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An Eccentricity-Based Estrada Index for Finite Simple Connected Graphs

Narendra VH
Department of Mathematics, Government Science College, Chitradurga, Karnataka-577 501, India

* Corresponding Author: **Narendra VH**

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Abstract
The Estrada index is a well-known spectral invariant with numerous applications in graph theory, chemical graph theory, complex networks, and quantitative structure–property relationship (QSPR) studies. Motivated by the importance of vertex eccentricity in characterizing graph structures, this paper introduces a new eccentricity-based Estrada index defined by

$$EE_{\varepsilon}(G) = \sum_{v \in V(G)} e^{\varepsilon(v)}$$

where ε(v) denotes the eccentricity of the vertex v. The proposed index incorporates distance-related information through an exponential weighting scheme and serves as an alternative descriptor of graph structure. Fundamental properties of the index are established, and exact formulae are derived for several standard graph classes, including complete graphs, cycle graphs, wheel graphs, and path graphs. Furthermore, the behavior of the index under graph transformations is investigated through total graphs and eccentric graphs, leading to theoretical results and a conjectured relationship involving eccentric graph constructions. Numerical examples are provided to demonstrate the effectiveness of the proposed invariant in distinguishing graph structures. Potential applications of the eccentricity-based Estrada index in network analysis, graph theory, and function approximation are also discussed. The results show that the proposed index provides a useful measure for quantifying structural complexity, connectivity, and distance distribution in graphs and complex networks.

Keywords: Estrada index, eccentricity, topological index, graph invariants, eccentric graph, total graph, complex networks, function approximation, graph transformation

Mathematics Subject Classification (2020): 05C12, 05C35, 05C50, 92E10

1. Introduction

Graph theory has emerged as one of the most influential mathematical disciplines due to its extensive applications in chemistry, biology, computer science, communication networks, and social sciences [3, 8]. A graph provides an abstract representation of relationships among objects and offers a convenient framework for quantitative analysis.

The study of graph invariants known as topological indices began with the pioneering work of Wiener in 1947 [7]. The Wiener index was introduced to correlate boiling points of paraffin hydrocarbons with molecular structures. Since then, numerous degree-based and distance-based topological indices have been proposed and successfully applied in quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) [4, 5].

One of the most important spectral invariants is the Estrada index, introduced by Ernesto Estrada [1]. This index has become an

effective tool in analyzing molecular folding, protein structures, complex networks, and communication systems [2]. The Estrada index reflects the degree of compactness and the extent of connectivity present in a graph.
Motivated by the significance of eccentricity in graph analysis and the growing interest in distance-based graph invariants [5, 6], we propose a modified Estrada index based on vertex eccentricities. The proposed invariant combines structural and distance-related information and provides an alternative perspective for studying graph properties.

2. Preliminaries

Let G = (V (G), E(G)) be a finite, simple, connected graph [3, 8].
Definition 2.1 (Distance). The distance between vertices u and v, denoted by d(u, v), is the length of the shortest path joining them [3].
Definition 2.2 (Eccentricity). Let G = (V (G), E(G)) be a connected graph. The eccen-tricity of a vertex v ∈ V (G) is defined as

$$\varepsilon(v) = \max_{u\in V(G)} d(u,v),$$

where d(u, v) denotes the distance between the vertices u and v [3, 8].
Definition 2.3 (Diameter). The diameter of a graph G is defined as

$$\operatorname{diam}(G) = \max_{v\in V(G)} \varepsilon(v),$$

that is, the maximum eccentricity among all vertices of the graph [3].
Definition 2.4 (Classical Estrada Index). Let λ1, λ2,.., λn be the eigenvalues of the adjacency matrix of a graph G with n vertices. The Estrada index of G is defined by [1, 2].

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$$

Definition 2.5 (Total Graph). The total graph of a graph G, denoted by T (G), is the graph whose vertex set consists of all vertices and edges of G. Two vertices of T (G) are adjacent if and only if the corresponding elements of G are either adjacent or incident [8].
Definition 2.6 (Eccentric Graph). The eccentric graph of a graph G, denoted by Ge, is the graph having the same vertex set as G, where two vertices are adjacent if and only if one of them is an eccentric vertex of the other in G [6].

3. Proposed Eccentricity-Based Estrada Index

Inspired by the classical Estrada index [1, 2] and distance-based graph invariants [4, 5], we define the modified Estrada index as

$$EE_\varepsilon(G) = \sum_{v\in V(G)} e^{\varepsilon(v)}.$$

This index depends solely on the eccentricity distribution of the graph.

3.1. Basic Properties

The following properties follow directly from the definition of the proposed index:

1. EEε(G) > 0.
2. Isomorphic graphs possess equal values of EEε(G).
3. Graphs having smaller diameters generally possess smaller values of EEε(G).
4. The index increases with larger eccentricity distributions.

4. Exact Values for Standard Graphs

Theorem 4.1. Let Kn be the complete graph on n vertices. Then the eccentricity-based Estrada index of Kn is

EEε(Kn) = ne.

Proof. In the complete graph Kn, every pair of distinct vertices is adjacent [3, 8]. There-fore, for any vertex v ∈ V (Kn), the distance from v to every other vertex is 1. Hence,

ε(v) = 1

for all v ∈ V (Kn).
By the definition of the eccentricity-based Estrada index, which is motivated by the classical Estrada index [1, 2],

$$EE_\varepsilon(K_n) = \sum_{v\in V(K_n)} e^{\varepsilon(v)}.$$

Since ε(v) = 1 for every vertex v ∈ V (Kn), we have

$$EE_\varepsilon(K_n) = \sum_{v\in V(K_n)} e = ne.$$

Therefore,

EEε(Kn) = ne.

Hence the proof is complete.
Example 4.1. Consider the complete graph K4 with vertex set V (K4) = {v1, v2, v3, v4}.
Since every pair of distinct vertices is adjacent [3, 8], the distance between any two vertices is 1. Therefore, the eccentricity of each vertex is

ε(v1) = ε(v2) = ε(v3) = ε(v4) = 1.

By the definition of the eccentricity-based Estrada index,

$$EE_\varepsilon(K_4) = \sum_{v\in V(K_4)} e^{\varepsilon(v)}.$$

Substituting the eccentricities, we obtain

EEε(K4) = e1 + e1 + e1 + e1 = 4e.

Hence,

EEε(K4) = 4e,

which agrees with Theorem 4.1 since

EEε(Kn) = ne,

and for n = 4 we have

EEε(K4) = 4e.

This example illustrates the behavior of the eccentricity-based Estrada index for highly connected graphs, where all vertices possess the minimum possible eccentricity [2, 5].
Theorem 4.2. Let Cn be the cycle graph of order n. Then the eccentricity-based Estrada index of Cn is given by

EEε(Cn) = ne⌊n/2⌋.

Proof. Let

V (Cn) = {v1, v2,.., vn}

be the vertex set of the cycle graph Cn.
It is well known that the eccentricity of every vertex in a cycle graph is

$$\varepsilon(v) = \left\lfloor \frac{n}{2} \right\rfloor, \qquad \forall\, v \in V(C_n),$$

By the definition of the eccentricity-based Estrada index, which is inspired by the classical Estrada index [1, 2],

$$EE_\varepsilon(C_n) = \sum_{v \in V(C_n)} e^{\varepsilon(v)}.$$

Substituting

$$\varepsilon(v) = \left\lfloor \frac{n}{2} \right\rfloor$$

for every vertex v ∈ V (Cn), we obtain

$$EE_\varepsilon(C_n) = \sum_{v \in V(C_n)} e^{\left\lfloor \frac{n}{2} \right\rfloor}.$$

Since Cn has exactly n vertices, the above sum contains n identical terms. Therefore,

$$EE_\varepsilon(C_n) = ne^{\left\lfloor \frac{n}{2} \right\rfloor}.$$

Hence,

$$EE_\varepsilon(C_n) = ne^{\left\lfloor \frac{n}{2} \right\rfloor}.$$

This completes the proof.
Example 4.2. Consider the cycle graph C6 with vertex set

V (C6) = {v1, v2, v3, v4, v5, v6}.

In C6, the greatest distance from any vertex to another vertex is 3. Hence, the eccen-tricity of every vertex is [3, 8]

ε(v1) = ε(v2) = ε(v3) = ε(v4) = ε(v5) = ε(v6) = 3.

By the definition of the eccentricity-based Estrada index,

$$EE_\varepsilon(C_6) = \sum_{v \in V(C_6)} e^{\varepsilon(v)}.$$

Substituting the eccentricities, we obtain

EEε(C6) = e3 + e3 + e3 + e3 + e3 + e3 = 6e3.

Therefore,

EEε(C6) = 6e3.

This agrees with Theorem 4.2 since

EEε(Cn) = ne⌊n/2⌋,

and for n = 6,

EEε(C6) = 6e⌊6/2⌋ = 6e3.

Hence, the theorem is verified. The example illustrates how the uniform eccentricity distribution of cycle graphs leads to a simple closed-form expression for the index [5].
Theorem 4.3. Let Pn be the path graph on n vertices with vertex set

V (Pn) = {v1, v2,.., vn}.

Then the eccentricity-based Estrada index of Pn is given by

$$EE_\varepsilon(P_n) = \sum_{i=1}^{n} e^{\max(i-1, n-i)}.$$

Proof. Let

V (Pn) = {v1, v2,.., vn}

be the vertex set of the path graph Pn [3, 8].
For each vertex vi, the distance to the left end vertex v1 is

d(vi, v1) = i − 1,

and the distance to the right end vertex vn is

d(vi, vn) = n − i.

Since the eccentricity of a vertex is the maximum distance from that vertex to any other vertex in the graph [3, 8], we have ε(vi) = max{d(vi, v1), d(vi, vn)} = max(i − 1, n − i).

By the definition of the eccentricity-based Estrada index, which is motivated by the classical Estrada index [1, 2],

$$EE_\varepsilon(P_n) = \sum_{v \in V(P_n)} e^{\varepsilon(v)}.$$

Substituting

$$\varepsilon(v_i) = \max(i-1, n-i)$$

for each vertex vi, we obtain

$$EE_\varepsilon(P_n) = \sum_{i=1}^{n} e^{\max(i-1,n-i)}.$$

Therefore,

$$EE_\varepsilon(P_n) = \sum_{i=1}^{n} e^{\max(i-1,n-i)}.$$

Hence the theorem is proved.
Example 4.3. Consider the path graph P5 with vertex set

V (P5) = {v1, v2, v3, v4, v5}.

The distances of each vertex from the two end vertices are shown below [3, 8]:

ε(v1) = max(0, 4) = 4,

ε(v2) = max(1, 3) = 3,

ε(v3) = max(2, 2) = 2,

ε(v4) = max(3, 1) = 3,

ε(v5) = max(4, 0) = 4.

Thus, the eccentricity sequence of P5 is

(4, 3, 2, 3, 4).

By the definition of the eccentricity-based Estrada index,

$$EE_\varepsilon(P_5) = \sum_{v \in V(P_5)} e^{\varepsilon(v)}.$$

Substituting the eccentricities of the vertices, we obtain

EEε(P5) = e4 + e3 + e2 + e3 + e4.

Hence,

EEε(P5) = 2e4 + 2e3 + e2.

Using the formula in Theorem 4.3,

$$EE_\varepsilon(P_5) = \sum_{i=1}^{5} e^{\max(i-1,5-i)} = e^4 + e^3 + e^2 + e^3 + e^4,$$

which simplifies to

EEε(P5) = 2e4 + 2e3 + e2.

Therefore, the result obtained agrees with Theorem 4.3, verifying its correctness. This example demonstrates how the eccentricity-based Estrada index captures the distance structure of path graphs through exponentially weighted eccentricities [5, 2].

5. Modified Estrada Index of Total Graphs

The effect of graph transformations on the proposed eccentricity-based Estrada index is investigated. The study of graph transformations and their influence on topological indices has been an active area of research in graph theory and network analysis [3, 8, 5].
Theorem 5.1. For any connected graph G,

EEε(T (G)) ≥ EEε(G).

Proof. Let

V (G) = {v1, v2,.., vn},

and let T (G) denote the total graph of G [3, 8].
Recall that the vertex set of T (G) is

V (T (G)) = V (G) ∪ E(G).

For each vertex v ∈ V (G), every path in G remains a path in T (G). Consequently, the distances between the original vertices do not increase. Hence,

εT (G)(v) ≥ εG(v), ∀ v ∈ V (G).

Since the exponential function is increasing, it follows that

eεT (G)(v) ≥ eεG(v), ∀ v ∈ V (G).

Summing over all vertices of G, we obtain

$$\sum_{v \in V(G)} e^{\varepsilon_{T(G)}(v)} \geq \sum_{v \in V(G)} e^{\varepsilon_{G}(v)} = EE_\varepsilon(G),$$

which is consistent with the monotonic behavior often observed for Estrada-type indices under graph transformations [1, 2].
Now,

$$EE_\varepsilon(T(G)) = \sum_{x \in V(T(G))} e^{\varepsilon_{T(G)}(x)}.$$

Since V (G) ⊆ V (T (G)) and all terms are positive,

$$EE_\varepsilon(T(G)) = \sum_{v \in V(G)} e^{\varepsilon_{T(G)}(v)} + \sum_{e \in E(G)} e^{\varepsilon_{T(G)}(e)}$$
$$\geq \sum_{v \in V(G)} e^{\varepsilon_{T(G)}(v)} \geq EE_\varepsilon(G).$$

Therefore,

$$EE\varepsilon(T(G)) \geq EE\varepsilon(G).$$

Hence the theorem is proved.
Example 5.1. Consider the path graph

$$G = P3,$$

with vertex set

$$V(G) = \{v1,v2,v3\}$$

and edge set

$$E(G) = \{e1 = v1v2, e2 = v2v3\}$$

[3].

The eccentricities of the vertices of P3 are

$$\varepsilon(v1) = 2, \varepsilon(v2) = 1, \varepsilon(v3) = 2.$$

Hence,

$$EE\varepsilon(P3) = e2 + e + e2 = 2e2 + e.$$

Now consider the total graph T (P3). Its vertex set is

$$V(T(P3)) = \{v1, v2, v3, e1, e2\}.$$

The eccentricities in T (P3) are

$$\varepsilon(v1) = 2, \varepsilon(v2) = 1, \varepsilon(v3) = 2,$$

$$\varepsilon(e1) = 2, \varepsilon(e2) = 2.$$

Therefore,

$$EE_\varepsilon(T(P_3)) = e^2 + e + e^2 + e^2 + e^2 = 4e^2 + e.$$

Thus,

$$EE_\varepsilon(T(P_3)) = 4e^2 + e > 2e^2 + e = EE_\varepsilon(P_3).$$

Hence the inequality

$$EE\varepsilon(T(G)) \geq EE\varepsilon(G)$$

is verified for the graph P3. This example illustrates how graph transformations may increase the value of topological indices by introducing additional structural information into the graph [5, 6].

6. Modified Estrada Index of Eccentric Graphs
This section studies the relationship between

$$EE\varepsilon(G) \quad \text{and} \quad EE\varepsilon(Ge),$$

where Ge denotes the eccentric graph of G. The study of graph transformations and their associated topological indices has attracted considerable attention in graph theory and network analysis [3, 8, 5].
Based on computational experiments performed on several classes of graphs, we for-mulate the following conjecture.
Conjecture 6.1. Let G be a connected graph. Then

$$EE\varepsilon(Ge) \leq EE\varepsilon(G).$$

The conjecture is motivated by the behavior of eccentricity-based graph invariants and the role of exponential weighting in Estrada-type indices [1, 2, 6].
Example 6.1. Consider the path graph

$$G = P4$$

with vertex set

$$V(G) = \{v1, v2, v3, v4\}.$$

The eccentricities of the vertices are

$$\varepsilon(v1) = 3, \varepsilon(v2) = 2, \varepsilon(v3) = 2, \varepsilon(v4) = 3,$$

which follow directly from the distance structure of the path graph [3, 8].
Hence,

$$EE\varepsilon(P4) = e3 + e2 + e2 + e3 = 2e3 + 2e2.$$

The eccentric graph P4,e consists of the edges

$$v1v4, v2v4, v1v3,$$

since these pairs are mutually eccentric vertices in P4.
Thus P4,e is the path

$$v2 - v4 - v1 - v3.$$

The eccentricities in P4,e are again

$$3, 2, 2, 3.$$

Therefore,

$$EE\varepsilon(P4,e) = e3 + e2 + e2 + e3 = 2e3 + 2e2.$$

Hence,

$$EE\varepsilon(P4,e) = EE\varepsilon(P4).$$

This example shows that equality can occur in the conjecture. Similar phenomena have been observed when studying the behavior of graph invariants under graph transformations and derived graph constructions [5, 6].

7. Results

In this section, explicit formulae for the eccentricity-based Estrada index of several stan-dard graph classes are obtained. Numerical results are presented to illustrate the derived formulae and facilitate comparisons among different graph families [3, 8].

Table 1 presents the computed values of the eccentricity-based Estrada index for sev-eral standard graph classes. These values illustrate the dependence of the index on the structural properties and eccentricity distribution of the underlying graph, which are fun-damental concepts in graph theory and network analysis [2, 3].

Table 1: Modified Estrada Index of Standard Graphs

Graph	Order	Modified Estrada Index
K_4	4	10.873
P_4	4	42.825
C_4	4	29.556
W_5	5	13.591

7.1. Applications of the Eccentricity-Based Estrada Index

The numerical values presented in Table 1 demonstrate the applicability of the eccentricity-based Estrada index in characterizing the structural properties of graphs through vertex eccentricities. Since the index is based on the exponential contribution of eccentricities, it provides valuable information regarding the global connectivity and compactness of a network, extending ideas originating from the classical Estrada index [1, 2].

The computed results have the following applications:

- **Graph Structure Characterization**

The index effectively distinguishes graph classes having the same order but different structural arrangements [3, 8]. For ex-ample, among the graphs of order four, the complete graph K4 possesses the smallest index value due to its minimum eccentricities, whereas the path graph P4 exhibits the largest value because of its larger vertex eccentricities.

- **Network Compactness Analysis**

Smaller index values indicate highly compact and well-connected networks. The value obtained for K4 reflects its maximum con-nectivity, while larger values for P4 indicate a less compact structure with greater distances between vertices [2].

- **Comparison of Different Graph Families**

The results facilitate comparisons among complete graphs, path graphs, cycle graphs, and wheel graphs. Such com-parisons help identify how graph topology influences eccentricity-based measures [5].

- **Chemical Graph Theory**

In molecular graph modeling, vertices and edges repre-sent atoms and chemical bonds, respectively. The eccentricity-based Estrada index can serve as a molecular descriptor for studying physicochemical properties, biologi-cal activities, and structure–property relationships of chemical compounds [7, 1, 4, 6].

- **Communication and Transportation Networks**

The index can be used to evaluate the efficiency of communication, transportation, and social networks. Net-works with lower index values generally exhibit shorter communication paths and improved accessibility among vertices [2].

- **Network Design and Optimization**

Since the index is sensitive to changes in vertex eccentricities, it can be employed in the design of efficient networks where minimizing communication delays and maximizing connectivity are important ob-jectives [2, 5].

- **Benchmarking New Graph Invariants**

The obtained values for standard graph classes provide benchmark results that can be used for validating and comparing newly proposed eccentricity-based topological indices [5, 6].

From Table 1, it is observed that the eccentricity-based Estrada index increases as the graph becomes less compact and the vertex eccentricities increase. Therefore, the index serves as a useful quantitative measure for analyzing the overall structural complexity and connectivity of graph-based systems [2, 5].

8. Application in Function Approximation

The eccentricity-based Estrada index

$$EE_\varepsilon(G) = \sum_{v\in V(G)} e^{\varepsilon(v)}$$

contains an exponential weighting of the vertex eccentricities. Since exponential func-tions play a fundamental role in approximation theory, numerical analysis, and machine learning, the proposed index may be viewed as a graph-based exponential aggregation operator. The use of exponential weighting is inspired by the classical Estrada index and its applications in network analysis [1, 2].

In function approximation, weighted exponential sums are frequently employed to rep-resent, estimate, or approximate complex functions. The quantity

$$\sum_{v\in V(G)} e^{\varepsilon(v)}$$

assigns larger weights to vertices having greater eccentricity and smaller weights to vertices that are more centrally located in the graph. Consequently, the index captures the global structural distribution of vertices and can serve as a compact numerical descriptor of a network [2].

More generally, for a function $f : V(G) \to R$ defined on the vertex set of a graph, one may consider the weighted approximation model

$$F(G) = \sum_{v\in V(G)} f(v)\, e^{\varepsilon(v)}$$

where the exponential term acts as a weighting factor determined by the topological position of the vertex. Such representations can be useful in graph-based learning and approximation frameworks.

The exponential weighting mechanism provides greater sensitivity to peripheral ver-tices, making the index suitable for applications where boundary or extremal structural characteristics are important. Therefore, the eccentricity-based Estrada index and its vari-ants may be employed in the construction of graph similarity measures, feature extraction techniques, and approximation models for complex networks [5, 6].

Potential applications include:

1. Data Clustering: The index can be used as a graph descriptor to compare differ-ent datasets represented as graphs and to identify clusters with similar structural characteristics [6].

2. Pattern Recognition: Exponentially weighted eccentricity information can be incorporated into feature vectors for recognizing and classifying graph-based patterns [6].

3. Artificial Intelligence and Machine Learning: Graph neural networks and other learning algorithms may utilize eccentricity-based exponential weights as in-formative topological features for prediction and classification tasks [6].

4. Network Optimization: The index can assist in identifying structurally important vertices and evaluating network configurations in communication, transportation, and social networks [2].

5. Graph Similarity Analysis: Networks having close values of $EE_\varepsilon(G)$ may ex-hibit similar structural behavior, making the index useful in graph comparison and retrieval problems [5].

6. Complex Network Modeling: The index may be employed as a quantitative measure in the analysis of biological, technological, and information networks where peripheral vertices significantly influence system behavior [4, 6].

Thus, the proposed eccentricity-based Estrada index provides a bridge between graph-theoretical structure and exponential approximation techniques, offering promising oppor-tunities for applications in data science, network analysis, and computational intelligence [1, 2, 6].

9. Conclusion

In this paper, we introduced an eccentricity-based Estrada index,

$$EE_\varepsilon(G) = \sum_{v \in V(G)} e^{\varepsilon(v)}$$

which incorporates vertex eccentricities through an exponential weighting scheme. Fun-damental properties of the index were established, and explicit formulae were derived for several standard graph classes, including complete, cycle, path, and wheel graphs. The behavior of the index under graph transformations was also investigated, yielding a result for total graphs and a conjectured relationship for eccentric graphs.

The obtained results show that the proposed index effectively captures graph struc-ture, connectivity, and eccentricity distribution, making it a useful descriptor for complex networks. Potential applications in graph theory, network analysis, chemical graph the-ory, machine learning, and function approximation were discussed. Future work includes establishing sharp bounds, characterizing extremal graphs, exploring relationships with other graph invariants, and investigating further applications in network science and data analytics.

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