Lower bounds for eccentricity-based parameters of graphs

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Abstract

For a connected graph G, the average eccentricity of G, written $\sigma_0(G)$, is the mean of the eccentricities of the vertices; the first Zagreb eccentricity index of G, written $\sigma_1(G)$, is the sum of the squares of the eccentricities, and the second Zagreb eccentricity index, written $\sigma_2(G)$, is the sum of the products of the eccentricities of pairs of adjacent vertices. We consider extremal problems for σ_0, σ_1, and σ_2 over connected n-vertex graphs in terms of other graph parameters. Specifically, we find the smallest values of σ_0, σ_1, and σ_2 over connected n-vertex graphs with fixed values of the chromatic number, number of vertices of degree 1, or number of cut-edges. We also characterize the corresponding extremal graphs.

Keywords: average eccentricity; Zagreb eccentricity index; chromatic number; cut-edge; topological index

1 Introduction

We consider n-vertex connected graphs. We write $d_G(u,v)$ for the distance between vertices u and v in a graph G. The *eccentricity* of a vertex $u \in V(G)$, denoted by $\varepsilon_G(u)$, is $\max_{v\in V(G)} d_G(u,v)$. The *radius* $r(G)$ and *diameter* $d(G)$ of a graph G are the minimum and maximum of $\varepsilon_G(u)$ over vertices $u \in V(G)$. Thus $r(G) \le \varepsilon_G(u) \le d(G)$ for $u \in V(G)$. Since eccentricity is infinite for disconnected graphs, we consider only connected graphs.

In chemical graph theory, graph invariants are called "topological indices", intended as numerical values reflecting structural properties. We consider some eccentricity-based invariants of connected 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 mainly study three eccentricity-based topological indices, called $\sigma_0, \sigma_1, \sigma_2$.

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The *average eccentricity* $\sigma_0(G)$ of G is defined by

$$\sigma_0(G) = \frac{1}{n} \sum_{u \in V(G)} \varepsilon_G(u),$$

where $n = |V(G)|$. This concept was introduced by Skorobogatov and Dobryninin [15] in mathematical chemistry as a molecular descriptor. Buckley and Harary [1] called it the "eccentric mean".

Many results about $\sigma_0(G)$ on n-vertex connected graphs have been obtained. Dankelmann et al. [2] gave upper bounds on $\sigma_0(G)$ in terms of minimum degree. Du and Ilić [3] resolved conjectures of the system AutoGraphiX about the relation between $\sigma_0(G)$ and the independence number, chromatic number, Randić index, and spectral radius. Dankelmann and Mukwembi [5] proved sharp upper bounds on $\sigma_0(G)$ in terms of the independence number, chromatic number, domination number, and connected domination number. Das et al. [6] presented lower and upper bounds for $\sigma_0(G)$ in terms of diameter, clique number, independence number, and the first Zagreb index. Ilić [10] resolved conjectures of AutoGraphiX about the relation between $\sigma_0(G)$ and the clique number, independence number, Randić index, minimum vertex degree and domination number. He et al. [11] gave sharp upper and lower bounds on $\sigma_0(G)$ for trees in terms of the number of leaves, domination number, and sizes of color classes. Tang and Zhou presented lower and upper bounds on $\sigma_0(G)$ for trees [16] and upper bounds on $\sigma_0(G)$ for unicyclic graphs [17]. Again, all these are for n-vertex connected graphs.

In analogy with the first and the second Zagreb indices (introduced in [9]), Vukičević and Graovac [18] introduced "Zagreb eccentricity indices" using vertex eccentricities instead of vertex degrees. The *first Zagreb eccentricity index* $\sigma_1(G)$ of a graph G is defined by

$$\sigma_1(G) = \sum_{u \in V(G)} \varepsilon_G^2(u),$$

and the *second Zagreb eccentricity index* $\sigma_2(G)$ of G is defined by

$$\sigma_2(G) = \sum_{uv \in E(G)} \varepsilon_G(u)\varepsilon_G(v).$$

Various results about the Zagreb eccentricity indices for n-vertex connected graphs have been obtained. Das et al. [4] obtained upper and lower bounds on σ_1 and σ_2 for trees and graphs and characterized the extremal graphs. Du et al. [7] found the trees with the three largest values of σ_1 and σ_2. Qi et al. [14] found the unicyclic graphs with the two largest values of σ_1 and the three largest values of σ_2. and σ_2 in terms of domination number, maximum degree, and size of the color classes; they also discussed the maximum over trees with given domination number. Qi and Du [13] found the trees with smallest values of σ_1. Xing et al. [20] determined the largest and smallest values of σ_1 and σ_2 over n-vertex trees with fixed diameter, and the smallest values over n-vertex trees with fixed matching number. Luo and Wu [12] studied the behavior of σ_1 and σ_2 under generalized hierarchical products of graphs.

These parameters are studied in detail on elementary graphs like trees, unicyclic, and bicyclic graphs due to their applications to molecular graphs. The graph-theoretical structures of the bonds in actual molecules tend to lie in these elementary classes of sparse graphs.

In this paper, we determine the smallest values of σ_0, σ_1, and σ_2 for n-vertex connected graphs with fixed chromatic number, number of vertices of degree 1, or number of cut-edges. We also characterize the corresponding extremal graphs. To describe the results, we introduce some notation and terminology.

Definition 1.1. Let $G+H$ denote the disjoint union of the graphs G and H, and let $G \oplus H$ be the *join* of G and H, obtained from $G+H$ by adding as edges all pairs consisting of one vertex of G and one vertex of H.

Let K_n denote the complete graph with n vertices, in which every two vertices form an edge. The *complement* $\overline{G}$ of a graph G is the graph with vertex set $V(G)$ in which vertices are adjacent if and only if they are not adjacent in G; thus $\overline{K}_n$ has no edges.

A *dominating vertex* in an n-vertex graph is a vertex of degree $n-1$. An *isolated vertex* is a vertex of degree 0. An *independent set* in a graph is a set of pairwise non-adjacent vertices. The *chromatic number* of a graph G, written $\chi(G)$, is the least k such that the vertex set can be expressed as the union of k independent sets.

A *pendant vertex* is a vertex of degree 1; a *pendant edge* is an edge with an endpoint of degree 1. A *cut-edge* of a connected graph is an edge whose deletion yields a disconnected graph.

The graphs minimizing σ_i over the classes we study all have dominating vertices, which ensures that all vertices have eccentricity at most 2.

When we fix the chromatic number to be 1 or n for an n-vertex graph, the only instances are $\overline{K}_n$ and K_n, so the extremal problems are trivial. For n-vertex graphs with chromatic number k, where $2 \le k \le n-1$, we show in Theorem 2.1 that $\sigma_0(G) \ge 2 - \frac{k-1}{n}$ and $\sigma_1(G) \ge 4n-k+3$, with equality in each case if and only if $G = K_{k-1} \oplus \overline{K}_{n+1-k}$. For σ_2, we show in Theorem 2.2 that the minimizing graphs always have the form $K_t \oplus (K_{k-t} + \overline{K}_{n-k})$, but the choice of t depends on the range of k compared to n.

For n-vertex graphs with k pendant vertices, we show in Theorem 3.4 that $\sigma_0(G) \ge 2 - \frac{1}{n}$ and $\sigma_1(G) \ge 4n-3$, each with equality if and only if G is any graph of the form $K_1 \oplus (H + \overline{K}_k)$, where H has no isolated vertex. We also prove in Theorem 3.4 that $\sigma_2 \ge 2(n-1) + 4\lceil (n-k-1)/2 \rceil$, with equality if and only if $G = K_1 \oplus (H + \overline{K}_k)$, where H is the $(n-k-1)$-vertex graph with fewest edges having no isolated vertex. We show in Corollary 3.5 that the extremal graphs are the same over the family of n-vertex graphs with k cut-edges.

We use the following observations in both sections. They are immediate, since dominating vertices have eccentricity 1, and all non-dominating vertices have eccentricity at least 2.

Lemma 1.2 ([7, 16]). *If G is an n-vertex connected graph with r dominating vertices, then*

$$\begin{aligned}\sigma_0(G) &\geq 2 - \frac{r}{n},\\ \sigma_1(G) &\geq 4n - 3r,\end{aligned}$$

with equality in each if and only if all the non-dominating vertices have eccentricity 2.

2 Fixed order and chromatic number

We consider first the extremal problem for the vertex-based parameters. As noted in the introduction, the problem is trivial when the chromatic number is 1 or n. When the vertices of a graph are partitioned into independent sets, the independent sets are called *color classes*.

Theorem 2.1. *If G is an n-vertex connected graph with chromatic number k, where $2 \leq k \leq n-1$, then $\sigma_0(G) \geq 2 - \frac{k-1}{n}$ and $\sigma_1(G) \geq 4n - 3k + 3$. Furthermore, each equality holds if and only if $G = K_{k-1} \oplus \overline{K}_{n+1-k}$.*

Proof. Let t be the number of dominating vertices in G (eccentricity 1). In a partition of G into k color classes, the dominating vertices must be in color classes of size 1. Since $k < n$, we have $t \leq k-1$. By Lemma 1.2, the bounds follow.

Equality in the bounds requires G to have $k-1$ dominating vertices. Hence any partition into independent sets has $k-1$ color classes of size 1. Since $\chi(G) = k$, the remaining vertices form an independent set. Hence $G = K_{k-1} \oplus \overline{K}_{n+1-k}$. Conversely, since the non-dominating vertices have eccentricity 2, by Lemma 1.2 equality holds for this graph. □

The result for the edge-based index is more difficult.

Theorem 2.2. *If G is an n-vertex connected graph with chromatic number k, where $n \geq 3$ and $2 \leq k \leq n-1$, then*

$$\sigma_2(G) \geq \begin{cases} 2n + 2 + 2k^2 - 6k & \text{if } 2 \leq k \leq \left\lfloor \frac{n+1}{2} \right\rfloor, \\ 8kn + 4k - 6k^2 - 2n^2 - 3n - 1 & \text{if } \left\lfloor \frac{n+1}{2} \right\rfloor < k < \left\lceil \frac{2n+1}{3} \right\rceil, \\ 2(k-1)n + \frac{5k}{2} - \frac{3k^2}{2} - 1 & \text{if } \left\lceil \frac{2n+1}{3} \right\rceil \leq k \leq n-1. \end{cases}$$

Furthermore, equality holds in the lower bound if and only if $G = K_t \oplus (K_{k-t} + \overline{K}_{n-k})$, where $t = 1$ in the first case, t is $4k - 2n - 2$ or $4k - 2n - 1$ in the second case, and $t = k-1$ in the third case.

Proof. Let G be a graph minimizing σ_2 among all n-vertex connected graphs with chromatic number k. Let T be the set of dominating vertices in G, with $t = |T|$. First suppose $t \geq 1$, so t vertices have eccentricity 1, and the remaining $n-t$ vertices all have eccentricity 2. Thus $\varepsilon(u)\varepsilon(v)$ is 1 when $u, v \in T$, 2 when one of them is in T, and 4 when $u, v \notin T$.

Now $G = K_t \oplus H$ with $\chi(H) = k - t$, so $|E(H)| \geq \binom{k-t}{2}$. Thus

$$\begin{aligned} \sigma_2(G) &\geq 1\binom{t}{2} + 2t(n-t) + 4\binom{k-t}{2} \\ &= \binom{t}{2} + 2t(n-2k+1) + 2k(k-1). \end{aligned}$$

Let $h(t) = \binom{t}{2} + 2t(n-2k+1)$. For G with fixed n and k, we may have various t. Nevertheless, when $t \geq 1$ we always have $\sigma_2(G) \geq h(t) + 2k(k-1)$. We obtain a lower bound by choosing t to minimize $h(t)$ (among graphs with $t \geq 1$). Achieving equality in the argument for the lower bound then requires $G = K_t \oplus (K_{k-t} + \overline{K}_{n-k})$.

Note that $h(t) - h(t-1) = (t-1) + 2(n-2k+1) = t - 4k + 2n + 1$. This difference is positive when $t > 4k - 2n - 1$ and negative when $t < 4k - 2n - 1$. Also, since $k < n$, we have $t \leq k - 1$. Thus $h(t)$ is minimized for some t in $\{1, 4k-2n-2, 4k-2n-1, k-1\}$. Also $h(4k-2n-2) = h(4k-2n-1)$, so h can be minimized at two integer values.

If $k \leq \lfloor \frac{n+1}{2} \rfloor$, then $4k - 2n - 1 \leq 1$, so h is minimized only at $t = 1$, and the only minimizing graph is $K_1 \oplus (K_{k-1} + \overline{K}_{n-k})$.

If $\lfloor \frac{n+1}{2} \rfloor < k < \lceil \frac{2n+1}{3} \rceil$, then $4k - 2n - 1 > 1$ and $4k - 2n - 2 < k - 1$, so h is minimized at two values, namely $4k - 2n - 2$ and $4k - 2n - 1$. Hence there are two minimizing graphs, both of the form $K_t \oplus (K_{k-t} + \overline{K}_{n-k})$, where t may be either of these values.

If $k \geq \lceil \frac{2n+1}{3} \rceil$, then $4k - 2n - 2 \geq k - 1$, so h is minimized only at $t = k - 1$, and the only minimizing graph is $K_{k-1} \oplus (K_1 + \overline{K}_{n-l})$.

It remains only to show that when $t = 0$, the value of $\sigma_2(G)$ with given n and k is always larger than the minimum found above. If $t = 0$, then each vertex in G has eccentricity at least 2, so $\varepsilon(u)\varepsilon(v) \geq 4$ for every edge. It is well known that every n-vertex connected graph with chromatic k has at least $\frac{1}{2}k(k-1) + (n-k)$ edges ([8]; see Exercise 5.2.6 in [19]). Thus

$$\begin{aligned} \sigma_2(G) &\geq 4\left[\frac{1}{2}k(k-1) + (n-k)\right] = 4n + 2k^2 - 6k \\ &> 2n + 2 + 2k^2 - 6k = h(1) + 2k(k-1). \end{aligned}$$

Since the value of $h(1)$ is always at least the smallest value of $h(t)$, the result follows. □

3 Fixed number of cut-edges or pendant vertices

For $n \geq 4$, let $\mathbf{G}_{n,k}$ be the set of n-vertex connected graphs with k cut-edges, where $1 \leq k \leq n-3$ (there are no n-vertex graphs with $n-2$ or at least n cut-edges, and those with $n-1$ cut-edges are the trees). Let $E'(G)$ be the set of cut-edges of G; note that the edges in $E'(G)$ are pendant edges or non-pendant edges. For $1 \leq k \leq n-3$, let $\mathbf{F}_{n,k}$ be the set of n-vertex graphs of the form $K_1 \oplus (H + \overline{K}_k)$, where H has minimum degree at least 1. Note that $\mathbf{F}_{n,k} \subseteq \mathbf{G}_{n,k}$.

For $n \geq 4$, let $\mathbf{H}_{n,k}$ be the set of n-vertex connected graphs with k vertices of degree 1, where $1 \leq k \leq n-1$. Obviously, $\mathbf{H}_{n,n-1} = \{K_{1,n}\}$ and $\mathbf{H}_{n,n-2}$ consists of the double-stars, which are graphs obtained from an edge uv by adding a and $n-2-a$ neighbors to u and v, respectively, where $1 \leq a \leq n-3$. For these graphs, the values of σ_i are easy to compute, so in studying $\mathbf{H}_{n,k}$ we restrict to $1 \leq k \leq n-3$.

Definition 3.1. Let uv be a non-pendant cut-edge of a graph G and let H and H' be the components of $G - uv$, with $u \in H$ and $v \in H'$, named so that $\varepsilon_H(u) \geq \varepsilon_{H'}(v)$. Construct the graph $\hat{G}$ from G by contracting the edge uv into u adding a pendant edge uz. We say that $\hat{G}$ is a *splinter* of G, called a "σ-transform" of G in [10].

Lemma 3.2 ([10])**.** *If $\hat{G}$ is a splinter of G, then $\sigma_0(\hat{G}) < \sigma_0(G)$.*

Lemma 3.3. *If $\hat{G}$ is a splinter of G, then $\sigma_1(\hat{G}) < \sigma_1(G)$ and $\sigma_2(\hat{G}) < \sigma_2(G)$.*

Proof. The proof is very similar to the proof of Lemma 3.2 in [10]. For the splinter operation, let u, v, H, H', z be as specified in Definition 3.1. Choose x and y so that $\varepsilon_H(u) = d_G(u,x)$ and $\varepsilon_{H'}(v) = d_G(v,y)$. Note that every vertex of $V(G) - \{v,y\}$ has eccentricity in G at least as large as in $\hat{G}$. As in Definition 3.1, $d_G(u,x) \geq d_G(v,y)$, so $\varepsilon_G(v) = 1 + d_G(u,x) = \varepsilon_{\hat{G}}(z)$ and $\varepsilon_G(y) = 1 + \varepsilon_{\hat{G}}(y)$. Hence each vertex contributes at least as much to $\sigma_i(G)$ as to $\sigma_i(\hat{G})$, and y contributes more. Thus the result follows. □

Theorem 3.4. *If $G \in \mathbf{H}_{n,k}$ with $1 \leq k \leq n-3$, then*

(i) $\sigma_0(G) \geq 2 - \frac{1}{n}$ *and* $\sigma_1(G) \geq 4n-3$, *each with equality if and only if* $G \in \mathbf{F}_{n,k}$;

(ii) $\sigma_2(G) \geq \begin{cases} 4n-2k-4 & \text{if } n-k \text{ is odd,} \\ 4n-2k-2 & \text{if } n-k \text{ is even,} \end{cases}$

with equality when $n-k$ is odd if and only if $G = K_1 \oplus (\frac{n-k-1}{2}K_2 + \overline{K}_k)$,
and equality when $n-k$ is even if and only if $G = K_1 \oplus (\frac{n-k-4}{2}K_2 + \overline{K}_k + P_3)$.

Proof. Given $G \in \mathbf{H}_{n,k}$, let t be the number of dominating vertices in G. Since G has at least one vertex of degree 1, we have $t \in \{0,1\}$.

By Lemma 1.2, $\sigma_0(G) \geq 2 - \frac{1}{n}$ and $\sigma_1(G) \geq 4n-3$, with equality if and only if $t = 1$, which implies $G \in \mathbf{F}_{n,k}$.

Now consider σ_2. If $t = 0$, then the k vertices of degree 1 have eccentricity at least 3, and all the other vertices have eccentricity at least 2. Since a connected n-vertex graph has at least $n-1$ edges,

$$\begin{aligned} \sigma_2(G) &\geq 2 \cdot 3 \cdot k + 2 \cdot 2 \cdot (n-k-1) \\ &= 4n + 2k - 4 > 4n - 2k - 2. \end{aligned}$$

If $t = 1$, then $G \in \mathbf{F}_{n,k}$. The one dominating vertex has eccentricity 1, all other vertices have eccentricity 2, and H has at least $\lceil (n-k-1)/2 \rceil$ edges since it has minimum degree at least 1. Thus

$$\begin{aligned}\sigma_2(G) &= 2(n-1) + 4|E(H)| \;\geq\; 2(n-1) + 4\left\lceil \frac{n-k-1}{2} \right\rceil \\ &= \begin{cases} 4n-2k-4 & \text{if } n-k \text{ is odd,} \\ 4n-2k-2 & \text{if } n-k \text{ is even.} \end{cases}\end{aligned}$$

The lower bound when $t = 0$ is strictly larger than this, and this is achievable, so σ_2 is minimized only when $t = 1$. Equality when $t = 1$ requires $|E(H)| = \lceil (n-k-1)/2 \rceil$. Thus H must consist of disjoint edges when $n-k-1$ is even, disjoint edges plus one path of two edges when $n-k-1$ is odd. That is, $G = K_1 \oplus (H + \overline{K}_k)$, where $H = \frac{n-k-1}{2} K_2$ if $n-k-1$ is even and $H = \frac{n-k-4}{2} K_2 + P_3$ if $n-k-1$ is odd. □

Corollary 3.5. *If $G \in \mathbf{G}_{n,k}$ with $1 \leq k \leq n-3$, then*

(i) $\sigma_0(G) \geq 2 - \frac{1}{n}$ *and* $\sigma_1(G) \geq 4n-3$, *each one with equality if and only if* $G \in \mathbf{F}_{n,k}$;

(ii) $\sigma_2(G) \geq \begin{cases} 4n-2k-4 & \textit{if } n-k \textit{ is odd,} \\ 4n-2k-2 & \textit{if } n-k \textit{ is even,} \end{cases}$

with equality when $n-k$ is odd if and only if $G = K_1 \oplus (\frac{n-k-1}{2} K_2 + \overline{K}_k)$,
and equality when $n-k$ is even if and only if $G = K_1 \oplus (\frac{n-k-4}{2} K_2 + \overline{K}_k + P_3)$.

Proof. Let G be a graph minimizing σ_i over $\mathbf{G}_{n,k}$, for $i \in \{0,1,2\}$. By Lemma 3.2 or Lemma 3.3, the k cut-edges of G must be pendant edges, which implies that G has k pendant vertices. Thus in fact $G \in \mathbf{H}_{n,k}$, and Theorem 3.4 yields the result. □

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