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.
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 \( K_k + K_{n-k} \), 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 $\delta_i \geq n \sum d_i$. 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 $G'$, $M_1 (P^k_n) \leq M_1 (G)$ 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 $G$, $M_1 (P^k_n) \leq M_1 (G)$.
2. For a maximally $k$-degenerate graph $G$, $M_2 (P^k_n) \leq M_2 (G')$.
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 $\delta$ or $\Delta$.

**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 $\delta$ or $\Delta$. 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 \(\delta\) or \(\Delta\).

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 \((n - 1)^k k^{n-k} (r^s \text{ means } r \text{ is listed } s \text{ times})\) 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. \(\square\)

### 3 Minimum \(M_1\) for Maximal \(k\)-degenerate Graphs

Estes and Wei [9] suggested that for a maximal \(k\)-degenerate graph \(G\), \(M_1 (P^k_n) \leq M_1 (G)\). 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 $4^{n-3}3^2$.

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 $i$th 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 $M_1(P_k^n)$.

For simple $k$-trees, $P_k^n$ 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

\[
\sum_{x \in N(u)} d(x) + \sum_{x \in N(v)} d(x) + (d(u) + 1)(d(v) + 1) = \sum_{x \in N[u]} d(x) + \sum_{x \in N(v)} d(x) + d(u)d(v) + d(v) + 1.
\]

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 $M_2(K_k + \overline{K}_{n-k}) = \binom{k}{2}(n-1)^2 + k(n-k)(n-1)$. \(\square\)
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 $G$, $M_2(P^k_n) \leq M_2(G)$. 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 $M_2(P^2_5) = 59$.

**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 $u \leftrightarrow v$.

**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 $u \leftrightarrow v$). 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 $u \leftrightarrow v$. \hfill \Box

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 $M_2(H) \leq M_2(G)$. 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. \hfill \Box

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 $G$ 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 $G$ when $n \geq 5$. 

A. BICKLE / AUSTRALAS. J. COMBIN. 89 (1) (2024), 167–178
Lemma 6.4. Any graph in $G$ with minimum $M_2$ is near-regular.

Proof. Let $G$ be a graph in $G$ 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 $u \leftrightarrow w$. 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 $G$ 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 $G$ 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 $M_2$.

<table>
<thead>
<tr>
<th>code</th>
<th>$M_2(G)$</th>
<th>code</th>
<th>$M_2(G)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1, 1, 4, 3)$</td>
<td>$32n - 106$</td>
<td>$(2, 0, 4, 2)$</td>
<td>$32n - 104$</td>
</tr>
<tr>
<td>$(1, 1, 3, 5)$</td>
<td>$32n - 104$</td>
<td>$(2, 0, 3, 4)$</td>
<td>$32n - 105$</td>
</tr>
<tr>
<td>$(1, 1, 2, 7)$</td>
<td>$32n - 108$</td>
<td>$(2, 0, 2, 6)$</td>
<td>$32n - 106$</td>
</tr>
<tr>
<td>$(1, 1, 1, 9)$</td>
<td>$32n - 109$</td>
<td>$(2, 0, 1, 8)$</td>
<td>$32n - 107$</td>
</tr>
<tr>
<td>$(1, 1, 0, 11)$</td>
<td>$32n - 110$</td>
<td>$(2, 0, 0, 10)$</td>
<td>$32n - 108$</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>$n$</th>
<th>min $M_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>12</td>
</tr>
<tr>
<td>4</td>
<td>33</td>
</tr>
<tr>
<td>5</td>
<td>51</td>
</tr>
<tr>
<td>6</td>
<td>86</td>
</tr>
<tr>
<td>7</td>
<td>116</td>
</tr>
<tr>
<td>8</td>
<td>147</td>
</tr>
<tr>
<td>9</td>
<td>178</td>
</tr>
</tbody>
</table>

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 $P_k^n$.

**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 $P^k_n$.

We claim there is a $k$-clique in $P^k_n$ 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 $M_2$ is minimized when $v$ is added adjacent to a root that minimizes relation $R$. Thus $T$ must be a $k$-tree also.

The proof of Estes and Wei is two pages, not including two pages of lemmas. The calculation of the formula for $M_2(P^k_n)$ 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 $vv$, 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

\[
2m(H) = \sum_{v \in V(H)} d_H(v) = \sum_{v \in N(u)} d_H(v) + \sum_{v \in N(w)} d_H(v) - d(x) + \sum_{v \in V(H) - N(u) - N(w)} d_H(v)
\]

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

\[
M_2(G) \leq M_2(H) + 2m(H) + 4 + 2n(G) + 5 \\
\leq [3(n-1)^2 + (n-1) - 19] + [4(n-1) - 6] + 4 + 2n + 5 \\
= 3n^2 + n - 18.
\]

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


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