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Zagreb indices of maximal k-degenerate graphs

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Abstract

A graph is maximal k-degenerate if every subgraph has a vertex of degree at most k, and the property does not hold if any new edge is added to the graph. A well-known subclass of maximal k-degenerate graphs is the k-trees. We explore the Zagreb indices $M_1(G) = \sum_v (d(v))^2$ and $M_2(G) = \sum_{uv} d(u)\, d(v)$ for maximal k-degenerate graphs of order $n \geq k+2$. Estes and Wei previously studied these indices mostly for k-trees, and made three claims about Zagreb indices of maximal k-degenerate graphs. We show that one of their claims is true, and two are false. We also provide shorter proofs of several existing results on Zagreb indices.

1 Introduction

In this paper, we consider the Zagreb indices of maximal k-degenerate graphs.

Definition 1.1. [13] A graph G is *k-degenerate* if the vertices of G can be successively deleted, so that when each vertex v is deleted, it has degree at most k in the remaining graph. A graph is *maximal k-degenerate* if no edges can be added without violating the property of being k-degenerate. A *k-leaf* is a degree-k vertex of a maximal k-degenerate graph.

The size of a maximal k-degenerate graph with order $n \geq k$ is $kn - \binom{k+1}{2}$ [13]. One class of maximal k-degenerate graphs is particularly important.

Definition 1.2. A *k-tree* is a graph that can be formed by starting with K_{k+1} and iterating the operation of adding a k-leaf adjacent to all the vertices of a k-clique of the existing graph. The neighborhood of a new k-leaf is its *root.* We refer to the process of adding k-leaves as *constructing* the graph.

The maximal 2-degenerate graphs of order 5 and 6 are shown in Figure 1.

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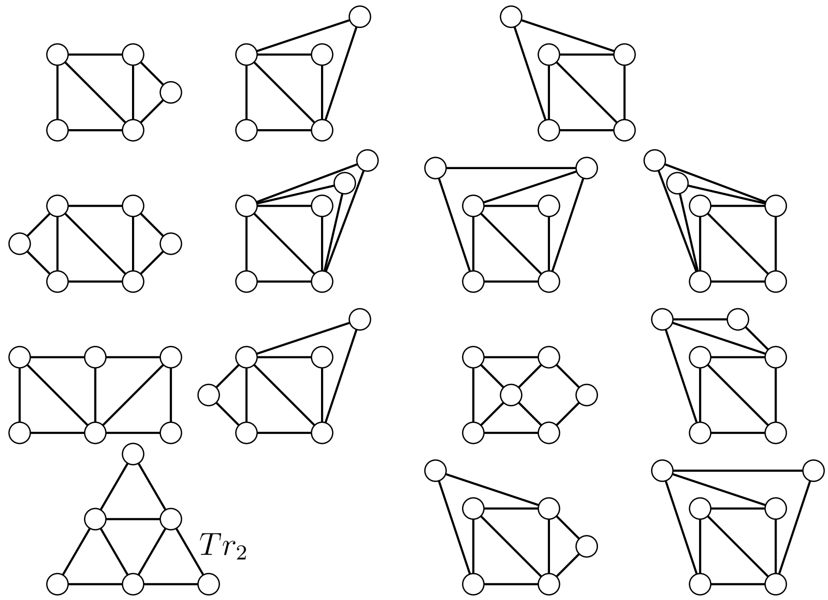


Figure 1: The maximal 2-degenerate graphs of order 5 and 6 are shown above. Those in the first column are outerplanar. Those in the second column are 2-trees, but not outerplanar. The rest are not 2-trees.

See [3] for a survey of maximal k-degenerate graphs and k-trees. One subclass of k-trees is of particular interest.

Definition 1.3. A *simple k-tree* is defined recursively by starting with K_{k+1} and iteratively adding a vertex adjacent to all vertices of a k-clique Q not previously used as the neighborhood of a k-leaf.

A *plane drawing* of a graph is a drawing in the plane that has no crossings. A graph is *outerplanar* if it has a plane drawing with all vertices on the boundary of the exterior region. A graph is a *maximal outerplanar graph (MOP)* if no edge can be added so that the resulting graph is still outerplanar.

The simple 2-trees are exactly the MOPs with order $n \geq 3$.

Definition 1.4. The *join* of graphs G and H, denoted $G + H$, has all possible edges between copies of G and H. The *k-star* with order n is $K_k + \overline{K}_{n-k}$, also denoted $S_{k,n-k}$. The *k^{th} power* G^k of a graph G adds all edges between pairs of vertices with distance at most k.

Any k-star is a k-tree. The k^{th} power of the path P_n, P_n^k, is a simple k-tree. These classes often occur as extremal graphs among all k-trees.

There are many results that bound graph parameters on maximal k-degenerate graphs, k-trees, and simple k-trees and determine the extremal graphs. See [4] for Albertson irregularity and sigma irregularity, and [3] for many other parameters. This paper focuses on two Zagreb indices.

Definition 1.5. The *first and second Zagreb indices* are $M_1(G) = \sum_v (d(v))^2$ and $M_2(G) = \sum_{uv} d(u)\, d(v)$.

These indices have applications to the study of chemical molecules. There are dozens of papers studying these indices on various graph classes. Nikolic et al. [15] survey M_1, M_2, and other related indices. Gutman and Das extend this work to survey M_1 [10] and M_2 [6]. Borovicanin et al. [5] survey bounds for Zagreb indices, and Gutman et al. [11] have a recent survey of related concepts. More recent papers on Zagreb indices include [7, 9, 12, 14, 16], and they contain references to many other such papers.

Das and Gutman [6, 10] showed that among trees, M_1 and M_2 are maximum for stars and minimum for paths. Hou et al. [12] found sharp bounds on M_1 and M_2 for MOPs. Estes [8] and Estes and Wei [9] studied M_1 and M_2 for k-trees and maximal k-degenerate graphs, proving several sharp bounds.

Estes and Wei [9] stated that "It may be interesting to show that for a maximally k-degenerate graph G and a k-degenerate graph G', $M_i\left(P_n^k\right) \leq M_i(G)$ for $1 \leq i \leq 2$ and $M_2(G') \leq M_2(S_{k,n-k})$." For clarity, we will separate out these three claims.

1. For a maximally k-degenerate graph G, $M_1\left(P_n^k\right) \leq M_1(G)$.
2. For a maximally k-degenerate graph G, $M_2\left(P_n^k\right) \leq M_2(G)$.
3. For a k-degenerate graph G', $M_2(G') \leq M_2(S_{k,n-k})$.

We will show that claim 3 is true, while claims 1 and 2 are false.

Definitions of terms and notation not defined here appear in [2]. In particular, $n(G)$ and $m(G)$ are the number of vertices and edges of G, respectively. The neighborhood of a vertex v is denoted $N(v)$, and the closed neighborhood is denoted $N[v]$. If vertices u and v are adjacent, we write $u \leftrightarrow v$, and if they are nonadjacent, we write $u \not\leftrightarrow v$.

2 Maximum M_1 for Maximal k-degenerate Graphs

Estes and Wei [9] found a sharp upper bound on M_1 for k-degenerate graphs. We will give an alternative proof of this result. Note that M_1 is determined only by the degree sequence of a graph. Thus we can define this for a sequence (which need not be graphic).

Definition 2.1. Let L be a (finite) list of numbers $d_1, \ldots, d_n$. The *Zagreb index of L* is

$$M_1(L) = \sum (d_i)^2 .$$

Lemma 2.2. *Let S be the set of all (finite) lists of integers $d_1, \ldots, d_n$ with $\Delta \geq d_1 \geq \ldots \geq d_n \geq \delta$ and fixed sum $\sum d_i$ satisfying $\delta n \leq \sum d_i \leq \Delta n$. Then the list with maximum M_1 in S is the list with at most one term that is not δ or Δ.*

Proof. Let L be a list in S, and denote $d_0 = \Delta$ and $d_{n+1} = \delta$. Suppose that there is more than one term that is not δ or Δ. Let i and j be indices ($1 \leq i < j \leq n$) such that $d_{i-1} > d_i \geq d_j > d_{j+1}$. Let L' be a list formed from L by replacing d_i with $d_i + 1$ and d_j with $d_j - 1$. Then L' is also in S. Now $M_1(L') = M_1(L) + (d_i + 1)^2 - (d_i)^2 +$

$(d_j-1)^2-(d_j)^2 = M_1(L)+2d_i+1-2d_j+1 > M_1(L)$. Thus we can successively increase M_1 until at most one term of the list is not δ or Δ. ☐

This can be applied to the degree sequences of maximal k-degenerate graphs.

Theorem 2.3. (Estes/Wei [9]) *Let G be a k-degenerate graph with order $n \geq k$. Then $M_1(G) \leq k(n-1)^2+(n-k)k^2$, and the k-degenerate graphs that maximize M_1 are the k-stars $K_k+\overline{K}_{n-k}$.*

Proof. Adding edges can only increase M_1, so we assume that G is maximal k-degenerate. The result is trivial when $n \in \{k, k+1\}$. A maximal k-degenerate graph has maximum degree $\Delta \leq n-1$, minimum degree $\delta = k$, and degree sum $2kn-k(k+1)$. The algorithm in Lemma 2.2 produces a unique list with maximum M_1 that satisfies these bounds. The list $(n-1)^k k^{n-k}$ (r^s means r is listed s times) must be this list, since it has sum $2kn-k(k+1)$ and all terms are $n-1$ or k. The M_1 of this list is clearly $k(n-1)^2+(n-k)k^2$. When $n \geq k+2$, the k-leaves of a maximal k-degenerate graph are nonadjacent. Thus k-stars are the only graphs with this list as their degree sequence, and $k(n-1)^2+(n-k)k^2$ is the value of M_1 on these graphs. ☐

3 Minimum M_1 for Maximal k-degenerate Graphs

Estes and Wei [9] suggested that for a maximal k-degenerate graph G, $M_1\left(P_n^k\right) \leq M_1(G)$. We will show that this is false. Note that since the definition of M_1 depends only on degrees, the graphs with minimum M_1 can be defined only by their degree sequence. There is a characterization of the degree sequences of maximal k-degenerate graphs.

Theorem 3.1. [1] *A nonincreasing sequence of integers $d_1, \ldots, d_n$ is the degree sequence of a maximal k-degenerate graph G if and only if*

$$k \leq d_i \leq \min\{n-1,\, k+n-i\}$$

and $\sum d_i = 2\left[k \cdot n - \binom{k+1}{2}\right]$ *for* $0 \leq i \leq n-1$.

We use this characterization to describe the graphs that minimize M_1.

Definition 3.2. A *near-regular sequence* is a nonincreasing sequence of integers $d_1, \ldots, d_n$ with $k \leq d_i \leq min\{n-1,\, k+n-i\}$ containing at most two consecutive integers other than those with $d_i = k+n-i$. A maximal k-degenerate graph is *near-regular* if it has a near-regular degree sequence.

Theorem 3.3. *Let S be a near-regular sequence of $n \geq k+1$ integers. Then any maximal k-degenerate graph with degree sequence S minimizes M_1.*

Proof. Let S be a graphic sequence for a maximal k-degenerate graph G. Let i and j be indices $(1 \leq i < j \leq n)$ such that $d_i > d_j+1$. Let L' be a list formed from L by replacing d_i with d_i-1 and d_j with d_j+1. Now $M_1(L') = M_1(L)+(d_i-1)^2-(d_i)^2+(d_j+1)^2-(d_j)^2 = M_1(L)-2d_i+1+2d_j+1 < M_1(L)$.

Thus we can successively decrease M_1 until we obtain a sequence with at most two distinct consecutive terms, except for those at the end with $d_i = k + n - i$. This degree sequence minimizes M_1 over all maximal k-degenerate graphs, and by Theorem 3.1, some maximal k-degenerate graph has this degree sequence. Thus any maximal k-degenerate graph with this degree sequence is extremal. □

When $k = 1$, the extremal graphs are paths. When $k = 2$ and $n \geq 5$, they are all those with degree sequence $4^{n-5}3^42$.

4 Minimum M_1 for k-trees

Estes and Wei [9] found the extremal graphs that minimize M_1 for k-trees. We provide a shorter proof of their result.

To facilitate an inductive proof, we define an order relation R on nonincreasing lists. For lists L with $d_1 \geq d_2 \geq \cdots \geq d_k$ and L' with $d'_1 \geq d'_2 \geq \cdots \geq d'_k$, we say $L \prec L'$ if $d_i \leq d'_i$ for all i. We minimize R if $L \prec L'$ for all lists L'.

Lemma 4.1. *Among all k-trees of order n, a k-clique that minimizes R occurs in P_n^k.*

Proof. This holds when $n = k$. Let T be a k-tree of order n containing a k-clique S. We can construct T starting with S and iteratively adding k-leaves. Each time we do, the new k-leaf and its neighbors induce K_{k+1}, and each new K_{k+1} has all but one vertex in common with the previous K_{k+1}. Thus for v_i, the ith vertex added (after the first $k + 1$), $|N(v_i) \cap S| \geq \max\{k + 1 - i, 0\}$. When $i \leq k$, equality is only possible when it is achieved for all smaller values of i. Thus minimizing R for S requires making each v_i adjacent to exactly $\max\{k + 1 - i, 0\}$ vertices in S. When $n \leq 2k+1$, this must produce P_n^k. For larger orders, P_n^k has a k-clique that minimizes R, but other graphs do also. □

Theorem 4.2. (Estes/Wei [9]) *The unique k-tree of order n that minimizes M_1 is P_n^k.*

Proof. We use induction on n, noting that the result is clear when $n \in \{k, k + 1\}$. Assume that for order r, P_r^k minimizes M_1. Let G be a k-tree with order $r + 1$ containing a k-leaf v. We know that $M_1(G - v)$ is minimized when $G - v = P_r^k$. We now show that when adding v to $G - v$, the increase in M_1 is minimum when v is rooted on a clique that minimizes relation R. Thus adding v results in P_{r+1}^k when $G - v = P_r^k$.

We add a new k-leaf v with neighborhood S and consider how this changes M_1. Note that v adds k^2 to M_1 regardless of S.

For each vertex $v_i \in S$, $d_G(v_i) = d_{G-v}(v_i) + 1$. Note that the difference between consecutive squares $(s + 1)^2 - s^2 = 2s + 1$ is smallest when s is smallest. Thus when $S = N(v)$ minimizes R, the increase in M_1 is minimized.

By Lemma 4.1, P_r^k has a k-clique that minimizes R over all cliques of k-trees of order r. This completes the proof. □

Estes and Wei's proof is about three pages, including essential lemmas. They also prove the (rather complicated) formula for $M_1\left(P_n^k\right)$.

For simple k-trees, P_n^k must also be the extremal graph for the lower bound. Estes [8] proved an upper bound on M_1 for simple k-trees and characterized the extremal graphs.

5 Maximum M_2 for Maximal k-degenerate Graphs

Estes and Wei [9] suggested that M_2 is maximized by k-stars over all maximal k-degenerate graphs. We will prove this. We could try induction adding one vertex at a time, but this runs into trouble. Instead, we add one edge at a time.

Lemma 5.1. *Increasing the degree of vertex u by 1 increases M_2 of the edges incident with u by $\sum_{x\in N(u)} d(x)$.*

Proof. When $uv \in E(G)$, increasing the degree of u by 1 increases the product for uv by $(d(u)+1)\,d(v) - d(u)\,d(v) = d(v)$. Thus the increase is $\sum d(x)$ over all neighbors of u. □

Definition 5.2. A *dominating vertex* of a graph is a vertex adjacent to all other vertices.

Theorem 5.3. *Let G be a k-degenerate graph with order $n \geq k$. Then $M_2(G) \leq \binom{k}{2}(n-1)^2 + k^2(n-k)(n-1)$, and the k-degenerate graphs that maximize M_2 are the k-stars $K_k + \overline{K}_{n-k}$.*

Proof. Adding edges can only increase M_2, so we only consider maximal k-degenerate graphs. The result is trivial when $n = k$. We use induction on n; assume the result holds for order r. Let G be a maximal k-degenerate graph with order $r+1$ that maximizes M_2, and v be a k-leaf. We consider $G - v$ and add the edges incident with v one by one. By Lemma 5.1, adding edge uv to G increases M_2 by

$$\begin{aligned} &\sum_{x\in N(u)} d(x) + \sum_{x\in N(v)} d(x) + (d(u)+1)(d(v)+1) \\ =&\sum_{x\in N[u]} d(x) + \sum_{x\in N(v)} d(x) + d(u)\,d(v) + d(v) + 1. \end{aligned}$$

Now $\sum_{x\in N[u]} d(x) \leq 2m$, with equality exactly when u is a dominating vertex. Since $d(v) = k$, $d(u)\,d(v)$ is maximized exactly when u is a dominating vertex and $\sum_{x\in N(v)} d(x)$ is maximized exactly when all neighbors of v are dominating vertices. Thus when successively adding edges incident with v, making all of its neighbors dominating vertices maximizes the increase in M_2. This is possible (only) when $G - v$ is a k-star, and $G - v$ has maximum M_2 when it is a k-star, so G is also. It is easily verified that $M_2\left(K_k + \overline{K}_{n-k}\right) = \binom{k}{2}(n-1)^2 + k(n-k)\,k(n-1)$. □

Estes and Wei [9] proved this result for the special case of k-trees. Their proof is about two pages.

6 Minimum M_2 for Maximal k-degenerate Graphs

Estes and Wei [9] suggested that for a maximally k-degenerate graph G, $M_2\left(P_n^k\right) \leq M_2(G)$. This is true when $k=1$, but false for every other value of k. The smallest counterexample occurs when $k=2$ and $n=5$. Let $K_4\bullet$ be formed by subdividing an edge of K_4. Then $M_2(K_4\bullet)=51$, while $M_2(P_5^2)=59$.

Definition 6.1. A *rotation* of edge vw to uw deletes vw and replaces it with uw.

Lemma 6.2. *Let G be a graph containing vertices u and v with $d(v)=a$ and $d(u)=b$, $a \geq b+2$, so that v has no neighbor with degree less than b, and u has no neighbor with degree greater than a. Let H be the result of rotating vw to uw. Then $M_2(H) \leq M_2(G)$, with equality only if $a=b+2$, all neighbors of v have degree b, all neighbors of u have degree a, and $u \nleftrightarrow v$.*

Proof. Assume the hypothesis. Note that there must be a vertex w in the neighborhood of v that is not in the neighborhood of u. Now M_2 is decreased at least $(a-1)b+ad(w)$ by removing vw and increased at most $ba+(b+1)d(w)$ by adding uw (equality requires $u \nleftrightarrow v$). Now $(a-1)b+ad(w)-(ba+(b+1)d(w)) = d(w)(a-b-1)-b \geq 0$, so rotating vw to uw decreases M_2 unless $a=b+2$, all neighbors of v have degree b, all neighbors of u have degree a, and $u \nleftrightarrow v$. □

Rotations can be used to find information about the structure of graphs that minimize M_2.

Lemma 6.3. *Any maximal k-degenerate graph with $n \geq k+3$ and minimum M_2 has one k-leaf.*

Proof. Let G be a maximal k-degenerate graph with $n \geq k+3$ with k-leaves u and w. Say $w \leftrightarrow v$, where v has largest degree among all neighbors of u and w (if not, exchange u and w). Form H by rotating vw to uw. Since v cannot be adjacent only to k-leaves, Lemma 6.2 implies that $M_2(H) < M_2(G)$. This reduces the number of k-leaves unless $d_H(v)=k$. In that case, rotate an edge incident with v to be adjacent with w, and repeat this process until no new k-leaf is produced. (This must occur since $n \geq k+3$, so $\Delta(G) \geq k+2$ unless $k=2$, $n=5$, and G has only one 2-leaf). The preceding operation can be iterated until we find a graph with smaller M_2 and only one k-leaf. □

This shows that Estes and Wei's suggestion is incorrect for all $n \geq k+3 \geq 5$.

We can determine the minimum value of M_2 for maximal 2-degenerate graphs by considering a larger class of graphs. Let $\mathbb{G}$ be the class of all graphs with size $m=2n-3$, minimum degree $\delta=2$, and exactly one 2-leaf (which is adjacent to a degree 3 vertex). The maximal 2-degenerate graphs with minimum M_2 are contained in $\mathbb{G}$ when $n \geq 5$.

Lemma 6.4. *Any graph in $\mathbb{G}$ with minimum M_2 is near-regular.*

Proof. Let G be a graph in $\mathbb{G}$ with 2-leaf u adjacent to a degree 3 vertex y and suppose G contains v with $d(v) = \Delta(G) > 4$. Note that G must contain at least five degree 3 vertices since its degree sum is $4n - 6$.

First assume $u \leftrightarrow v$. Let w be a vertex with $d(w) = 3$ so that $u \not\leftrightarrow w$. We rotate uv to uw, decreasing M_2 by Lemma 6.2.

Now assume $u \not\leftrightarrow v$. Let w and x be vertices with $d(w) = d(x) = 3$ so that $v \leftrightarrow w$ and $w \not\leftrightarrow x$, and $x \neq y$. We rotate vw to wx, resulting in a graph with M_2 no larger by Lemma 6.2.

We successively apply rotations, each time decreasing the degree of a vertex with degree above 4. Eventually, it is not possible for all neighbors of (the vertex designated) x to have maximum degree, so M_2 is decreased. Thus we see that any graph minimizing M_2 over $\mathbb{G}$ has maximum degree $\Delta \leq 4$, so it must be near-regular. □

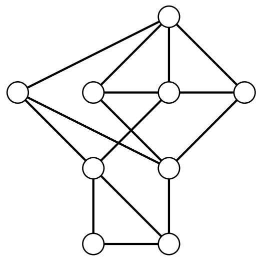
Let an $f - g$ edge be an edge that joins vertices of degrees f and g. Since graphs in $\mathbb{G}$ can only have degrees 2, 3, and 4, we can consider all possible types of $f - g$ edges for all possible values of f and g. A maximal 2-degenerate graph with $\Delta = 4$ has mostly 4-4 edges. Let G be maximal 2-degenerate with $\Delta = 4$ with a 2-3 edges, b 2-4 edges, c 3-3 edges, and d 3-4 edges. Then

$$M_2(G) = 6a+8b+9c+12d+16(2n-3-(a+b+c+d)) = 32n-48-10a-8b-7c-4d.$$

By Lemma 6.3, G has one 2-leaf, so $1 \leq a \leq 2$ and $a + b = 2$. We can list all possibilities for edges other than 4-4 edges using a code (a, b, c, d). These are contained in the following table, along with the resulting formula for M_2.

code	$M_2(G)$	code	$M_2(G)$
$(1,1,4,3)$	$32n-106$	$(2,0,4,2)$	$32n-104$
$(1,1,3,5)$	$32n-107$	$(2,0,3,4)$	$32n-105$
$(1,1,2,7)$	$32n-108$	$(2,0,2,6)$	$32n-106$
$(1,1,1,9)$	$32n-109$	$(2,0,1,8)$	$32n-107$
$(1,1,0,11)$	$32n-110$	$(2,0,0,10)$	$32n-108$

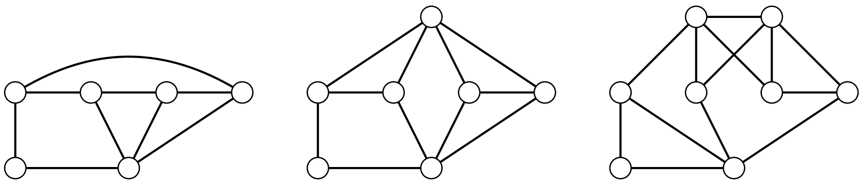
Note that $(1, 1, 0, 11)$ gives the smallest values for M_2. We can solve the problem of minimizing M_2 for maximal 2-degenerate graphs by demonstrating the existence of graphs with code $(1, 1, 0, 11)$. Note that such a graph must have $n \geq 9$, since there must be at least one 4-4 edge for a triangle to exist, and there are 11 3-4 edges. The following graph works for $n = 9$, and it can be extended to all larger orders by adding a new 2-leaf adjacent to the old 2-leaf and its degree 3 neighbor.



This implies the following.

Theorem 6.5. *The minimum possible value of* $M_2(G)$ *over all maximal 2-degenerate graphs of order* $n \geq 9$ *is* $32n-110$, *and the extremal graphs are all near-regular graphs with code* $(1,1,0,11)$.

We can also determine the minimum of M_2 for smaller maximal 2-degenerate graphs. For $n \in \{3,4,5\}$, K_3, $K_4 - e$, and $K_4\bullet$ (formed by subdividing an edge of K_4) are clearly extremal. For $n = 6$, deleting a 2-leaf must produce $K_4\bullet$. For $n = 7$, there are two degree 4 vertices, and hence at most 7 3-4 edges. For $n = 8$, we have seen that code $(1,1,0,11)$ is not possible. Graphs achieving the minimum for $n \in \{6,7,8\}$ are shown below.



The minimum values of M_2 for small n are shown in the following table.

n	3	4	5	6	7	8	9
min M_2	12	33	51	86	116	147	178

The argument used to characterize maximal 2-degenerate graphs with minimum M_2 does not generalize easily to larger values of k.

Conjecture 6.6. Any maximal k-degenerate graph with minimum M_2 is near-regular.

7 Minimum M_2 for k-trees

Estes and Wei [9] found the extremal graphs that minimize M_2 for k-trees. We provide a shorter proof of their result.

Theorem 7.1. (Estes/Wei [9]) *The unique* k*-tree of order* n *that minimizes* M_2 *is* P_n^k.

Proof. This holds when $n = k$. We use induction on n. Assume the result holds for k-trees of order at most n and let T be a k-tree of order $n+1 \geq k+1$. Let v be a k-leaf of T rooted on S and $H = T - v$.

Among all k-trees of order n, we seek a k-clique for which the increase in M_2 will be minimum when it is the root of a new k-leaf. We successively add all edges between v and $S = \{v_1, \ldots, v_k\}$. By Lemma 5.1, the increase in M_2 is

$$A(S) = \sum_{i=1}^{k} \left(\sum_{u_j \in N(v_i)} d_H(u_j) + i - 1 \right) = \sum_{i=1}^{k} \left(\sum_{u_j \in N(v_i)} d_H(u_j) \right) + \binom{k}{2}$$

for existing edges and $k\left(\sum d_H(v_i) + k\right)$ for new edges. The latter is clearly minimized when $\sum d_H(v_i)$ is smallest. By Lemma 4.1, this occurs for a k-clique of P_n^k.

We claim there is a k-clique in P_n^k that minimizes $A(S)$. Say we start constructing H with S and consider the change in $A(S)$ when a new k-leaf x is added. Now $A(S)$ increases by k for each vertex in S that x is adjacent to (and this will increase further if x has other neighbors). When x is adjacent to $y \notin S$, $A(S)$ increases by 1 for each neighbor of y in S. Thus at each step, the increase in $A(S)$ is minimized when each newly added vertex has as few neighbors in S as possible and its neighbors not in S have as few neighbors in S as possible. Further, minimizing these quantities in each step requires minimizing them in all previous steps. As in Lemma 4.1, this occurs when $T - v$ is a k-tree.

By induction, M_2 is minimized when $T - v$ is a k-tree. We have seen that the increase in M_2 is minimized when v is added adjacent to a root that minimizes relation R. Thus T must be a k-tree also. $\square$

The proof of Estes and Wei is two pages, not including two pages of lemmas. The calculation of the formula for $M_2\left(P_n^k\right)$ is in a 3.5 page lemma.

8 Maximum M_2 for MOPs

Hou et al. [12] found an upper bound on M_2 for simple 2-trees (MOPs). We present a shorter proof.

Theorem 8.1. (Hou et al. [12]) *For any MOP G with order $n \neq 6$, $M_2(G) \leq 3n^2 + n - 19$. Equality is achieved exactly by fans $P_{n-1} + K_1$.*

Proof. This is easily verified when $4 \leq n \leq 7$. We use induction on order n. Assume the result holds for MOPs of order less than n and let G be a MOP of order $n \geq 8$.

Assume G has a 2-leaf v with neighbors u and w, and $H = G - v$. By assumption, $M_2(H) \leq 3(n-1)^2 + (n-1) - 19$, with equality only if H is a fan. When we add v to H, we first add edge vw, then uv. This adds 1 to $d_H(w)$, increasing M_2 by $\sum d_H(v_i)$, $v_i \in N(w)$ by Lemma 5.1. Then this adds 1 to $d_H(u)$, increasing M_2 by $\sum d_H(v_i) + 1$, $v_i \in N(u)$. We also add $2(d_H(w) + d_H(u) + 2)$ due to uv and vw. Thus

$$M_2(G) = M_2(H) + \sum_{N(u)} d_H(v_i) + \sum_{N(w)} d_H(v_i) + 1 + 2(d_H(w) + d_H(u) + 2).$$

Note that the neighborhoods of u and w in H overlap on a single vertex x, so $d_H(w) + d_H(u) \leq n$. Now

$$2m(H) = \sum_{V(H)} d_H(v_i) = \sum_{N(u)} d_H(v_i) + \sum_{N(w)} d_H(v_i) - d(x) + \sum_{V(H)-N(u)-N(w)} d_H(v_i)$$

and x has at most 4 neighbors in $N(u) \cup N(w)$. Thus

$$\begin{aligned} M_2(G) &\leq M_2(H) + 2m(H) + 4 + 2n(G) + 5 \\ &\leq \left[3(n-1)^2 + (n-1) - 19\right] + [4(n-1) - 6] + 4 + 2n + 5 \\ &= 3n^2 + n - 18. \end{aligned}$$

Now x only has 4 neighbors in $N(u) \cup N(w)$ when H is not a fan, so $M_2(G) \leq 3n^2 + n - 19$. Equality requires $d_H(w) + d_H(u) = n$. If H were not a fan, deleting a 2-leaf whose neighbors do not neighbor all vertices of H and adding one that does must increase M_2 by the argument above. Thus H is a fan, so G is also. □

The proof of Hou et al. is about four pages. Note that $n = 6$ has an exceptional case, as $M_2(P_5 + K_1) = 95 < 96 = M_2(Tr_2)$ (see Figure 1).

References

[1] A. Bickle, Structural results on maximal k-degenerate graphs, *Discuss. Math. Graph Theory* 32 (4) (2012), 659–676.

[2] A. Bickle, "Fundamentals of Graph Theory", American Math Society (2020).

[3] A. Bickle, A survey of maximal k-degenerate graphs and k-trees, *Theory and Applications of Graphs* 0 (1) (2024) Article 5

[4] A. Bickle and Z. Che, Irregularities of maximal k-degenerate graphs, *Discrete Applied Math.* 331 (2023), 70–87.

[5] B. Borovicanin, K. C. Das, B. Furtulaxi and, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* 78 (2017), 17–100.

[6] K. Das and I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* 52 (2004), 103–112.

[7] K. Das, K. Xu and J. Nam, Zagreb indices of graphs, *Front. Math. China* 10 (3) (2015), 567–582.

[8] J. Estes, "On k-trees and Special Classes of k-trees", PhD Thesis, The University of Mississippi, (2012).

[9] J. Estes and B. Wei, Sharp bounds of the Zagreb indices of k-trees, *J Comb Optim.* 27 (2014), 271–291.

[10] I. Gutman and K. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* 50 (2004), 83–92.

[11] I. Gutman, E. Milovanović and I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graphs Comb.* 17 (1) (2020), 74–85.

[12] A. Hou, S. Li, L. Song and B. Wei, Sharp bounds for Zagreb indices of maximal outerplanar graphs, *J Comb Optim.* 22 (2011), 252–269.

[13] D. R. Lick and A. T. White, k-degenerate graphs, *Canad. J. Math.* 22 (1970), 1082–1096.

[14] B. Liu and Z. You, A survey on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* 65 (2011), 581–593.

[15] S. Nikolic, G. Kovacevic, A. Milicevic and N. Trinajstic, The Zagreb indices 30 years after, *Croat. Chem. Acta* 76 (2003), 113–124.

[16] K. Xu, The Zagreb indices of graphs with a given clique number, *Appl Math Lett.* 24 (2011), 1026–1030.

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