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ORIGINAL RESEARCH

Exploring the SDE index: a novel approach using eccentricity in graph analysis

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Abstract
In this article, we present an enhanced version of the symmetric division deg index (*sdd*-index) known as symmetric division eccentric index or *SDE* index, for short. Unlike its predecessor, *SDE* employs eccentricity instead of vertex degree to assess the properties of a graph G. In this paper, we first give some bounds for *SDE* index of a connected graph G with fixed size m. For two connected graphs G_1 and G_2 of order n_1 and n_2, employing these bounds, we compute the *SDE* index for two classes of graph products, e.g., the Cartesian product and Corona product. As an application, we determine the structure of graphs with two non-equi-centric edges. Our theorems generalize the recent results for the extended adjacency index of a graph. Besides, this research significantly contributes to the comprehension of graph analysis techniques and offers valuable insights into the relationship between *SDE* and various graph properties.

Keywords Symmetric division deg index · Eccentricity · Vertex degree

Mathematics Subject Classification Primary: 05C09 · Secondary: 05C12 · 05C70

1 Introduction

Graph theory, a fundamental area of mathematics, plays a pivotal role in modelling real-world networks and understanding their intricate structures. In this paper, we present an advanced variant of the symmetric division degree index (*SDD*-index)

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called as symmetric division eccentric index (or shortly *SDE* index) which leverages eccentricity instead of vertex degree for evaluating graph properties.

The *SDD*-index has been widely used to measure the distribution of edges in a graph. However, by incorporating eccentricity, the *SDE* index offers a refined perspective on graph analysis. Eccentricity captures the notion of how far a vertex is from other vertices in terms of shortest path lengths, providing a more comprehensive evaluation of graph structure.

The primary objective of this study is to explore new bounds and new properties of the *SDE* index as well as investigate its relationship with other prominent graph indices. Specifically, we will examine the graph invariants such as the first and second Zagreb indices, harmonic index, atom-bond-connectivity index, Randic index, the size of the graph automorphism group, and the sum connectivity index. By calculating these indices and analyzing their correlations with *SDE*, we aim to gain a deeper understanding of the interplay between different graph measures and the enhanced *SDE* index.

Understanding such relationships can lead to valuable applications in various fields, including network analysis, network modelling, and biological network characterization. Moreover, uncovering the connections between the *SDE* index and established graph indices may offer new insights into graph properties that were previously unexplored.

In the subsequent sections of this paper, we will introduce the methodology behind the calculation of the *SDE* index and graph indices. We will then present our findings on the correlation between *SDE* and other indices, highlighting any significant patterns or observations. Finally, we will discuss the implications of our results and potential avenues for future research.

In conclusion, by introducing the *SDE* index and investigating its relationships with various graph indices, this paper contributes to the advancement of graph theory and provides a deeper understanding of graph properties.

2 Preliminary results

We denote a graph by $G = (V, E)$, where $V(G)$ represents the set of vertices and $E(G)$ represents the set of edges. In this paper, all graphs are assumed to be simple, connected, and undirected.

The Cartesian product of two graphs, G and H, denoted as $G_1 \times G_2$, results in a new graph with the vertex set $V(G) \times V(H)$. Two vertices (g_1, h_1) and (g_2, h_2) are adjacent if and only if either $g_1 = g_2$ and $h_1h_2 \in E(H)$, or if $h_1 = h_2$ and $g_1g_2 \in E(G)$. To obtain further information on other terms related to graph theory, refer to [14]. The corona product of two graphs G_1 and G_2, represented as $G_1 \circ G_2$, is obtained by taking $|V(G_1)|$ copies of G_2 and connecting each vertex of the i-th copy with the corresponding vertex $v_i \in V(G_1)$, see for example [5]. It follows that the number of vertices in $G_1 \circ G_2$, denoted by $|V(G_1 \circ G_2)|$, is given by $|V(G_1)|$ $(1+|V(G_2)|)$, and the number of edges, denoted by $|E(G_1 \circ G_2)|$, is calculated as $|E(G_1)| + |V(G_1)|(|(V(G_2)|+|E(G_2)|)$, see [8].

The distance between two vertices $u, v \in V$, denoted as $d(u, v)$, is defined as the length of the shortest path between vertices u and v in graph G. The eccentricity of a vertex v, denoted as $\varepsilon(v)$, is the maximum distance from v to any other vertex in G:

$$\varepsilon(v) = max(d(u, v));\ \text{for all } u \in V(G).$$

The radius of a graph G, denoted as $r(G)$, is the minimum eccentricity among all vertices:

$$r(G) = min(\varepsilon(v));\ \text{for all } v \in V(G).$$

The diameter of a graph G, denoted as $d(G)$, is the maximum eccentricity among all vertices [1]:

$$d(G) = max(\varepsilon(v));\ \text{for all } v \in V(G).$$

A vertex v of G is called a central vertex if $\varepsilon(v) = r(G)$ and center $C(G)$ of G is the collection of all such vertices in G. A graph is referred to as a self-centered graph if $r(G) = d(G)$. In other words, in a self-centered graph, the eccentricity is the same for all vertices in the graph. This can be equivalently stated as the radius and diameter of the graph, which represent the smallest and largest eccentricities, respectively, being equal. Within this piece, we introduce the notion of an "equi-centric" edge (or **ec**-edge for short) in a graph, which refers to an edge, where both ends have equal eccentricity. By defining and identifying equi-centric edges, we can gain deeper insights into the structural properties of graphs. By an equi-centric edge, we mean an edge that endpoints have the same eccentricity. An edge which is not equi-centric is called a non-equi-centric edge (or **nec**-edge for short). This means that for such an edge, the maximum distance from each endpoint to any other vertex in the graph is identical.

A graph G is called as **nec**-graph if G has no **ec**-edge. Equi-centric edges play a significant role in understanding and analyzing various graph structures. Identifying equi-centric edges can be valuable in several applications. For example, in social network analysis, detecting equi-centric edges may provide insights into individuals who exhibit similar influence or centrality within a network. Additionally, in transportation networks, identifying equi-centric edges could highlight roads or paths, where travel time remains constant regardless of the starting or ending point. Studying equi-centric edges contributes to the broader understanding of graph properties and helps uncover hidden patterns or connections within complex networks. By exploring the characteristics and implications of equi-centric edges, researchers and practitioners can enhance their analyses and make informed decisions in a wide range of fields.

A pendant edge in a graph refers to an edge that is incident to only one vertex. In other words, one end of the edge connects to a vertex while the other end remains unconnected. A cut edge, also known as a bridge, is an edge in a graph whose removal increases the number of connected components in the graph. In other words, if we remove a cut edge from a graph, the graph becomes disconnected or split into two or more separate parts.

The edge connectivity number of a graph is the minimum number of edges that must be removed in order to disconnect the graph. It represents the minimum number of edges that need to be remove in order to separate the graph into multiple disconnected components.

A leaf node, also known as a leaf vertex or terminal vertex, refers to a node in a graph that has only one edge connected to it. Here we denote leaf nodes by LF.

Graph indices are numerical quantities associated with graphs that provide insights into their structural properties and can be used to analyze various aspects of graph behavior. In this paper, we focus on several important graph indices: the graph independence number, first and second Zagreb index, harmonic index, ABC index, Randic index, size of the graph automorphism group, and sum connectivity index.

The graph independence number, denoted as $\alpha(G)$, is the maximum cardinality of an independent set in a graph G. An independent set is a subset of vertices in which no two vertices are adjacent.

One of the most graph indices is the widely recognized Zagreb index presented in [9]. When considering a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ can be defined as follows:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2,$$
$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v),$$

where $d_G(v)$ denotes the degree of vertex v in graph G.

The harmonic index, represented as $H(G)$, is a graph property initially presented in reference [4]. It is computed for a given graph G using the following formula:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)}.$$

The atom-bond-connectivity index (or shorting the ABC index) is determined by the following formula [3]:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}.$$

The Randic index, denoted as $R(G)$, is a molecular descriptor originally developed for chemical compounds but applicable to graphs as well. It is defined as the sum of the reciprocal square roots of the degrees of all vertices in a graph G. The $R(G)$ captures the complexity and branching patterns of a graph and is defined as [12]

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

The size of the automorphism group, denoted as $|Aut(G)|$, represents the number of automorphisms of a graph G. An automorphism is an isomorphism from a graph to itself, preserving both the vertex set and the edge set. The size of the graph automorphism group reflects the symmetry and structural regularity of a graph.

The sum connectivity index, denoted as $SC(G)$ is defined as [16]

$$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$

The symmetric division degree index (SDD-index) was defined by Vukičević [13] as follows:

$$SDD(G) = \sum_{uv \in E(G)} \left[\frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)} \right].$$

In this way, we define the *SDE* index based on eccentricities of vertices as follows:

$$SDE(G) = \sum_{uv \in E(G)} \left[\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} \right].$$

In graph theory, a theta graph (denoted as Θ-graph) is a specific type of connected graph that consists of three internally disjoint paths, each with a length of at least one edge, connecting two vertices (u and v) with lengths k, l, and m, where k, l, and m are non-negative integers. The three paths are mutually disjoint, meaning they do not share any vertices or edges except for the endpoints u and v.

Several studies have been conducted to explore the relationship between network properties and graph parameters. Ghorbani et al. [7] focused on investigating various topological indices such as the first Zagreb index, second Zagreb index, spectral radius, Randic index, Laplacian Estrada index, Laplacian Energy, Harary index, Estrada index, energy, Balaban index and atom-bond connectivity across different networks. Additionally, the authors in [6] examined networks of fullerene molecules. In this paper, our objective is to explore the correlation between graph indices and the generalized symmetric division degree index *SDE* in protein networks. Our focus will be on investigating and analyzing how changes in graph indicators impact the *SDE*. This research aims to enhance our understanding of network behavior and the factors influencing it.

Example 2.1 Here, we determine the SDE index of a star graph on n vertices. Since surrounded vertices have an eccentricity of two and the eccentricity of the central vertex is one, we obtain

$$SDE(S_n) = \sum_{uv \in E(S_n)} \left[\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} \right] = \sum_{uv \in E(S_n)} \left[\frac{1}{2} + \frac{2}{1} \right] = \frac{5}{2}(n-1).$$

The star graph is a special case of an edge-transitive graph. In general, we have the following theorem.

Theorem 2.1 *Let G be a graph with size m. Then*

i) $2m \leq SDE(G) \leq \frac{5}{2}m$,

ii) *If G is an edge-transitive graph, then $SDE(G) = 2m$ or $SDE(G) = m(\frac{r}{d} + \frac{d}{r})$, where r and d are the radius and diameter of the graph, respectively.*

Proof First, we show that for an edge $e = uv$, $\varepsilon(u) = \varepsilon(v)$ or $\varepsilon(u) = \varepsilon(v) + 1$. Suppose $\varepsilon(u) \neq \varepsilon(v)$, there exists a path P of length $\varepsilon(u)$ between u and a vertex such as u_n that is $P = u, u_1, u_2, u_3 \ldots u_n$. Clearly, if $v \notin \{u, u_1, u_2, \ldots, u_n\}$ then $\varepsilon(v) > \varepsilon(u)$ which is a contradiction. Since u and v are adjacent, without loss of generality, we can assume that $u_1 = v$ and we are done.
$i)$ Given that for each edge $e = uv$, since $|\varepsilon(u) - \varepsilon(v)| \leq 1$, we have following two cases:

- If $\varepsilon(u) = \varepsilon(v)$, then $\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} = 2$,
- If $\varepsilon(u) \neq \varepsilon(v)$, then $\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} \leq \frac{5}{2}$.

This completes the proof of the first claim.
$ii)$ Assume that G is edge-transitive. If G is vertex-transitive, then G is self-centered and so $SDE(G) = 2m$. If G is edge-transitive but not vertex-transitive, since the action of $Aut(G)$ on the edges is transitive, for each edge $e = uv$ and an arbitrary vertex w, we have $\varepsilon(w) \in \{r, d\}$ and by discussion before the proof of Part $i)$ the proof is complete. □

Example 2.2 Now consider the path graph P_n with vertices $v_1, v_2, \ldots, v_n$. It is easy to see that $\varepsilon(v_1) = \varepsilon(v_n)$, $\varepsilon(v_2) = \varepsilon(v_{n-1})$, etc. This leads us to conclude that if n is even, then we have

$$SDE(P_n) = \sum_{uv \in E(P_n)} \left[\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} \right]$$
$$= 2 \times \left[\frac{n-1}{n-2} + \frac{n-2}{n-1} + \frac{n-2}{n-3} + \cdots + \frac{n - \frac{n-2}{2}}{n - \frac{n}{2}} + \frac{n - \frac{n}{2}}{n - \frac{n-2}{2}} \right]$$
$$+ \left[\frac{n - \frac{n}{2}}{n - \frac{n}{2}} + \frac{n - \frac{n}{2}}{n - \frac{n}{2}} \right].$$

And if n is odd, we obtain

$$
\begin{aligned}
SDE(P_n) &= \sum_{uv \in E(P_n)} \left[\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} \right] \\
&= 2 \times \left[\left(\frac{n-1}{n-2} + \frac{n-2}{n-1} \right) + \left(\frac{n-2}{n-3} + \frac{n-3}{n-2} \right) + \cdots \right. \\
&\quad \left. + \left(\frac{n - \frac{n+1}{2}}{n - \frac{n-1}{2}} + \frac{n - \frac{n-1}{2}}{n - \frac{n+1}{2}} \right) \right].
\end{aligned}
$$

Example 2.3 It is well-known that for a tree T, the center $C(T)$ is isomorphic to K_1 or K_2. The star graph S_n is an example for which $C(S_n) \cong K_1$ and for the bistar tree $S_{m,n}$, we have $C(S_{m,n}) \cong K_2$. This leads us to conclude

$$
\begin{aligned}
SDE(S_{m,n}) &= \sum_{uv \in E(S_{m,n})} \left[\frac{\varepsilon(u)}{\varepsilon(v)} + \frac{\varepsilon(v)}{\varepsilon(u)} \right] \\
&= (\frac{2}{2} + \frac{2}{2}) + m \times (\frac{2}{3} + \frac{3}{2}) + n \times (\frac{2}{3} + \frac{3}{2}) \\
&= \frac{13}{6}(m+n) + 2.
\end{aligned}
$$

3 Results

This section begins with the establishment of bounds for the *SDE* index in a graph, providing valuable information about its potential range. The aim of this section is to obtain bounds for SDE index. Besides, we characterize graphs with no or with two **ec**-edges.

Theorem 3.1 *Consider two graphs G_1 and G_2 of respectively orders n_1 and n_2 with sizes m_1 and m_2. Then*

1. *If both G_1 and G_2 are self-centered, then*

$$SDE(G_1 \times G_2) = 2n_1m_2 + 2n_2m_1.$$

2. *If one of the graphs G_1 or G_2 is not self-centered, then*

$$SDE(G_1 \times G_2) < \frac{13}{6}n_1m_2 + 2n_2m_1.$$

Equality holds if and only if $G_1 \cong S_{n_1}$ and $G_2 \cong K_{n_2}$.

Proof By definition of the Cartesian product of two graphs, we have:

$$|E(G_1 \times G_2)| = |E(G_1)|.|V(G_2)| + |E(G_2)|.|V(G_1)|,$$

and

$$\varepsilon_{G_1\times G_2}(u_i, v_j) = \varepsilon_{G_1}(u_i) + \varepsilon_{G_2}(v_j).$$

1. If both G_1 and G_2 are self-centered, then $G_1 \times G_2$ is self-centered and we are done.

2. Suppose $X = G_1 \times G_2$. Without loss of generality, suppose that G_2 is not self-centered, then

$$\begin{aligned}
SDE(X) &= \sum_{[(u_i,v_j),(u_k,v_l)]\in E(X)(u_i,v_j)\neq(u_k,v_l)} \left[\frac{\varepsilon_X(u_i, v_j)}{\varepsilon_X(u_k, v_l)} + \frac{\varepsilon_X(u_k, v_l)}{\varepsilon_X(u_i, v_j)}\right] \\
&= \sum_{[(u_i,v_j),(u_i,v_l)]\in E(X)v_jv_l\in E(G_2)} \left[\frac{\varepsilon_X(u_i, v_j)}{\varepsilon_X(u_i, v_l)} + \frac{\varepsilon_X(u_i, v_l)}{\varepsilon_X(u_i, v_j)}\right] \\
&\quad + \sum_{[(u_i,v_j),(u_k,v_j)]\in E(X)u_iu_k\in E(G_1)} \left[\frac{\varepsilon_X(u_i, v_j)}{\varepsilon_X(u_k, v_j)} + \frac{\varepsilon_X(u_k, v_j)}{\varepsilon_X(u_i, v_j)}\right].
\end{aligned}$$

So

$$SDE(X) = \sum_{u_i\in V(G_1)} \sum_{v_jv_l\in E(G_2)} \left[\frac{\varepsilon_{G_1}(u_i)+\varepsilon_{G_2}(v_j)}{\varepsilon_{G_1}(u_i)+\varepsilon_{G_2}(v_l)} + \frac{\varepsilon_{G_1}(u_i)+\varepsilon_{G_2}(v_l)}{\varepsilon_{G_1}(u_i)+\varepsilon_{G_2}(v_j)}\right] \tag{1}$$

$$+ \sum_{v_j\in V(G_2)} \sum_{u_iu_k\in E(G_1)} \left[\frac{\varepsilon_{G_1}(u_i)+\varepsilon_{G_2}(v_j)}{\varepsilon_{G_1}(u_k)+\varepsilon_{G_2}(v_j)} + \frac{\varepsilon_{G_1}(u_k)+\varepsilon_{G_2}(v_j)}{\varepsilon_{G_1}(u_i)+\varepsilon_{G_2}(v_j)}\right]. \tag{2}$$

In the second term, the edges between graphs G_2 are considered and it is clear that in these edges, the eccentricities of two ends of an edge have the same value. Therefore the second term is equal to $2n_2m_1$. Furthermore, consider that the function f by $f(x) = \frac{a+x}{a+(x+1)} + \frac{a+(x+1)}{a+x}$ is decreasing. This implies that the maximum value of this function occurs when the eccentricities of all vertices in G_1 are one, and in G_2, the eccentricities are 1 and 2, for each edge. Consequently, we have

$$\begin{aligned}
SDE(G_1 \times G_2) &\leq n_1 \sum_{v_jv_l\in E(G_2)} \left[\frac{1+1}{1+2} + \frac{1+2}{1+1}\right] + 2n_2m_1 \\
&= \frac{13}{6} n_1m_2 + 2n_2m_1.
\end{aligned}$$

□

Theorem 3.2 *Consider two graphs G_1 and G_2 of orders n_1 and n_2, respectively. Then*

$$SDE(G_1 \circ G_2) \leq SDE(G_1) + n_1SDE(G_2) + n_1n_2\left(\frac{13}{6}\right).$$

Equality holds if and only if $G_1 \cong K_{n_1}$.

Proof The edges of the corona graph $G_1 \circ G_2$ can be partitioned into three distinct subsets as follows:

$$E_1 = \{e \in E(G_1 \circ G_2), e \in E(G_1)\},$$
$$E_2 = \left\{e \in E(G_1 \circ G_2), e \in E(G_{2_i}), i = 1, 2, \ldots, V(G_1)\right\},$$
$$E_3 = \left\{e \in E(G_1 \circ G_2), e = uv, u \in V(G_{2_i}), i = 1, 2, ..., V(G_1), v \in V(G_1)\right\},$$

and

$$\varepsilon_{G_1 \circ G_2}(u) = \begin{cases} \varepsilon(u) + 1 & \text{if } u \in V(G_1) \\ \varepsilon(u) + 2 & \text{if } u \in V(G_2) \end{cases}.$$

Then

$$\begin{aligned} SDE(G_1 \circ G_2) =& \sum_{uv \in E_1} \left[\frac{\varepsilon_{G_1 \circ G_2}(u)}{\varepsilon_{G_1 \circ G_2}(v)} + \frac{\varepsilon_{G_1 \circ G_2}(v)}{\varepsilon_{G_1 \circ G_2}(u)}\right] \\ &+ \sum_{u'v' \in E_2} \left[\frac{\varepsilon_{G_1 \circ G_2}(u')}{\varepsilon_{G_1 \circ G_2}(v')} + \frac{\varepsilon_{G_1 \circ G_2}(v')}{\varepsilon_{G_1 \circ G_2}(u')}\right] \\ &+ \sum_{u''v'' \in E_3} \left[\frac{\varepsilon_{G_1 \circ G_2}(u'')}{\varepsilon_{G_1 \circ G_2}(v'')} + \frac{\varepsilon_{G_1 \circ G_2}(v'')}{\varepsilon_{G_1 \circ G_2}(u'')}\right] \\ =& \sum_{uv \in E_1} \left[\frac{\varepsilon_{G_1}(u)+1}{\varepsilon_{G_1}(v)+1} + \frac{\varepsilon_{G_1}(v)+1}{\varepsilon_{G_1}(u)+1}\right] \\ &+ \sum_{u'v' \in E_2} \left[\frac{\varepsilon_{G_2}(u')+2}{\varepsilon_{G_2}(v')+2} + \frac{\varepsilon_{G_2}(v')+2}{\varepsilon_{G_2}(u')+2}\right] \\ &+ \sum_{u''v'' \in E_3} \left[\frac{\varepsilon_{G_1 \circ G_2}(u'')}{\varepsilon_{G_1 \circ G_2}(v'')} + \frac{\varepsilon_{G_1 \circ G_2}(v'')}{\varepsilon_{G_1 \circ G_2}(u'')}\right] \\ \leq& \sum_{uv \in E_1} \left[\frac{\varepsilon_{G_1}(u)}{\varepsilon_{G_1}(v)} + \frac{\varepsilon_{G_1}(v)}{\varepsilon_{G_1}(u)}\right] \\ &+ n_1 \sum_{u'v' \in E_2} \left[\frac{\varepsilon_{G_2}(u')}{\varepsilon_{G_2}(v')} + \frac{\varepsilon_{G_2}(v')}{\varepsilon_{G_2}(u')}\right] \\ &+ \sum_{u''v'' \in E_3, u'' \in V_1, v'' \in V_2} \left[\frac{2}{3} + \frac{3}{2}\right] \\ \leq& SDE(G_1) + n_1 SDE(G_2) + n_1 n_2 (\tfrac{13}{6}). \end{aligned}$$

If $G_1 \cong K_{n_1}$, then clearly the equality holds. Conversely, if equality holds then all vertices of G_1 are adjacent and for each vertex $u \in V(G_1)$ and $v \in V(G_2)$, we have $\varepsilon_{G_1}(u) = 2$ and $\varepsilon_{G_2}(v) = 3$ and this completes the proof. □

Proposition 3.1 *Let G be a graph of order n, size m and t well-connected vertices. Then*

$$SDE(G) = \frac{1}{2} t(n - t) + 2m.$$

Proof Since the diameter of the graph is two, the eccentricity of each vertex is either one or two. Assume that the graph has t well-connected vertices. In this case, the following formula can be inferred:

$$
\begin{aligned}
SDE(G) &= t(n-t)\left(\frac{1}{2}+\frac{2}{1}\right)+\frac{t(t-1)}{2}\left(\frac{1}{1}+\frac{1}{1}\right)\\
&\quad+\left(m-t(n-t)-\frac{t(t-1)}{2}\right)\left(\frac{2}{2}+\frac{2}{2}\right)\\
&=\frac{1}{2}t(n-t)+2m.
\end{aligned}
$$

□

Theorem 3.3 *A graph G has diameter two, and all of its edges are* ***nec*** *if and only if* $G \cong S_n$.

Proof If $G \cong S_n$, it is evident that the conditions of the problem are satisfied. Let G be a graph with diameter two and all edges are **nec**. Therefore, there exist vertices like w_i and w_j such that there is a path of length two, such as w_i, w_k, w_j between them. Therefore, $\varepsilon(w_i)$, $\varepsilon(w_k)$ and $\varepsilon(w_j)$ are 2, 1, and 2, respectively and the degree of vertex w_k is $n-1$. Suppose the vertex w_i is adjacent to another vertex say w_t. If the eccentricity of w_t is one, the edge $w_t w_k$ has an eccentricity of one at both ends which contradicts the assumption of the problem. If $\varepsilon(w_t) = 2$, then the eccentricity of both ends of $w_i w_t$ is two, a contradiction. We can conclude that a vertex like w_t cannot exist, and except for w_k, the degree of other vertices is one and so $G \cong S_n$. □

Note 1. It is not difficult to prove that every tree of order greater than 3, has at least three **nec**-edges.

Note 2. If a graph G has at least three distinct eccentricities, then G has at least three **nec**-edges.

Theorem 3.4 *If G is* ***nec****-graph, then the diameter of the graph is even.*

Proof Let the diameter of graph G be d. Therefore, there exists a path, $v_1, v_2, v_3, \ldots, v_{d+1}$, where all $\varepsilon(v_1), \varepsilon(v_2), \ldots, \varepsilon(v_{d+1})$ are distinct.

Knowing that two ends of an edge have either equal eccentricities or their difference is 1, we conclude $\varepsilon(v_1) = \varepsilon(v_{d+1}) = d$ and $\varepsilon(v_2) = \varepsilon(v_d) = d-1$. By using proof by contradiction, assume that the diameter of the graph is odd. In this case, we will show that along the path $v_1, v_2, v_3, \ldots, v_{d+1}$, there exists an edge e in the center, and the eccentricities of endpoints of e are the same.

As shown in Table 1, the possible values for the eccentricities of two ends of a median edge($v_{d+1/2}$, $v_{d-(d-3)/2}$), are as follows: when $(d+1)/2$ is odd, they are d, $d-2, d-4 \ldots d-((d-3)/2+1)$ and when $(d+1)/2$ is even, the possible values are $d-1, d-3, d-5, \ldots, d-((d+1)/2-1)$. In both cases, the minimum difference is 2 and cannot represent the eccentricities of two ends of an edge. □

Corollary 3.1 *If a graph has diameter* $d = 2k+1$*, then there exists at least one* ***ec*** *edge.*

Corollary 3.2 *There is no graph with diameter three, in which all edges are* ***nec****.*

Theorem 3.5 *There is no graph with exactly one* ***nec****-edge.*

Table 1 The contribution of different eccentricities of vertices

v_1, v_{d+1}	v_2, v_d	v_3, v_{d-1}	v_4, v_{d-2}	v_5, v_{d-3}	…	$v_{d+1/2}, v_{d-(d-3)/2}$ $(d+1)/2$ is odd	$(d+1)/2$ is even
d	$d-1$	d	$d-1$	d	…	d	$d-1$
		$d-2$	$d-3$	$d-2$		$d-2$	$d-3$
				$d-4$		$d-4$	$d-5$
						.	.
						.	.
						.	.
						$d-((d-3)/2+1)$	$d-((d+1)/2-1)$

Proof Suppose $e = uv$ is the only **nec**-edge. Assume P is the longest path containing e, where $P = w_1 w_2 \dots w_i u v w_{i+3} \dots w_{d+1}$. Since, according to the assumption, all edges are **ec**-edge except e, we obtain

$$\varepsilon(w_1) = \varepsilon(w_2) = \dots = \varepsilon(w_i) = \varepsilon(u) = d,$$

and neccesarily $\varepsilon(v) = d - 1$. This means that

$$d - 1 = \varepsilon(v) = \varepsilon(w_{i+3}) = \dots = \varepsilon(w_{d+1}),$$

a contradiction with $d(w_1, w_{d+1}) = d$. □

Theorem 3.6 *If the graph G has exactly two* **nec** *edges, then both of them are pendants.*

Proof Suppose G has two **nec** edges say $e = uv$ and $e' = u'v'$ and the other edges are **ec**. We demonstrate that the edges e and e' are located on the longest path in the graph. Let $\varepsilon(u) = \alpha$, $\varepsilon(v) = \alpha - 1$, $\varepsilon(u') = \beta$ and $\varepsilon(v') = \beta - 1$. Since the graph is connected, there exists a path P between e and e'. All edges on P are **ec**, so we conclude that $\alpha = \beta$ and the eccentricity is either α or $\alpha - 1$, for all vertices and the diameter of G is equal to α. On the other hand, except for e and e', all edges are **ec**, then the eccentricity of endpoints of an edge is either α or $\alpha - 1$. However, if there are some edges where the eccentricity of their endpoints is α while in remaining edges it is $\alpha - 1$, the graph structure will resemble Fig. 1, where the edges e and e' are cut edges which contradicts the fact α is diameter. Therefore, the eccentricity of endpoints of all edges in the graph is either α or $\alpha - 1$, but not both. If they are α, then vertices u' and v' are not adjacent to any other vertex and their degree is 1. If the eccentricity of endpoints of all edges is $\alpha - 1$, then vertices u and v are not adjacent to any other vertex and their degree is 1. □

Theorem 3.7 *Let G be a graph ($G \ncong S_n$) with size $m \geq 4$ and diameter $d \geq 2$. Then*

$$2(m-2) + 2(\frac{d}{d-1} + \frac{d-1}{d}) \leq SDE(G) \leq \frac{5}{2}m - \frac{1}{2}.$$

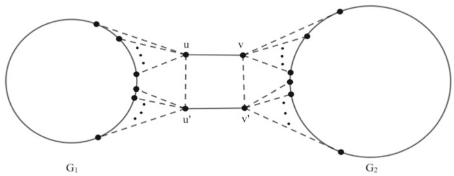


Fig. 1 The structure of the graph in Theorem 3.6

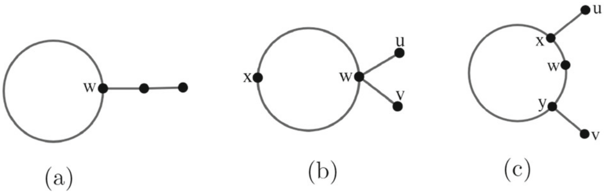


Fig. 2 Graph G in Theorem 3.7

The equality holds for lower bound for $G+2e$, where G is a Θ-graph and upper bound holds for two graphs S_m+e and $(K_{\frac{m-1}{2}})^c+K_2$.

Proof For the lower bound, if G is not self-centered, then by Theorem 3.5, it has at least two pendant edges. If any rooted tree T_v attached to a vertex of C_n is of order greater than 3, then by Note 1 we have a contradiction. If $|T_v|=3$, then G is isomorphic with one of the graphs depicted in Fig. 2. □ □

In Fig. 2a, G has more than two **nec**-edges, a contradiction. Suppose two pendant edges uw and vw are attached to C_n at vertex w. Without loss of generality, we can suppose the eccentricity of u or v holds with vertex x. Thus two vertices adjacent with x have the same eccentricity equal $\epsilon(w)$ which yields at least three **nec**-edges, a contradiction.

Finally, suppose two pendant edges are attached to C_n at different vertices such as x and y, see Fig. 2c.

Let w lies in a shortest xy-path, where $d(w,x)\le[\frac{n}{4}]$. It is clear that $\epsilon(w)=\frac{n}{2}$ while $d(w,u)=[\frac{n}{4}]+1$ or $d(w,v)=[\frac{n}{4}]+1$. Hence, three vertices u,x,w have distinct eccentricities, a contradiction. Thus the lower bond equality holds holds for the graph $G+2e$, where G is Θ-graph.

For the upper bound, obviously, the difference between eccentricities of vertices located on an edge is zero or one. Suppose r denotes the radius of graph G and G has exactly k equi-centric edges, then

$$SDE(G)=\sum_{uv\in E(G)}\left[\frac{\varepsilon(u)}{\varepsilon(v)}+\frac{\varepsilon(v)}{\varepsilon(u)}\right]$$
$$\le 2+2+\cdots+2+(m-k)\left[\frac{r}{r+1}+\frac{r+1}{r}\right]. \tag{3}$$

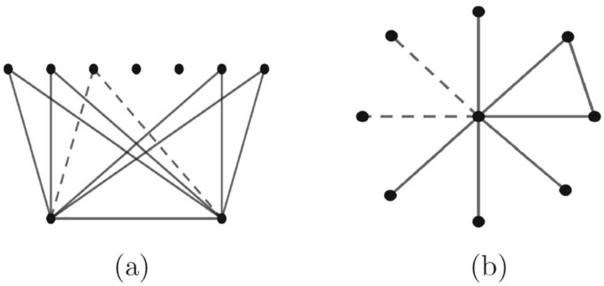


Fig. 3 All structures of graphs given in Theorem 3.7

Since the function f by $f(x) = \frac{x}{x+1} + \frac{x+1}{x}$ is decreasing, the maximum value of SDE occurs for $r = 1$ and therefore

$$SDE(G) \leq \frac{5}{2}m - \frac{k}{2}.$$

It is clear that the maximum value of (1) occurs when $k = 1$. In the following, we show that the equality holds for the upper bound in graphs isomorphic with one of the structures shown in Fig. 3. The graph G has exactly one **ec**-edge say uv. The values of $\varepsilon(v)$ and $\varepsilon(u)$ can be either one or two.

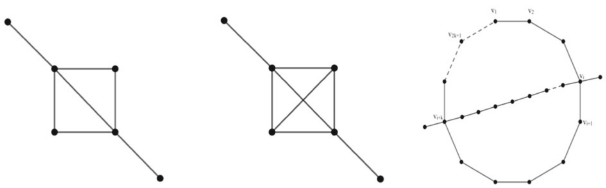
1) Assume that $\varepsilon(v) = \varepsilon(u)$= 1 and consider an arbitrary vertex w. Suppose on the contrary that w is adjacent to a vertex z, then either the eccentricity of both ends of wz is two, a contradiction, or one of them is two and the other is one. Without loss of generality, suppose the eccentricity of vertex z is one. In this case, both ends of uz have the same eccentricity, a contradiction. This yields a graph with structure (a) as shown in Fig. 3.

2) Assume that $\varepsilon(v) = \varepsilon(u)$= 2. There are two paths, namely $P_1 = u, s, w$ and $P_2 = v, t, z$. Since the eccentricity of u and v is two, the eccentricity of s and t must be one. Clearly, s and t are adjacent implying that the edge st is **ec**, a contradiction. Therefore, we conclude s and t can not be distinguished, and the desired paths are $P_1 = u, s, w$ and $P_2 = v, s, z$. Similarly, it is not difficult to see that two vertices w and z are not adjacent, and the graph has a structure as depicted in Fig. 3.7b.

Example 3.1 It should be noted that there many classes of graphs satisfying the lower bound condition of Theorem 3.7, but among them, a Θ-graph has the minimum number of edges. For example, two graphs Fig. 4 have exactly two **nec**-edges but graph Fig. 4a has 7 edges while Fig. 4b has 8 edges. To construct a class of graphs satisfying in the conditions of Theorem 3.7, we consider a cycle graph of length $2k + 1$. Then, we add a path of length $k - 1$ between two vertices in the cycle, namely v_i and v_{i+k}. Finally, we add two pendant edges to vertices u and v. The structure of these graphs can be observed in Fig. 4c.

Theorem 3.8 *Let G be a connected graph with size $m \geq 4$ and diameter $d = 3$. Then*

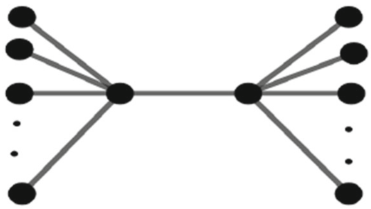
$$SDE(G) \geq \frac{13}{6}m - \frac{1}{6}.$$



(a) (b) (c)

Fig. 4 The structure of graphs in Example 3.1

Fig. 5 Bistar graph $S_{a,b}$: A graph structure showing equality in Theorem 3.8



The equality holds for the bistar graph $S_{a,b}$.

Proof Suppose the number of **ec**-edges is k, then according to Theorem 3.7, we have

$$SDE(G) \geq 2k + (m-k)\left[\tfrac{d}{d-1} + \tfrac{d-1}{d}\right].$$

Considering $d = 3$, the inequality can be rewritten as

$$SDE(G) \geq 2k + (m-k)\left[\frac{3}{2} + \frac{2}{3}\right] = 2k + \frac{13}{6}(m-k) = \frac{13}{6}m - \frac{1}{6}k. \qquad (4)$$

So, the minimum value of $SDE(G)$ with diameter three is $\frac{13}{6}m - \frac{1}{6}$. In the following, we show all structures with equality in Eq. 4 are isomorphic with the bistar graph $S_{a,b}$. Since the diameter of G is three, there exists a path of length three say $P = w_1w_2w_3w_4$. Since $\varepsilon(w_1) = \varepsilon(w_4)= 3$, $\varepsilon(w_2)$ and $\varepsilon(w_3)$ are 2 or 3. Since there is exactly one **ec**-edge, we conclude $\varepsilon(w_2)$ and $\varepsilon(w_3)$ are not three simultaneously. Therefore, either $\varepsilon(w_2) = \varepsilon(w_3) = 2$ or $\varepsilon(w_2) = 2$ and $\varepsilon(w_3) = 3$.

1) At first suppose $\varepsilon(w_2) = \varepsilon(w_3)= 2$. For each arbitrary vertex z, we have $\varepsilon(z) \neq 1$, because otherwise $d(w_1, w_4) = 2$, a contradiction. Thus we may assume that $\varepsilon(z) = 2$, then z is not adjacent to w_2 or w_3 and so it is adjacent to w_1 or w_4, but not both. Without loss of generality, assume that z is adjacent to w_1, then $d(z, w_4) > 3$, a contradiction. Hence $\varepsilon(z) = 3$ and thus z is not adjacent to w_1 or w_4. Suppose z is adjacent to both w_2 and w_3, there exists a path of the length of three from z to a vertex like s. If this path passes through w_2 or w_3, the structure (b) in Fig. 6 occurs and if $\varepsilon(t) = 2$ then the edge tw_3 is **ec**. In the case that $\varepsilon(t) = 3$, the edge ts is **ec**. If this path passes through w_1 or w_4, the structure (a) in Fig. 6 occurs and edge w_4s is **ec**. Finally, if P does not contain vertices w_1, w_2, w_3 and w_4, then the structure (c) occurs in Fig. 6 and one of

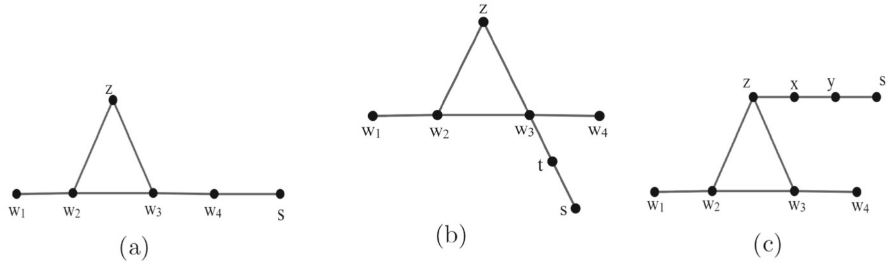


Fig. 6 Different positions of vertex s with respect to z

the edges ys or xy are **ec**. In all cases, the number of **ec**-edges is greater than one, a contradiction. □

Hence, z is adjacent to one of the vertices w_2 or w_3. This implies that all vertices except w_i's (i=1,2,3,4) have an eccentricity equal to three. If there are edges between these vertices, then the number of ec-edges is greater than two, a contradiction. Consequently, all of them are pendant edges and we are done.

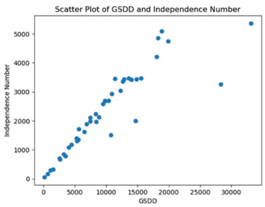
4 Analyzing protein networks

Proteins play a crucial role in various biological processes and are often represented as networks to understand their structural and functional properties, see [2, 10, 11, 15]. In this section, we extend our investigation of *SDE* index by analyzing real protein networks.

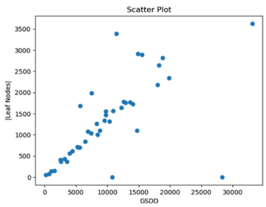
Essential proteins play critical roles in cell processes such as development and survival. Table 2 reports the correlation coefficients between the *SDE* index and several

Table 2 Correlation analysis of *SDE* index with the topological indices

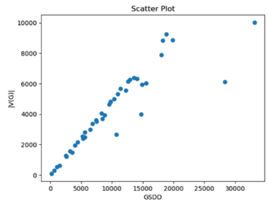
	SDE	α	$\|LF\|$	$\|V\|$	$\|E\|$	R	H	ABC	SC	M_1	M_2	$\|A\|$
SDE	1	0.89	0.66	0.90	1	0.89	0.88	0.99	0.97	0.91	0.80	0.52
α	0.89	1	0.86	0.99	0.89	0.99	0.99	0.94	0.97	0.62	0.45	0.35
$\|LF\|$	0.66	0.86	1	0.83	0.66	0.81	0.78	0.74	0.75	0.42	0.26	0.38
$\|V(G)\|$	0.90	0.99	0.83	1	0.90	0.99	0.99	0.95	0.98	0.64	0.47	0.36
$\|E(G)\|$	1	0.89	0.66	0.90	1	0.89	0.88	0.99	0.97	0.91	0.80	0.52
$R(G)$	0.89	0.99	0.81	0.99	0.89	1	0.99	0.94	0.98	0.62	0.44	0.03
$H(G)$	0.88	0.99	0.78	0.99	0.88	0.99	1	0.93	0.97	0.60	0.42	0.30
ABC	0.99	0.94	0.74	0.95	0.99	0.94	0.93	1	0.99	0.84	0.71	0.48
SC	0.97	0.97	0.75	0.98	0.97	098	0.97	0.99	1	0.76	0.61	0.41
M_1	0.91	0.62	0.42	0.64	0.91	0.62	0.60	0.84	0.76	1	0.98	0.64
M_2	0.80	0.45	0.26	0.47	0.80	0.44	0.42	0.71	0.61	0.98	1	0.67
$\|A\|$	0.52	0.35	0.38	0.36	0.52	0.03	0.30	0.48	0.41	0.64	0.67	1



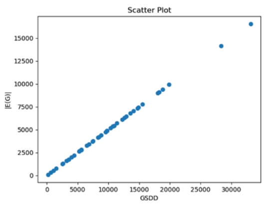
(a) Scatter map showing the relationship between *SDE* and α.



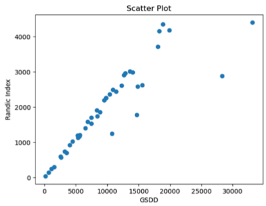
(b) Scatter map showing the relationship between *SDE* and $|LF|$.



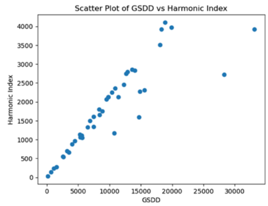
(c) Scatter map showing the relationship between *SDE* and $|V|$.



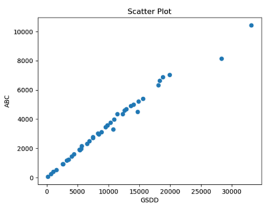
(d) Scatter map showing the relationship between *SDE* and $|E|$.



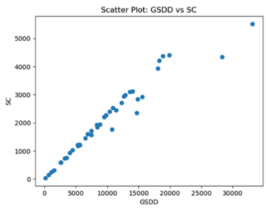
(e) Scatter map showing the relationship between *SDE* and R.



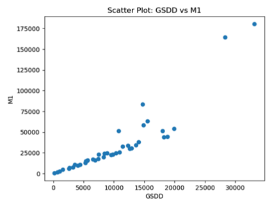
(f) Scatter map showing the relationship between *SDE* and H.



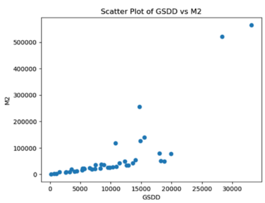
(g) Scatter map showing the relationship between *SDE* and ABC.



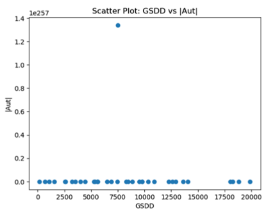
(h) Scatter map showing the relationship between *SDE* and SC.



(i) Scatter map showing the relationship between *SDE* and M_1.



(j) Scatter map showing the relationship between *SDE* and M_2.



(k) Scatter map showing the relationship between *SDE* and $|A|$.

Fig. 7 Scatter maps showing the relationship between *SDE* and different graph properties graph invariants including the indepence number $\alpha = \alpha(G)$, $|LF|$, $|V|$, $|E|$, R, H, ABC, SC, M_1, M_2, and $|A| = |Aut(G)|$. Each correlation coefficient represents the strength and direction of the relationship between the *SDE* index and the corresponding network property. We observed a strong linear correlation between SDE and M_2 and R. In other words, upon analyzing the results, we infer that *SDE* index exhibits a strong positive correlation with $|E|$, ABC, SC, M_1, $|V|$, α, R, H, and M_2, respectively. The implications of these correlation analysis results are significant for understanding protein network properties.

These findings can guide further research in protein network analysis and contribute to the development of more accurate computational models for predicting protein functions and identifying potential therapeutic targets. It evaluates whether the coefficients of all predictors collectively exhibit a significant deviation from zero. Overall, the correlation analysis between the *SDE* index and topological indices provides valuable insights into the intricate nature of protein networks. By unravelling the relationships between network properties, we can deepen our understanding of protein network organization and its implications in biological networks.

In Table 3 the coefficient for M_2 is estimated as 0.05284 with a standard error of 0.0009274. It is highly statistically significant (p-value $< 2e - 16$), implying that M_2 has a strong positive impact on *SDE*. For a one-unit increase in M_2, *SDE* is expected to increase by approximately 0.05284 units, while keeping all other variables constant. The coefficient for R is estimated as 3.743 with a standard error of 0.01499. It is highly statistically significant (p-value $<2e - 16$), indicating that R has a strong positive impact on *SDE*. For a one-unit increase in R, *SDE* is expected to increase by approximately 3.743 units, while keeping all other variables constant. The coefficient for $|A|$ is estimated as $-7.136e - 256$ (which is essentially zero) with a standard error of 0. The coefficient being effectively zero suggests that $|A|$ may not be contributing significantly to the model, and its inclusion in the regression equation may not be appropriate. Therefore, we remove $|A|$ and perform the regression again.

In Table 4 the estimated coefficient for M_2 is $2.983e - 02$. It indicates that a one unit increase in M_2 is associated with an estimated increase of 0.02983 units in the predicted value of *SDE*. The estimated coefficient for R is 4.010e+00. This suggests

Table 3 Results of the linear regression model for the variables *SDE*, $|A|$, M_2, and R

	Estimate	Std. error	T value	Pr(> $|t|$)
(Intercept)	–1.201e+01	1.411e+01	−0.852	0.401
M_2	5.284e−02	9.274e−04	56.979	<2e-16 ***
$\|A\|$	−7.136e−256	0.000e+00	$-\infty$	<2e-16 ***
R	3.743e+00	1.499e−02	249.707	<2e-16 ***
Residual standard error	44.5 on 31 degrees of freedom			
Multiple R-squared	0.9999			
Adjusted R-squared	0.9999			
F-statistic	1.65e+05 on 3 and 31 DF			
p value	$< 2.2e{-16}$			

Table 4 Results of the linear regression model for the variables *SDE*, M_2, and *R*

	Estimate	Std. Error	T value	Pr(> |t|)
(Intercept)	2.014e+02	1.549e+02	1.30	0.201
M_2	2.983e−02	7.537e−04	39.58	<2e–16 ***
$R(G)$	4.010e+00	7.547e−02	53.14	<2e–16 ***
Residual standard error	510.9 on 39 degrees of freedom			
Multiple R-squared	0.995			
Adjusted R-squared	0.9947			
F-statistic	3872 on 2 and 39 DF			
p value	< 2.2e−16			

that a one-unit increasing in R is associated with an estimated increase of 4.01 units in the predicted value of *SDE*. The R-squared is 0.995, meaning that approximately 99.5 percent of the variability in *SDE* can be explained by the independent variables (M_2 and R) included in the model. The adjusted R-squared (Adjusted R-squared) is 0.9947, which is slightly lower than the R-squared value but still indicates a highly effective model in explaining the relationship between *SDE* and the predictors. The F-statistic tests the overall significance of the regression model. It assesses whether the coefficients of all predictors are jointly different from zero. In this case, the F-statistic is 3872 with degrees of freedom (DF) of 2 and 39. The associated p-value is $< 2.2e-16$, which is extremely low. This suggests that the overall regression model is highly significant, indicating that at least one of the predictors (M_2 or R) is significantly related to *SDE*. In summary, the regression analysis indicates that both M_2 and R are highly significant predictors of *SDE*. The model explains a large proportion of the variability in *SDE*, as evident from the high R-squared value. The overall regression model is also highly significant, suggesting that it provides valuable information for predicting and understanding the relationship between *SDE* and the predictors. The regression equation for the variables *SDE*, M_2, and R, as shown in Table 4, can be written as:

$$SDE = 201.4 + 0.02983M_2 + 4.01R.$$

5 Conclusion

In this article, we introduced the *SDE* index as a new version of the *SDD*-index in graphs, which utilizes eccentricity instead of vertex degrees for graph analysis. Through our investigation, we determined the limits of the *SDE* index and explored its relationship with other graph properties. We have found significant correlations between *SDE* and various graph properties. Furthermore, the strong positive associations between *SDE* and indices like R and H suggest the central and diverse roles played by proteins with higher *SDE* values in the network. Additionally, the nearly perfect correlation between *SDE* and the ABC index emphasizes the crucial involve-

Table 5 Exploring the topological indices of a collection of 42 proteins

No			α	$\|LF\|$	$\|V\|$	$\|E\|$	R	H	ABC	SC	M_1	M_2	$\|A\|$	SDE
1	7KR0		1999	1104	3995	7365	1772.39	1591.53	4505.01	2356.72	83596.0	256556.0	1.63E+422	14730.05
2	7TX0		5368	3625	10018	16561	4400.78	3917.29	10429.85	5519.27	180512.0	565251.0	1.52E+828	33126.63
3	7KQO		3468	2886	6037	7776	2625.47	2308.60	5402.52	2932.08	63208.0	139784.0	3.80E+510	15552.05
4	7KQP		3444	2912	5947	7428	2587.63	2274.61	5214.36	2846.91	58486.0	126527.0	6.22E+500	14856.31
5	7NTK		3457	3385	5661	5706	2442.83	2125.69	4356.26	2445.14	32502.0	42572.0	1.58E+453	11417.47
6	7QCR		1504	0	2668	5376	1246.60	1169.63	3306.74	1765.68	51200.0	117488.0	6.83E+487	10754.92
7	7TUQ		1083	564	1960	2012	924.75	875.9	1466.02	935.59	9488.0	10728.0	8.92E+43	4024.295
8	6Z4U		700	405	1263	1282	592.86	558.8	937.35	596.34	6052.0	6839.0	1.98E+28	2564.316
9	6HN3		779	366	1480	1771	700.72	666.16	1225.83	757.42	10768.0	18391.0	3.95E+49	3544.679
10	2CME		2672	1551	4817	4893	2259.48	2128.13	3580.47	2273.81	23130.0	26132.0	3.72E+122	9786.885
11	5TY3		2114	1988	3524	3741	1529.33	1339.13	2795.05	1566.35	23014.0	35380.0	1.34E+257	7486.228
12	5HK1		2939	1561	5310	5446	2497.61	2359.2	3982.13	2526.98	25750.0	28995.0	3.4E+152	10922.49
13	6YG9		2583	1341	4641	4761	2188.49	2071.92	3468.12	2212.60	22590.0	26030.0	5.63E+109	9523.129
14	2ACF		3044	1644	5552	6132	2608.51	2460.67	4359.39	2718.61	33780.0	50024.0	2.31E+179	12272.04
15	7DJR		1352	696	2489	2792	1172.13	1108.22	1978.93	1231.55	15464.0	22869.0	6.04E+88	5590.006
16	2C35		5104	2814	9236	9414	4345.62	4104.93	6874.61	4380.68	44352.0	49980.0	2.1E+208	18828.09
17	4XBM		2690	1319	4996	5176	2365.41	2248.1	3762.89	2404.68	24422.0	27684.0	4.3745E+99	10352.55
18	2IHC		1882	1076	3382	3440	1587.48	1496.0	2515.36	1598.46	16260.0	18350.0	9.04626E+74	6880.22
19	5FS8		2127	1095	3938	4424	1855.46	1755.55	3131.05	1950.79	24526.0	36269.0	9.6834E+119	8848.218
20	3DK9		4207	2179	7880	9010	3713.47	3514.22	6335.31	3934.20	51328.0	78789.0	1.595E+245	18033.06
21	4A7U		1305	697	2394	2671	1123.78	1059.57	1895.66	1176.91	14934.0	22469.0	2.57606E+75	5352.417

Table 6 Exploring the topological indices of a collection of 42 proteins

No			α	$\|LF\|$	$\|V\|$	$\|E\|$	R	H	ABC	SC	M_1	M_2	$\|A\|$	SDE
22	1RYO		1393	706	2534	2632	1196.65	1134.43	1910.80	1216.89	12646.0	14834.0	1.5325E+54	5264.035
23	1PL4		3437	1753	6257	6453	2953.89	2799.47	4699.84	2995.73	30518.0	34591.0	2.1661E+127	12906.21
24	1T7H		162	72	307	337	145.99	139.32	240.65	152.33	1712.0	2176.0	16777216	674.4466
25	1R3S		3266	0	6104	14156	2879.13	2726.77	8151.11	4341.58	164400.0	521920.0	4.87E+1134	28313.04
26	2F8A		1628	841	2982	3253	1404.08	1327.67	2329.82	1458.46	17140.0	23409.0	1.79E+88	6507.354
27	1N45		1987	1034	3600	3719	1696.88	1605.90	2708.87	1722.00	17724.0	20318.0	1.19E+88	7440.017
28	7F60		3352	1775	6151	6309	2904.08	2752.33	4591.41	2936.16	29734.0	33672.0	5.3E+123	12618.67
29	6W37		285	142	522	539	246.72	234.1	392.53	250.42	2542.0	2873.0	4.4E+12	1078.095
30	7JX6		842	436	1557	1607	735.42	697.3	1169.56	746.08	7600.0	8627.0	8.30767E+34	3214.054
31	7LUZ		57	57	91	90	38.87	33.48	69.55	38.57	510.0	651.0	1.91E+08	180.3158
32	1JR2		2238	1262	4059	4154	1905.81	1796.95	3033.52	1924.58	19806.0	22675.0	2.32031E+91	8308.329
33	3HCN		3424	1726	6334	7032	2987.18	2828.59	5000.35	3125.55	38046.0	54243.0	4.8E+191	14071.51
34	4EEW		671	363	1225	1314	576.01	543.89	944.42	593.45	6790.0	8964.0	5.19E+33	2628.048
35	5F0P		4863	2644	8828	9115	4155.49	3927.32	6626.73	4211.95	43934.0	51660.0	8.6549E+243	18251.02
36	7NTJ		1719	1686	2809	2820	1211.84	1054.22	2156.85	1211.01	15944.0	20588.0	1.635E+223	5640.936
37	6A73		2701	1470	4814	4893	2262.00	2134.4	3579.70	2277.46	23038.0	25846.0	1.2E+118	9790.655
38	3FGH		323	147	620	774	292.97	278.08	529.35	322.69	4996.0	8970.0	5.66684E+22	1548.034
39	2OBV		1969	998	3696	4223	1743.18	1651.04	2969.79	1845.57	24188.0	38009.0	3.05555E+90	8446.789
40	1T5Z		1185	610	2162	2218	1021.56	968.94	1614.07	1033.05	10432.0	11783.0	2.28E+46	4436.632
41	6SJA		3474	1766	6386	6801	3017.00	2860.58	4894.46	3100.51	34100.0	43015.0	3.4888E+137	13603.82
42	2FLU		4744	2337	8858	9940	4184.36	3968.58	7040.82	4400.95	54178.0	77831.0	2.7E+211	19883.96

ment of proteins with high *SDE* values. Regression analysis confirms the significance of M_2 and R as predictors for *SDE*, with the model explaining a substantial proportion of its variability. Overall, our findings contribute to advancing graph analysis and understanding the intricate interplay between *SDE* and other graph characteristics.

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Declarations

Conflict of interest The authors declare no conflict of interest.

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