2.2. *Let t be a decreasing edge-weight index function with positive second derivative and negative third derivative. If also $(z-1)t(z)$ is increasing and strictly concave, then the following hold:*

(a) $zt(z+j)$ is increasing and concave for $j \in \mathbb{N}$,

(b) the function h is increasing and strictly concave, and

(c) the function h is strictly subadditive ($h(a+b) < h(a)+h(b)$ for $a,b \ge 1$ and $a+b \ge 3$).

Proof. With positive second derivative, t is strictly convex, so $t(z+2)-t(z+1)$ increases with z. Since the third derivative is negative, the first difference $t(z+2)-t(z+1)$ has negative second derivative and is a concave function of z.

(a) The claim holds by assumption for $j=1$. If follows by induction on j from

$$zt(z+j) = (z+1)t(z+1+j-1) - t(z+j),$$

since the first term is increasing and concave (by the induction hypothesis), and $t(z+j)$ is decreasing and convex.

(b) Note that

$$(z-2)t(z+1) + 2t(z+2) = zt(z+1) - 2[t(z+1) - t(z+2)],$$

where the first term is increasing and strictly concave. Since also $t(z+1)-t(z+2)$ is decreasing and convex, $(z-2)t(z+1)+2t(z+2)$ is increasing and strictly concave.

(c) We compute

$$\begin{aligned} h(a)+h(b) &= (a-3)t(a) + (b-3)t(b) + 2t(a+1) + 2t(b+1) + 2t(4) \\ &> (a+b-3)t(a+b) + 2t(a+b+1) + t(4) \;=\; h(a+b). \end{aligned}$$

To see this, note that $h(a)+h(b)$ is a sum of $a+b$ values of t, corresponding to the $a+b$ edges in $\hat{S}_a + \hat{S}_b$. Similarly, $\hat{S}_{a+b}$ has $a+b$ edges, and the expression for $h(a+b)$ sums $a+b$ values of t. The arguments a, b, $a+1$, and $b+1$ are all at most $a+b$, and $4 \le a+b+1$, so term-by-term the contribution to $h(a+b)$ is smaller than the contribution to $h(a)+h(b)$. □

The assumed properties hold when $t(z) = z^{-\alpha}$ with $0 < \alpha < 1$, since $z^{-\alpha}$ is increasing and has higher derivatives alternating in sign.

A *locally minimal edge* in G is an edge uv such that $d_G(u) = \min_{w \in N(v)} d_G(w)$ and $d_G(v) = \min_{w \in N(u)} d_G(w)$. Locally minimal edges exist, because every edge with least weight in G is locally minimal.

Lemma 2.3. *Let t be as in Lemma 2.2. If uv is a locally minimal edge in G, then $t(G) > t(G-uv)$.*

Proof. Since uv is locally minimal in G, we have $d_G(u) \le d_G(w)$ for $w \in N_G(v)$ and $d_G(v) \le d_G(w)$ for $w \in N_G(u)$. With $j = d_G(u)$ and $k = d_G(v)$, convexity of t allows us to replace each term in the sums below with $t(j+k-1) - t(j+k)$. We have

$$\begin{aligned} t(G) - t(G-uv) &= t(j+k) - \sum_{w \in N_G(u)-\{v\}} [t(j-1+d_G(w)) - t(j+d_G(w))] \\ &\quad - \sum_{w \in N_G(v)-\{u\}} [t(k-1+d_G(w)) - t(k+d_G(w))] \\ &\ge t(j+k) - (j+k-2)[t(j+k-1) - t(j+k)] \\ &= (j+k-1)t(j+k) - (j+k-2)t(j+k-1) \;>\; 0, \end{aligned}$$

where the final inequality uses that $(z-1)t(z)$ increases with z. □

A *leaf* is a vertex of degree 1.

Theorem 2.4. *Let t be as in Lemma 2.2. If $G \in \hat{\mathbf{Q}}_n - \{\hat{S}_n\}$, then $t(G) > h(n)$.*

Proof. It suffices to show that if $G \in \hat{\mathbf{Q}}_n - \{\hat{S}_n\}$, then G does not have the smallest t-index among the graphs in $\hat{\mathbf{Q}}_n$. We use induction on n. Note first for the cycle C_n that $t(C_n) = nt(4)$, while $h(n) = t(4) + 2t(n+1) + (n-3)t(n)$. Since t is decreasing, $t(C_n) > h(n)$ for $n \ge 4$. For $n = 3$, only C_n contains a cycle (and $C_n = \hat{S}_n$). For $n > 3$, consider $G \in \hat{\mathbf{Q}}_n$.

Case 1: $\delta(G) \ge 2$. Let e be a locally minimal edge, and let $G' = G - e$. By Lemma 2.3, $t(G) > t(G')$. Thus if $G' \in \hat{\mathbf{Q}}_n$, then G does not achieve the minimum. We have $G' \in \hat{\mathbf{Q}}_n$ unless e is a cut-edge or e belongs to every cycle in G; in the latter case G' is connected. If e belongs to more than one cycle, then the symmetric difference of the two cycles contains a cycle that omits e. If G has only one cycle, then $G = C_n$ (considered above) or $\delta(G) = 1$.

In the remaining case, G' is disconnected; let G_1 and G_2 be the components of G'. If G_1 or G_2 fails to contain a cycle, then $\delta(G) = 1$, since every tree with at least one edge has at least two leaves. With $n_i = |V(G_i)|$, the induction hypothesis yields $t(G) > t(G') = t(G_1) + t(G_2) \ge h(n_1) + h(n_2) \ge h(n)$, since h is subadditive.

Case 2: $\delta(G) = 1$. Let r be the maximum number of leaves adjacent to a single vertex in G. Let v be a vertex of highest degree in G among those adjacent to r leaves, and let $k = d_G(v)$. Let $q = k - r$, so v has q neighbors with degree at least 2.

If $q = 0$, then G is disconnected or a star, both forbidden from $\hat{\mathbf{Q}}_n$.

If $q = 1$, then let x be the neighbor of v with degree at least 2. Define G' by replacing the edge wv with the edge wx for all $w \in N(v) - \{x\}$. Note that $G' \in \hat{\mathbf{Q}}_n$. The moved edges and all edges other than vx have larger weight in G' than in G, and no edge has smaller weight in G' than in G, so $t(G') < t(G)$. Thus G does not maximize t over $\hat{\mathbf{Q}}_n$.

Hence we may assume $q \ge 2$. Let u be a leaf neighbor of v, and let $G' = G - u$. Note that $G' \in \hat{\mathbf{Q}}_{n-1}$. By the induction hypothesis, $t(G') \ge h(n-1)$, with equality only if $G' = \hat{S}_{n-1}$, in which case $G = \hat{S}_n$. Hence it suffices to show $t(G) - t(G') \ge h(n) - h(n-1)$.

In computing $t(G) - t(G')$, we include $t(k+1)$ for the edge uv. For $w \in N(v) - \{u\}$, we include $t(k + d_G(w)) - t(k - 1 + d_G(w))$. Since t is convex and decreasing, the latter contribution is smallest (most negative) when $d_G(w) = 1$, next when $d_G(w) = 2$. Hence $t(G) - t(G')$ is smallest when $q = 2$, and we have

$$t(G) - t(G') \ge (k-2)t(k+1) + 2t(k+2) - (k-3)t(k) - 2t(k+1) = h(k+1) - h(k).$$

By Lemma 2.2, h is increasing and strictly concave. Thus $t(G) - t(G') \ge h(n) - h(n-1)$. Equality requires $k = n-1$ and $q = 2$, in which case $G = \hat{S}_n$. □

Since $t(S_n) < t(\hat{S}_n)$ when t satisfies the given conditions, it would be interesting to know which trees have t-index smaller than $\hat{S}_n$. There are not many. Let S_n^j denote the n-vertex tree obtained from the star S_{n-j} by subdividing j edges. Already $\sigma(S_n^2) > \sigma(\hat{S}_n)$ when $n \geq 6$, and $\sigma(S_n^1) > \sigma(\hat{S}_n)$ when $n \geq 43$. Always $\sigma(T_n) > \sigma(\hat{S}_n)$, where T_n is obtained from S_{n-2} by subdividing one edge twice. For $n \geq 43$, it seems that $\hat{S}_n$ is actually the connected graph other than the star that has the smallest sum-connectivity index.

3 Eliminating Pendant Paths

We now turn our attention to the maximization problem. A *pendant path* at a vertex u of degree at least 3 in a graph G is a path with endpoint u whose internal vertices have degree 2 in G and whose endpoint other than u has degree 1 in G. Our goal in this section is to show that whenever G has a pendant path and t is a gradual function, it is possible to replace one edge with another to reduce the number of pendant paths and increase the t-index (with certain possible exceptions). This approach was used in [15] when $t(z) = 1/\sqrt{z}$ to maximize t over n-vertex trees; for trees it suffices to show that a maximizing graph cannot have two pendant paths at a single vertex, as generalized here in Lemma 3.2.

Lemma 3.1. *Let t be a gradual function. Let G be a graph having a pendant path P of length l at u, with w the endpoint of P opposite u. Given $vx \in E(G)$, let $G' = G - vx + xw$. Let $k = d_G(v)$ and $j = d_G(x)$. Under either of the following conditions, $t(G') > t(G)$:*

(a) vx is the first edge of a pendant path at v and $k \geq 4$.

(b) $u = v$, the edge vx is not on P, and $l = 1$ or $j \leq 3$.

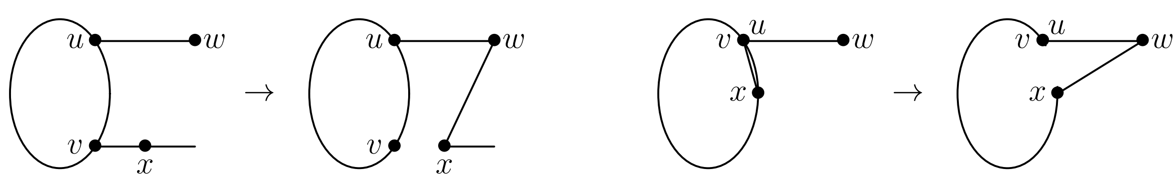

Figure 1: Transformations in Lemma 3.1

Proof. In changing from G to G', the contribution to t from edges incident to vx increases, since their weight decreases. Such gains may be arbitrarily small, so we ignore them, except possibly for the edge other than vx incident to x in case (a). Note that in each case $k \geq 3$.

Replacing vx with wx changes weight from $k + j$ to $j + 2$. The edge incident to w in G changes weight from 3 to 4 if $l > 1$, and from $d_G(u) + 1$ to $d_G(u) + 2$ if $l = 1$.

If $k \geq 4$ and $j \leq 2$, then

$$\begin{aligned} t(G') - t(G) &> t(4) - t(3) + t(j+2) - t(j+k) \\ &\geq t(4) - t(3) + t(j+2) - t(j+4) \\ &\geq t(4) - t(3) + t(4) - t(6) \ \geq \ 0. \end{aligned}$$

Here we first used that t is decreasing, then $j \le 2$ and convexity, then condition (1). This completes the proof of (a).

When $u = v$, we also consider the contribution from the edge incident to u on P. It changes from $t(k+2)$ to $t(k+1)$ if $l > 1$, but it does not change if $l = 1$. If $l > 1$, then we first use condition (3) to reduce to the case $k = 3$, then convexity to reduce to $j = 3$, and finally condition (1), yielding

$$\begin{aligned} t(G') - t(G) &> t(k+1) - t(k+2) + t(4) - t(3) + t(j+2) - t(j+k) \\ &\ge t(4) - t(5) + t(4) - t(3) + t(j+2) - t(j+3) \\ &\ge [t(4) - t(5)] + [t(5) - t(6)] - [t(3) - t(4)] \;\ge\; 0. \end{aligned}$$

When $u = v$ and $l = 1$, the new edge wx replaces the edge vx with larger weight; we have $t(G') - t(G) > t(j+2) - t(j+k) > 0$. □

The conditions on t in Lemma 3.1 can be weakened when there are two pendant paths at a vertex. We will use this to show that for more general t the path maximizes the t-index over n-vertex trees. A similar observation handles unicyclic graphs.

Lemma 3.2. *Let t be a decreasing convex function such that $t(3) - t(4) < t(4) - t(6)$, If G is a graph with two pendant paths at a vertex u, and G' is obtained from G by detaching one of those paths from u and attaching it to the endpoint of the other path, then $t(G') > t(G)$.*

Proof. Let x be the neighbor of u along the detached pendant path. Let w be the other endpoint of the other pendant path at u. With $v = u$, this puts us in the setting of Lemma 3.1 with $j \le 2$ and with vx being the first edge of a pendant path at v. If $k = d_G(v) \ge 4$, then (a) applies, using only condition (1).

For $k = 3$, we show that the argument for (b) holds under the weaker hypotheses stated here. Condition (3) of gradual functions is not needed when $k = 3$ to reduce to $k = 3$; we already have $k = 3$. When also $j \le 2$, we can apply (1). That is,

$$t(4) - t(5) + t(4) - t(3) + t(4) - t(5) > [t(4) - t(5)] + [t(5) - t(6)] - [t(3) - t(4)] > 0.$$

Hence $t(G') > t(G)$. □

Theorem 3.3. *If t is a decreasing convex function such that $t(3) - t(4) < t(4) - t(6)$, then*

(1) over n-vertex trees the t-index is maximized uniquely by the path, and

(2) over n-vertex unicyclic graphs the t-index is maximized uniquely by the cycle.

Proof. (1) Let G be an n-vertex tree other than a path. Among the vertices with degree at least 3 in G, let u be one such that at most one component of $G - u$ is not a path; it is a leaf of the smallest subtree of G containing all the vertices of degree at least 3. At u there are at least two pendant paths. By Lemma 3.2, combining them yields another n-vertex tree G' with $t(G') > t(G)$. Hence no n-vertex tree other than a path can maximize t.

(2) Among unicyclic n-vertex graphs, choose G to maximize the t-index. By Lemma 3.2, G consists of a cycle with 0 or 1 pendant path at each vertex. Now each pendant path is attached at a vertex v of degree 3 on the cycle in G, and its neighbor on the cycle has degree at most 3. In the proof of Lemma 3.1(b), when $d_G(v) = 3$ as is the case here, we do not need to invoke condition (3) in the definition of gradual function to make the reduction to the case where the degree is 3. Hence the weaker condition here suffices. Hence the transformation in Lemma 3.1(b) can be applied to absorb a pendant path into the cycle to yield a unicyclic graph with larger t-index. We conclude that G itself must be a cycle. □

Generally speaking, when t is a gradual function and we maximize the t-index over a family of graphs, the results in this section allow us to eliminate pendant paths. They can remain only in quite special situations, which we summarize here.

Lemma 3.4. *Let t be a gradual function, and P be a pendant path at a vertex v in a graph G. A graph G' with $t(G') > t(G)$ is obtained by reattaching P at a leaf of G or by replacing an edge incident to v with an edge to the other endpoint of P (transformation (b) of Lemma 3.1) unless (1) $d_G(v) = 3$, or (2) $d_G(v) \geq 4$ and P is the only pendant path in G. In either case, every neighbor of v not on P has degree at least 4, and P has length at least 2.*

Proof. Lemma 3.2 applies when there is more than one pendant path at a vertex, even under weaker hypotheses on t. Part (a) of Lemma 3.1 applies when $d_G(v) \geq 4$ if there is another pendant path; hence G' fails to exist when $d_G(v) \geq 4$ only if G has no pendant path other than P. Part (b) of Lemma 3.1 applies when P has length 1 or when v has a neighbor not on P with degree at most 3 in G. □

4 The Form of Maximizing Quasi-trees

Our main aim in this section is to show that when G is an n-vertex quasi-tree maximizing t, deleting a focal vertex leaves a path, and in fact the graph is a cycle plus chords from the focal vertex to consecutive vertices on the cycle.

When G is a quasi-tree, operations (a) and (b) of Lemma 3.1 produce a quasi-tree G'. Hence the conclusions of Lemma 3.4 apply when we choose G to maximize t over quasi-trees.

Lemma 4.1. *Let t be a gradual function, and let G be an n-vertex quasi-tree maximizing t. If $\hat{u}$ is a focal vertex of G, then every vertex of G other than $\hat{u}$ has degree at most 3 in G.*

Proof. Let T be the tree $G - \hat{u}$, and let w be a leaf of T; note that $d_G(w) \leq 2$. Suppose that T has a vertex whose degree in G is at least 4. Let v be such a vertex farthest from w in T. Let v' and w' be their neighbors along the path joining them in T (see Figure 2).

A leaf of T has degree at most 2 in G. Thus v cannot be a leaf of T. After allowing for v' and possibly $\hat{u}$, still v has at least two neighbors that are farther than v from w in T; let x and x' be such neighbors of v. By the choice of v, we have $d_G(x), d_G(x') \leq 3$. Hence G does not have a pendant path at v, by Lemma 3.4.

Let $G' = G - vx + xw$. Note that G' is a quasitree, since w is in the component of $T - vx$ not containing x. It suffices to show $t(G') > t(G)$.

For consistency with earlier notation, let $k = d_G(v)$ and $j = d_G(x)$; we have $k \geq 4$ and $j \leq 3$. In turning G into G', weight $k + j$ on vw is replaced with weight $j + 1 + d_G(w)$ on xw. The $k - 1$ other edges at v lose weight, and the $d_G(w)$ edges at w gain weight.

Specifically, reducing the weight on vx' and losing the edge vx gives us at least $t(k+2) - t(k+3) - t(j+k)$ (using convexity) as the part of the change due to these two edges. When this expression is written as $t(k+2) - t(k+3) - t(j-1+k+1)$, condition (3) implies that its value does not decrease as k increases (over $k \geq 2$) for fixed j with $j \leq 4$. Hence in proving $t(G') > t(G)$ we may assume $k = 4$. For the other contributions, we consider two cases.

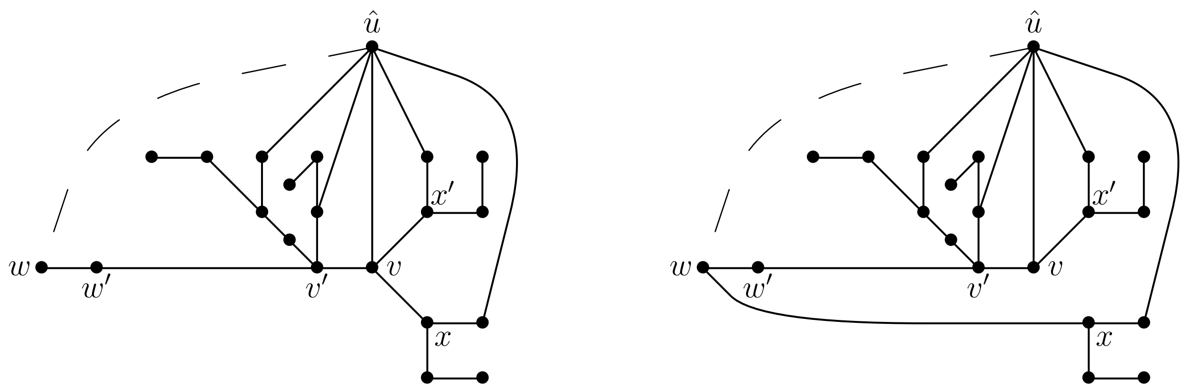

Figure 2: Transformation in Lemma 4.1

Case 1: $d_G(w) = 1$. In this case, $d_G(w') = 2$, since G has no pendant path of length 1, by Lemma 3.4. Since $k \geq 4$ and $j \leq 3$, and t is decreasing and convex, incorporating $t(xw)$ and the change in $t(ww')$ yields

$$\begin{aligned} t(G') - t(G) &> t(k+2) - t(k+3) - t(j+k) + t(j+2) + t(4) - t(3) \\ &\geq t(6) - t(7) - t(j+4) + t(j+2) + t(4) - t(3) \\ &\geq [t(6) - t(7)] + [t(5) - t(7)] - [t(3) - t(4)]. \end{aligned}$$

From $t(6) - t(7) + t(6) - t(7) \geq t(4) - t(5)$ (condition (2)), we obtain $t(5) - t(7) + t(6) - t(7) \geq t(4) - t(6)$. Condition (1) then applies to yield $t(G') - t(G) > 0$.

Case 2: $d_G(w) = 2$. In this case, $w\hat{u} \in E(G)$. The only edges gaining weight are ww' and $w\hat{u}$. In order to bound the decrease in t due to $w\hat{u}$, we prove a lower bound on $\omega(w\hat{u})$. Let

$r = \omega(vv')$. We can follow $r-2$ edge-disjoint paths in T from $\{v, v'\}$ to leaves (or directly to $\hat{u}$). Each path has a last vertex with degree greater than 2 in T. By Lemma 3.1, G does not have two pendant paths at one vertex, and hence each path leaving $\{v, v'\}$ yields a neighbor of $\hat{u}$ (except possibly one pendant path at v or v'). Thus $d_G(\hat{u}) \geq r-3$. We conclude that increasing the weight on $w\hat{u}$ may lose as much as $t(r-1) - t(r)$, but decreasing the weight on vv' gains $t(r-1) - t(r)$, so the total contribution from $w\hat{u}$ and vv' is nonnegative. Now $\omega(xw) = j+3$, and the contribution from ww' is at least $t(5) - t(4)$, by convexity. Hence

$$\begin{aligned} t(G') - t(G) &> t(k+2) - t(k+3) - t(j+k) + t(j+3) + t(5) - t(4) \\ &\geq t(6) - t(7) - t(j+4) + t(j+3) + t(5) - t(4) \\ &\geq [t(6) - t(7)] + [t(6) - t(7)] - [t(4) - t(5)] \geq 0. \end{aligned}$$

The last step uses condition (2), yielding $t(G') > t(G)$. □

Lemma 4.2. *Let t be a gradual function. If G with focal vertex $\hat{u}$ is a graph maximizing the t-index among graphs in $\mathbf{Q}'_n$, then $G - \hat{u} = P_{n-1}$.*

Proof. By Lemma 4.1, all vertices except $\hat{u}$ have degree at most 3 in G. Since Proposition 3.4 requires all neighbors of vertices incident to pendant paths to have degree at least 4, there is thus no pendant path at any vertex of G. As before, let $T = G - \hat{u}$. If $T \neq P_{n-1}$, then T has a vertex of degree 3. Let w be a leaf of T, with neighbor w', and let v be a vertex farthest from w in T among the vertices with degree 3 in T. Let v' be the neighbor of v on the path to w in T, and let x and x' be the other neighbors of v in T (see Figure 3). By the choice of v and the fact that G has no pendant path, $d_G(x) = d_G(x') = 2$.

Let $G' = G - vx + xw$; we show $t(G') > t(G)$. Since $d_G(v) = 3$ and $d_G(w) = 2$, the weight on the moved edge does not change. Weight increases on ww' and $w\hat{u}$; it decreases on vv' and vx'. Let $j = d_G(v')$ and $k = d_G(\hat{u})$. Since $\hat{u}$ is adjacent to every leaf in T, we have $k \geq 3$. Also $j \in \{2, 3\}$ and $d_G(w') \geq 2$. Thus

$$t(G') - t(G) \geq t(j{+}2) - t(j{+}3) + t(4) - t(5) - [t(k{+}2) - t(k{+}3)] - [t(4) - t(5)] > 0,$$

since $j < k$. The case $v = w'$ is included in this analysis. □

Theorem 4.3. *Let t be a gradual function. Let $G_n(c)$ be a graph obtained from the cycle C_n by adding chords from one vertex $\hat{u}$ to c consecutive other vertices. If G with focal vertex $\hat{u}$ is a graph maximizing the t-index among graphs in $\mathbf{Q}'_n$, then G has the form $G_n(c)$ for some c. For $c > 1$,*

$$t(G_n(c)) = 2t(c+4) + ct(c+5) + c[t(6) - t(4)] + \alpha_n,$$

where $\alpha_n = (n-2)t(4) - [t(4) - t(5)] + [t(5) - t(6)]$.

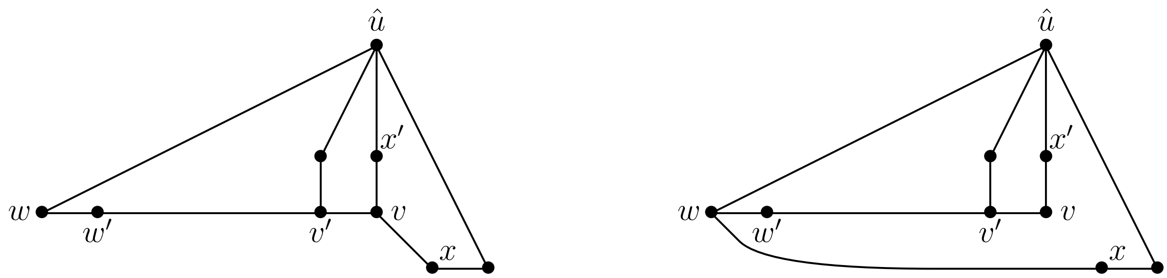

Figure 3: Transformation in Lemma 4.2

Proof. By Lemma 4.2, $G - \hat{u}$ is a path; call it $\hat{P}$. We also know that G has no pendant path, so $\hat{u}$ is adjacent to the endpoints of $\hat{P}$. Let $c = d_G(\hat{u}) - 2$, and let b be the number of components of the subgraph induced by the neighbors of $\hat{u}$ other than the endpoints of $\hat{P}$. We compute

$$t(G) = 2t(c+4) + ct(c+5) + (c-b)t(6) + 2bt(5) + (n-2-c-b)t(4).$$

The terms involving b sum to $b([t(5) - t(6)] - [t(4) - t(5)])$, which is negative since t is decreasing and convex. Therefore, for fixed positive c we attain the maximum when $b = 1$, which means that the chords are incident to consecutive vertices of $\hat{P}$, and they may be any c consecutive vertices. When $c = 0$, we have $G = C_n$, and the formula reduces to $t(C_n) = nt(4)$. □

Let $g_n(c) = t(G_n(c))$. For $c \geq 2$, we have

$$g_n(c) - g_n(c-1) = 2[t(c+4) - t(c+3)] + c[t(c+5) - t(c+4)] + t(c+4) + [t(6) - t(4)].$$

The contributions within brackets are negative, but $t(c+4)$ is positive. Significantly, the difference is independent of n. Thus when t is reasonably well behaved and n is large, there may be a fixed value of c such that $G_n(c)$ is the extreme graph.

Now we specialize to the sum-connectivity index.

Theorem 4.4. *Let $t(z) = 1/\sqrt{z}$. In $\mathbf{Q}_n$, the graphs maximizing the t-index are those indicated by $G_n(c)$, where $c = n-3$ if $n \leq 32$ and $c = 30$ if $n \geq 33$.*

Proof. With $g_n(c) = t(G_n(c))$, we have $g_n(0) < nt(4)$ and $g_n(1) > 4t(5) + t(6) + (n-4)t(4)$. Thus $g_n(1) - g_n(0) = t(6) - 4[t(4) - t(5)] \approx .197 > 0$, so it is always better to add at least one chord to the cycle. Also $g_n(2) - g_n(1) = 2t(6) + 2t(7) - 2t(5) - t(4) \approx .178$, so initially $g_n(c)$ is increasing. Since the difference is independent of n, it suffices to show that the derivative of the formula for the difference is negative and that the difference hits 0 between $c = 29$ and $c = 30$. We have

$$g_n(c) = \frac{2}{\sqrt{(c+4)}} + \frac{c}{\sqrt{c+5}} + \frac{c-1}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{n-c-3}{2}$$

From the derivative of the difference, we know that $g_n(c)$ is increasing for $c \leq 29$ and decreasing for $c \geq 30$. Always $c \leq n-3$. Thus the maximum occurs at $c = n-3$ for $n \leq 32$. Comparing $g_n(29) \approx \frac{n}{2} + 1.54699$ with $g_n(30) \approx \frac{n}{2} + 1.64754$ shows that the maximum occurs at $c = 30$ when $n \geq 33$. Thus the result follows. □

5 Maximization for Bounded Degree

An n-vertex quasi-tree has at most $2n-3$ edges. One way to define families that allow denser graphs is to bound the maximum degree. In this final section we show that the result of Zhou and Trinajstić [15] for maximizing the sum-connectivity index over such families extends in a straightforward way to maximizing a gradual index. We follow the steps of their proof.

Theorem 5.1. *Let t be an edge-weight index such that t is decreasing and $zt(z)$ is strictly increasing in z. If G is an n-vertex graph with $\Delta(G) = k$, then $t(G) \leq \frac{1}{2}nkt(2k)$, with equality if and only if G is k-regular. In particular, K_n is the unique n-vertex graph with largest t-index.*

Proof. For such a graph G, let $m_{i,j}$ denote the number of edges of G having endpoints of degrees i and j. Let n_i be the number of vertices with degree i. Counting the edges incident to vertices of degree i yields $in_i = m_{i,i} + \sum_{j=1}^{k} m_{i,j}$. With also $n = \sum n_i$, we have $n_k = n - \sum_{i=1}^{k-1} \frac{1}{i}(m_{i,i} + \sum_{j=1}^{k} m_{i,j})$. Thus

$$m_{k,k} = \frac{1}{2}\left(kn_k - \sum_{i=1}^{k-1} m_{k,j}\right) = \frac{kn}{2} - \frac{k}{2} \sum_{\substack{1 \leq i \leq j \leq k \\ (i,j) \neq (k,k)}} \left(\frac{1}{i} + \frac{1}{j}\right) m_{i,j}.$$

For the t-index, we compute

$$\begin{aligned} t(G) &= t(2k)m_{k,k} + \sum_{\substack{1 \leq i \leq j \leq k \\ (i,j) \neq (k,k)}} t(i+j)m_{i,j} \\ &= t(2k)\frac{kn}{2} + \sum_{\substack{1 \leq i \leq j \leq k \\ (i,j) \neq (k,k)}} \left(t(i+j) - t(2k)\frac{k}{2}\left(\frac{1}{i} + \frac{1}{j}\right)\right) m_{i,j} \end{aligned}$$

We are given that t is decreasing and $\frac{1}{2}zt(z)$ is strictly increasing with z. For $1 \leq i \leq j \leq k$ and $(i,j) \neq (k,k)$, we use $\frac{1}{i} + \frac{1}{j} \geq \frac{2}{\sqrt{ij}}$ and $2k > 2\sqrt{ij}$ and $\sqrt{ij} \leq \frac{i+j}{2}$ to compute

$$\frac{1}{2}\left(\frac{1}{i} + \frac{1}{j}\right) k\, t(2k) > \frac{1}{\sqrt{ij}}\sqrt{ij}\; t(2\sqrt{ij}) \geq t(i+j).$$

Therefore, $t(G) \leq t(2k)\frac{kn}{2}$, with equality if and only if $m_{i,j} = 0$ when $1 \leq i \leq j \leq k$ and $(i,j) \neq (k,k)$; that is, when G is k-regular. Since $zt(z)$ is increasing, the bound increases with k. □

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