Some new results on the sum of squares of eccentricity in graphs*

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Abstract

The sum of the squares of eccentricity (SSE) over all vertices of a connected graph is a new graph invariant proposed in [13] and further studied in [14, 15]. In this paper, we report some further mathematical properties of SSE. We give sharp lower bounds for SSE among all n-vertices connected graphs with given independence number, vertex-, and edge-connectivity, respectively. Addtionally, we give explicit formulas for SSE of Cartesian product of two graphs, from which we deduce SSE of C_4 nanotube and nanotorus.

Keywords: Distance; Eccentricity; connectivity; independence number; C_4 nanotube and nanotorus.

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1 Introduction

All graphs considered in this paper are simple and connected. Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, we use $d_G(v)$ to denote the degree of a vertex v in G. The distance between two vertices u and v, namely, the length of the shortest path between u and v is denoted by $d_G(u, v)$. The **eccentricity** of a

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vertex v in a graph G is defined to be $ec_G(v) = \max\{d_G(u, v) | u \in V(G)\}$. Other notation and terminology not defined here will conform to those in [2].

The oldest and well-studied distance-based graph invariant $W(G)$, also termed as **Wiener index** in chemical or mathematical chemistry literature [4, 6], associated with a connected graph G is defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$.

Recently, some eccentricity-based graph invariants or molecular topological indices in mathematical chemistry, such as **eccentricity connectivity index** [1, 5, 9, 11, 12] and **eccentricity distance sum** [7, 8] have been proposed and studied. Also, the **average eccentricity** of a graph was investigated in [3].

The sum of the squares of eccentricity (SSE) over all vertices of a graph and the sum $\sum_{uv \in E(G)} ec_G(u) ec_G(v)$ are called, respectively, the **first and second normalized Zagreb eccentricity indices** G in [13], where the authors compared these two graph invariants for all n-vertices trees and unicyclic graphs, where m is the size of G.

In [14], Wen first gave upper and lower bounds for SSE among n-vertices connected graphs. Then he gave a lower bound for SSE in terms of Wiener index and an upper bound for SSE in terms of the first Zagreb index among n-vertices connected graphs. Finally, he gave a Nordhaus-Gaddum-type bound for SSE. The same author [15] characterized the cactus with the minimum SSE among all n-vertex cacti. As an application, he obtained the tree and unicyclic graph with the minimum SSE. Finally, he gave explicit formulas for SSE of double graph and iterated double graph of a given nontrivial connected graph.

In this paper, we report some further mathematical properties of SSE. We give lower bounds for SSE among all n-vertex connected graphs with given independence number, vertex-, and edge-connectivity, respectively. Additionally, we give explicit formulas for SSE of Cartesian product of two graphs, from which we deduce SSE of C_4 nanotube and nanotorus.

2 Lower bounds for SSE involving other graph parameters

The following result is obvious, whose proof is omitted here.

Lemma 1. *Let G be a nontrivial connected graph with at least three vertices. If G is not isomorphic to K_n, then $SSE(G) > SSE(G + e)$, where*

$e \in E(\overline{G})$.

A vertex subset S of a graph G is said to be an **independent set** of G, if the subgraph induced by S is an empty graph. Then $\beta = \max\{|S| : S \text{ is an independent set of } G\}$ is said to be the **independence number** of G.

Let G and H be two vertex-disjoint graphs. The **join** of graphs G and H, denoted by $G \vee H$, is defined as a graph whose vertex set is $V(G) \cup V(H)$ and edge set is $E(G) \cup E(H) \cup \{xy | x \in V(G), y \in V(H)\}$.

Theorem 1. *Let G be an n-vertex connected graph with independence number β. Then*

$$SSE(G) \geq n + 3\beta$$

with equality if and only if $G \cong \beta K_1 \vee K_{n-\beta}$.

Proof. Let G_{min} be a graph chosen among all n-vertex connected graphs with independence number β such that G_{min} has the smallest SSE. Let S be a maximal independent set in G_{min} with $|S| = \beta$. Since adding edges into a graph will decrease its SSE by Lemma 1, each vertex x in S is adjacent to every vertex y in $G_{min} - S$. Moreover, the subgraph induced by vertices in $G_{min} - S$ is a clique in G_{min}. So $G_{min} \cong \beta K_1 \vee K_{n-\beta}$. An elementary calculation gives $SSE(\beta K_1 \vee K_{n-\beta}) = 2^2 \cdot \beta + 1 \cdot (n - \beta) = n + 3\beta$, as claimed. □

The **vertex-connectivity** is the minimum number of vertices whose deletion from a connected graph disconnects it, and the **edge-connectivity** is the minimum number of edges whose deletion from a connected graph disconnects it.

Theorem 2. *Let G be an n-vertex connected graph with vertex-connectivity k. Then*

$$SSE(G) \geq 4n - 3k$$

with equality if and only if G is of the form $K_k \vee (K_{n_1} + K_{n_2})$.

Proof. We choose G_{min} to be the graph such that G_{min} has the smallest SSE within all connected graphs with n vertices and vertex-connectivity k. Let C be a vertex-cut of G_{min} such that $|C| = k$ and let $G_{min} - C = G_1 \cup G_2 \cup \cdots \cup G_t$ $(t \geq 2)$. By Lemma 1, we must have $t = 2$, for otherwise, we can adding edges between any two components, resulting in a new graph G' with vertex-connectivity k and a strictly smaller SSE than that of G_{min}, a contradiction to our choice of G_{min}.

The same reason leads us to that both G_1 and G_2 are cliques of G_{min} and that any vertex in $G_1 \cup G_2$ is adjacent to each vertex in C. Let n_i

denote the order of G_i. Thus, we have $G_{min} \cong K_k \vee (K_{n_1} + K_{n_2})$, as claimed. $\square$

In the following theorem, we show that $K_k \vee (K_1 \cup K_{n-1-k})$ also minimizes SSE among all n-vertex connected graphs with edge-connectivity k.

Theorem 3. *Let G be an n-vertex connected graph with edge-connectivity k. Then*

$$SSE(G) \geq 4n - 3k$$

with equality if and only if G is of the form $K_k \vee (K_{n_1} + K_{n_2})$.

Proof. Let $f(x) = 4n - 3x$. It is easily seen that $f(x)$ is a strictly decreasing function. Suppose that G is a graph on n vertices with edge-connectivity k.

If G has the vertex connectivity λ, then we have $\lambda \leq k$. It is known from Theorem that $SSE(G) \geq f(\lambda)$. Now, $f(\lambda) \geq f(k)$ and we get $SSE(G) \geq f(k) = 4n - 3k$. It is easy to check that the equality holds if and only if G is of the form $K_k \vee (K_{n_1} + K_{n_2})$.

This completes the proof. $\square$

3 SSE of Cartesian product graphs and its chemical applications

Let R and S denote a C_4 **nanotube** and **nanotorus**, respectively. In this section, we give explicit formulas for the sum of squares of eccentricity of these two nano structures.

The **Cartesian product** $G_1 \times G_2 \times \cdots \times G_k$ of graphs $G_1, G_2, \ldots, G_k$ has the vertex set $V(G_1) \times V(G_2) \times \cdots V(G_k)$, in which two vertices $(u_1, u_2, \ldots, u_k)$ and $(v_1, v_2, \ldots, v_k)$ are adjacent if they differ in exactly one position, say in i-th, and u_iv_i is an edge of G_i. It is well known (see [10]) that for $G = G_1 \times G_2 \times \cdots \times G_k$ and its two vertices $u = (u_1, u_2, \ldots, u_k)$ and $v = (v_1, v_2, \ldots, v_k)$, we have $d_G(u, v) = \sum_{i=1}^{k} d_G(u_i, v_i)$.

Then we have the following relation

$$ec_{G_1 \times G_2}(u_1, u_2) = ec_{G_1}(u_1) + ec_{G_2}(u_2). \tag{1}$$

As introduced in [3], for a graph G, we use $\xi(G) = \sum_{v \in V(G)} ec_G(v)$ to denote the **total eccentricity** of G.

Theorem 4. *Let G_1 and G_2 be graphs of order n_1 and n_2, respectively. Then*

$$SSE(G_1 \times G_2) = n_2 SSE(G_1) + n_1 SSE(G_2) + 2\xi(G_1)\xi(G_2).$$

Proof. By the definition of SSE and above equation (1), we have

$$\begin{aligned} SSE(G_1 \times G_2) &= \sum_{(u_1,u_2)\in V(G_1\times G_2)} (ec_{G_1\times G_2}(u_1,u_2))^2 \\ &= \sum_{u_1\in V(G_1),\, u_2\in V(G_2)} (ec_{G_1}(u_1) + ec_{G_2}(u_2))^2 \\ &= \sum_{u_1\in V(G_1),\, u_2\in V(G_2)} (ec_{G_1}(u_1))^2 + \\ &\quad \sum_{u_1\in V(G_1),\, u_2\in V(G_2)} (ec_{G_2}(u_2))^2 + \\ &\quad 2\sum_{u_1\in V(G_1)} ec_{G_1}(u_1) \sum_{u_2\in V(G_2)} ec_{G_2}(u_2) \\ &= n_2 SSE(G_1) + n_1 SSE(G_2) + 2\xi(G_1)\xi(G_2). \end{aligned}$$

This completes the proof. □

Note that $R = P_n \times C_m$ and $S = C_n \times C_m$. In order to compute the sum of squares of eccentricity of R and S, we need only to compute the sum of squares of eccentricity of P_n and C_n by Theorem 4.

For any vertex v in C_n,

$$ec_{C_n}(v) = \begin{cases} \frac{n}{2}, & 2 \mid n; \\ \frac{n-1}{2}, & 2 \nmid n. \end{cases} \quad (2)$$

If we label vertices of the path P_n consecutively as $v_1, \ldots, v_n$, then for $1 \le i \le \lfloor \frac{n}{2} \rfloor$, we have

$$ec_{P_n}(v_i) = n - i \quad (3)$$

and for $\lfloor \frac{n}{2} \rfloor + 1 \le i \le n$, we have

$$ec_{P_n}(v_i) = i - 1. \quad (4)$$

By the definition of the sum of squares of eccentricity and the equations (1)–(4), we have

$$SSE(P_n) = \begin{cases} \frac{7n^3-9n^2+2n}{12}, & 2 \mid n; \\ \frac{7n^3-9n^2-n+3}{12}, & 2 \nmid n \end{cases} \quad (5)$$

and

$$SSE(C_n) = \begin{cases} \frac{n^3}{4}, & 2 \mid n; \\ \frac{n(n-1)^2}{4}, & 2 \nmid n. \end{cases} \tag{6}$$

Moreover,

$$\xi(P_n) = \begin{cases} \frac{3n^2-2n}{4}, & 2 \mid n; \\ \frac{3n^2-2n-1}{4}, & 2 \nmid n \end{cases} \tag{7}$$

and

$$\xi(C_n) = \begin{cases} \frac{n^2}{2}, & 2 \mid n; \\ \frac{n(n-1)}{2}, & 2 \nmid n. \end{cases} \tag{8}$$

In view of the equations (5)–(8),

$$SSE(R) = \begin{cases} \frac{3m^3n+7mn^3+9m^2n^2-6m^2n-9mn^2+2mn}{12}, & 2 \mid n, 2 \mid m; \\ \frac{3m^3n+7mn^3+9m^2n^2-12m^2n-18mn^2+11mn}{12}, & 2 \mid n, 2 \nmid m; \\ \frac{3m^3n+7mn^3+9m^2n^2-6m^2n-9mn^2-3m^2-mn+3m}{12}, & 2 \nmid n, 2 \mid m; \\ \frac{3m^4n-9m^3n+7mn^3+9m^2n^2+3m^2n-18mn^2-3m^2+2mn+6m}{12}, & 2 \nmid n, 2 \nmid m \end{cases}$$

and

$$SSE(S) = \begin{cases} \frac{m^3n+mn^3+2m^2n^2}{4}, & 2 \mid n, 2 \mid m; \\ \frac{m^3n+mn^3+2m^2n^2-2m^2n-2mn^2+mn}{4}, & 2 \mid n, 2 \nmid m; \\ \frac{m^3n+mn^3+2m^2n^2-2m^2n-2mn^2+mn}{4}, & 2 \nmid n, 2 \mid m; \\ \frac{m^3n+mn^3+2m^2n^2-4m^2n-4mn^2+4mn}{4}, & 2 \nmid n, 2 \nmid m. \end{cases}$$

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